IMPROVED FOKKER-PLANCK EQUATION FOR RESONANCE-LINE SCATTERING

George B. Rybicki

Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, MA 02138; grybicki@cfa.harvard.edu Received 2006 March 1; accepted 2006 April 22

ABSTRACT

A new Fokker-Planck equation is developed for treating resonance-line scattering, which is especially relevant to the treatment of $Ly\alpha$ in the early universe. It is a "corrected" form of the equation of Rybicki & Dell'Antonio that now obeys detailed balance, so the approach to thermal equilibrium is properly described. The new equation takes into account the energy changes due to scattering off moving particles, the recoil term of Basko, and stimulated scattering. One result is a surprising unification of the equation for resonance-line scattering and the Kompaneets equation. An improved energy exchange formula due to resonance-line scattering is derived. This formula is compared to previous formulas of Madau and coworkers and Chen & Miralda-Escudé.

Subject headings: atomic processes — cosmology: theory — radiation mechanisms: general — radiative transfer

1. INTRODUCTION

The scattering of radiation in resonance lines plays an important role in many parts of astrophysics, including stellar atmospheres, diffuse nebulae, and active galactic nuclei. In the early universe, resonance scattering in the hydrogen Ly α line has been shown to be an crucial process for understanding the state of the primordial gas during the recombination era (Peebles 1968; Zel'dovich et al. 1969). It can also can play a critical role in determining the populations of the fine structure levels in the ¹S level of hydrogen (Wouthuysen 1952; Field 1958, 1959) and thus affect the formation of the 21 cm line, observations of which promise to be an important source of information about the early universe (Hogan & Rees 1979; Madau et al. 1997; Tozzi et al. 2000). It may also play a role in direct heating of the gas (Madau et al. 1997; Chen & Miralda-Escudé 2004; Hirata 2006; Pritchard & Furlanetto 2006).

The theoretical description of resonance-line scattering is based on a redistribution function R, which gives the probability that an initial photon state will be scattered into some final photon state. The level of description of these photon states depends on the problem treated. For this paper we confine our attention to problems where the radiation field is sufficiently isotropic that only the angle-averaged form of the redistribution function needs to be used and where the radiation can also be considered to be unpolarized. The redistribution function then depends only on the initial ν' and final ν frequencies of the scattered photon; that is, $R(\nu,\nu')$.

For Ly α and other resonance-line scattering in low-density media, coherent scattering in the atom's rest frame from a natural (Lorentz) profile is appropriate. When one accounts for the Doppler effect due to atoms with a Maxwellian velocity distribution, a scattered photon will have its frequency decreased or increased depending on the components of the atomic velocity along the initial and final photon directions. The appropriate redistribution function under these conditions was first derived by Henyey (1940) and, following Hummer (1962), is usually denoted $R_{II}(\nu,\nu')$. For many cases in astrophysics, R_{II} captures the dominant physics for resonance-line transfer.

The solution of line transfer problems using a full redistribution function $R_{\rm II}$ is not trivial, since all frequencies are coupled together. However, there is an important class of problems where an approximate formulation can effectively used, namely, when the radiation field is sufficiently smooth on the scale of the Doppler width of the line. Then it is possible to derive a Fokker-Planck (F-P) type of transfer equation, where the redistribution is taken into account by a second-order differential operator over frequency space. An equation of this type was first given by Unno (1952), and improvements were made subsequently by Harrington (1973), Basko (1981), and Rybicki & Dell'Antonio (1994, hereafter RD94).

Another effect on redistribution is the loss of photon energy during scattering due to the recoil of the atom. This is completely analogous to the ordinary Compton effect, but is smaller by the ratio of the mass of an electron to the mass of an atom. The recoil effect was first discussed by Field (1959) for the case of resonance scattering with zero natural line width (R_I in the notation of Hummer 1962). Adams (1971) qualitatively considered recoil for R_{II} in the context of Ly α scattering in the neutral hydrogen of the Galactic disk. Basko (1981) derived the appropriate generalization of R_{II} including the recoil redistribution function and showed that it led to a simple additional term in the F-P formulation. RD94 showed how the Basko term could be included in their F-P equation and how it affected its solutions.

In all the cases treated by Adams (1971), Basko (1981), and RD94, the recoil term did not seem to be important, at least for its effect on the radiation field itself. However, Madau et al. (1997) argued that the atomic recoil in Ly α scattering could be an important heating mechanism for the intergalactic medium before reionization, basing their analysis on a simple formula that included recoil but no other effect. This was also investigated by Chen & Miralda-Escudé (2004), who found a much lower heating rate using the RD94 F-P equations with the Basko term.

A strong motivation for the present paper is to understand better the difference between the results of Madau et al. (1997) and Chen & Miralda-Escudé (2004) regarding energy exchange. It seems clear that Chen & Miralda-Escudé (2004) must be at least partially right: if the radiation field were thermal at the same temperature as the gas, then no net energy exchange should occur, so the simple formula of Madau et al. (1997) cannot be of general validity. On the other hand, the formulation of Chen & Miralda-Escudé (2004) did not take detailed balance fully into account, so the matter deserves further investigation.

Another motivation for this paper is the issue of the 21 cm spin temperature and how it depends on Ly α transfer. According to the Wouthuysen-Field effect (Wouthuysen 1952; Field 1958, 1959), the radiation field near Ly α comes into thermal equilibrium with the kinetic temperature of the gas, and this Ly α field then imposes that same spin temperature on the 21 cm line. Any transfer equation, either through using a full redistribution function or through a F-P approximation, should correctly incorporate this thermal requirement, since small errors in calculation could have large effects on predictions of 21 cm radiation.

It should be obvious that an accurate determination of energy exchange rates and 21 cm spin temperatures is critically dependent on being able to formulate the interaction of radiation and matter in a thermodynamically correct way. Deguchi & Watson (1985) showed that this will be true if the redistribution functions satisfy certain "detailed balance" relations. However, no known form of R_{II} satisfies these relations exactly, so Deguchi & Watson (1985), in their investigations of the recombination era, found a method of "correcting" the usual R_{II} such that its values did not change very much, but enough to satisfy detailed balance. Deguchi & Watson (1985) applied their correction method to the redistribution functions directly and solved the equations numerically; they did not consider how this might change any associated F-P method.

A review of the basic equations is given in § 2. In § 3 we introduce a simple correction scheme, different from that of Deguchi & Watson (1985), which can be used to produce a redistribution function–satisfying detailed balance, and in § 4 we use this correction scheme to derive a new, corrected F-P equation. This F-P equation incorporates the RD94 diffusion term and the Basko recoil term, plus a new term that describes stimulated scattering and another that accounts for the correct phase space factors; acting together, these terms ensure detailed balance and the approach to the proper thermal radiation field. In § 5 we demonstrate the close analogy between the new corrected F-P equation and the Kompaneets equation. In § 6 we use the new F-P equation to derive an energy exchange rate formula. This is compared to the formulas of Madau et al. (1997) and of Chen & Miralda-Escudé (2004).

2. BASIC EQUATIONS

We consider the time dependence of the radiation field in a homogeneous and isotropic medium. This idealized problem allows one to develop equations applicable to more complex situations under the isotropic scattering approximation, much as is done for the analogous Kompaneets equation. When dealing with scattering problems, it is often easier to use intensities based on photon numbers rather than energies, and this is done here. Because of the isotropic assumption, the radiation is determined by the mean intensity $J(\nu)$.

For simplicity of presentation, we write all of our transfer equations for the special case of the time dependence of a homogeneous, static medium, very much as in the spirit of the usual Kompaneets equation (Kompaneets 1957; Rybicki & Lightman 1979). One should interpret the right-hand side of such equations as "emission minus absorption" terms, which can be incorporated into other transfer equations as needed. In particular, we do not include a term accounting for the expansion of the medium, which, if needed, should be included on the left-hand side as part of the transfer operator. For cases that involve spatial transfer, one can also use the results here in an "isotropic scattering approximation" by appropriate modification of the absorption terms; that is, by adding back the isotropic absorption term and subtracting the proper anisotropic absorption term.

For many applications the process of stimulated scattering is not important, and most of the discussions of resonance-line scattering have explicitly or implicitly neglected it. In that case the time dependence of the radiation is then governed by the transfer equation,

$$\frac{1}{c\chi}\frac{\partial J}{\partial t} = \int R(\nu,\nu')J(\nu') - R(\nu',\nu)J(\nu)\,d\nu' = -\varphi(\nu)J(\nu) + \int R(\nu,\nu')J(\nu')\,d\nu'.$$
(1)

Here $R(\nu,\nu')$ is the $R_{\rm II}$ redistribution function and $\varphi(\nu)$ is the Voigt line profile function, related to the redistribution function by

$$\varphi(\nu) = \int R(\nu', \nu) \, d\nu', \tag{2}$$

and which is normalized to unity:

$$\int_0^\infty \varphi(\nu) \, d\nu = 1. \tag{3}$$

The quantity χ is given by

$$\chi = \frac{h\nu_0}{4\pi} N_1 B_{12}, \tag{4}$$

where ν_0 is the line center frequency, N_1 is the population of the lower level, and B_{12} is the upward Einstein *B*-coefficient for the resonance transition.

When stimulated scattering is important, it can be taken into account through additional factors in the transfer equation (1 + n), where $n(\nu) = c^2 J(\nu)/2\nu^2$ is the photon occupation number:

$$\frac{1}{c\chi}\frac{\partial J}{\partial t} = \int [1+n(\nu)]R(\nu,\nu')J(\nu') - [1+n(\nu')]R(\nu',\nu)J(\nu)\,d\nu'.$$
(5)

It is important to note that the same redistribution functions appear in both equations (1) and (5); that is, they are independent of whether stimulated scattering takes place or not. Therefore, it is possible to determine the properties of the redistribution functions for cases without stimulated processes and then use them in equation (5) when necessary.

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Both equations (1) and (5) conserve photons, as can be proved by integration over ν and interchanging ν and ν' in one of the two terms on the right. As such, photon conservation is built into the transfer equations themselves and does not depend on a particular symmetry or other property of the redistribution functions. This is as it should be, since scattering does not change photon number.

The difficulty of solving transfer problems using the full redistribution functions has led to some simplified formulations that are adequate under special circumstances. One important fact is that the redistribution function is significantly nonzero only for frequencies ν and ν' that do not differ by many Doppler widths. In many cases of interest the radiation field in the neighborhood of line center is sufficiently smooth such that for a given value of ν , the relevant values of $J(\nu')$ can be represented by a Taylor series up to second order in the difference $\nu' - \nu$. This makes it possible to replace the frequency integrations on the right-hand side of the transfer equation with an equivalent second-order differential operator. The resultant transfer equation is known as a Fokker-Planck equation.

There have been a number of F-P formulations for the R_{II} redistribution problem given in the literature. They fall into two categories: first, there are ones that are based on the standard R_{II} redistribution function (Henyey 1940; Hummer 1962), which consider the spreading of radiation on scattering but neglect recoil. These formulations give an expression for the integral of the redistribution function and the intensity by means of a differential operator,

$$\int R(\nu,\nu')J(\nu')\,d\nu' = \varphi(\nu)J(\nu) + \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\left[D(\nu)\frac{\partial J(\nu)}{\partial\nu}\right],\tag{6}$$

where $R = R_{II}$. Here

$$\Delta\nu_{\rm D} = \left(\frac{2kT\nu_0^2}{m_a c^2}\right)^{1/2} \tag{7}$$

is the usual Doppler width and $D(\nu)$ is the "diffusion" coefficient, essentially a second moment of the redistribution function. This implies the F-P transfer equation (without stimulated processes):

$$\frac{1}{c\chi}\frac{\partial J}{\partial t} = \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\left[D(\nu)\frac{\partial J(\nu)}{\partial\nu}\right].$$
(8)

The different F-P formulations differ in what they take for $D(\nu)$. The first such formulation by Unno (1955) (see also Harrington 1973) took

$$D(\nu) = \frac{\Gamma}{4\pi^2 |\nu - \nu_0|^2},$$
(9)

which is an asymptotic result for the second moment, strictly applicable only in the wings of the line. Basko (1981) used a nonsingular form of equation (9),

$$D(\nu) = \frac{\Gamma/4\pi^2}{(\nu - \nu_0)^2 + (\Gamma/4\pi)^2},$$
(10)

equal to the natural line profile, but did not justify this choice. RD94 rigorously calculated the second moment of R_{II} using the full R_{II} redistribution function. Their fundamental result is given in their equation (A13) for the second moment of the redistribution function including angular dependence. Averaging that result over angle depends on whether an isotropic or dipole phase function is assumed. The two results are, in terms of physical frequency,

$$D(\nu) = \varphi(\nu) + (1/3)\Delta\nu_D^2 \varphi''(\nu) \qquad (\text{RD94 isotropic}), \tag{11}$$

$$D(\nu) = \varphi(\nu) + (7/20)\Delta\nu_{\rm D}^2\varphi''(\nu) \qquad \text{(RD94 dipole)}.$$
(12)

In fact, RD94 adopted a version without the second derivative:

$$D(\nu) = \varphi(\nu)$$
 (RD94 adopted). (13)

Their main rationale for this choice was that either the first or second moment needed to be altered in order to preserve particle conservation, and equation (13) was the simplest way of doing this. Others (Madau et al. 1997; Chen & Miralda-Escudé 2004; Hirata 2006) have used the RD94 approximation with this form for $D(\nu)$.

For much of the formal developments in this paper, $D(\nu)$ will be left general, and only later will particular choices be made. One should point out that all of the expressions given in equations (9)–(13) for $D(\nu)$ are asymptotically equivalent in the line wings, so it is only near the line core that differences occur. A desire for a nonsingular result argues against equation (9). Although RD94 is somewhat ambiguous as to the correct form, it seems clear that the correct cutoff for the asymptotic wing region should occur on the scale of the Doppler width; this argues against Basko's choice (eq. [10]), which implies that this scale is the natural width. In § 5, the choice for $D(\nu)$ will be discussed further.

The second category of F-P equations take recoil into account. This was done first by Basko (1981), who gave the following generalization of the F-P equation (eq. [8]):

$$\frac{1}{c\chi}\frac{\partial J}{\partial t} = \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\left\{D(\nu)\left[\frac{\partial J(\nu)}{\partial\nu} + \frac{hJ}{kT}\right]\right\},\tag{14}$$

in which the new term hJ/kT accounts for the recoil. Basko used the value in equation (10) for $D(\nu)$. RD94 introduced a slight variation of Basko's generalized equation by using equation (13) for $D(\nu)$, which was subsequently employed by Chen & Miralda-Escudé (2004). This equation with recoil will not be used directly in our derivation of a corrected F-P equation, although we will compare our results with it later. Unless indicated to the contrary, the term "uncorrected F-P equation" will refer strictly to equation (8).

3. DETAILED BALANCE AND "CORRECTED" REDISTRIBUTION

In order to describe correctly the approach to thermal equilibrium, the redistribution function must satisfy a certain symmetry condition known as detailed balance. This is a result of the microscopic reversibility of the scattering process, along with the inclusion of appropriate phase-space factors and the fact that the scattering particles obey a Maxwellian velocity distribution at temperature *T*.

Deguchi & Watson (1985, hereafter DW85) considered the detailed balance relations satisfied by redistribution functions. Their result was stated for the redistribution function using energy-based intensities, and they also used opposite ordering of the arguments ν and ν' . Accounting for these differences, the DW85 result translates in our notation to

$$R(\nu',\nu)\nu^2 e^{-h\nu/kT} = R(\nu,\nu')\nu'^2 e^{-h\nu'/kT}.$$
(15)

In most cases of line transfer, one usually deals with frequencies ν and ν' that are very close to the line center frequency and thus very close to each other. Then equation (15) can be approximated by the symmetry relation

$$R^*(\nu',\nu) = R^*(\nu,\nu').$$
(16)

We have added the asterisk to denote redistribution functions satisfying the special symmetry in equation (16) rather than in equation (15). In fact, the usual redistribution functions used in line transfer calculations are clearly approximate in that they satisfy equation (16) rather than equation (15) (e.g., Hummer 1962).

Approximations such as equation (16) are satisfactory for many applications. However, as described in \S 1, there are cases where one needs a formulation that includes enough physics to ensure the detailed balance relation (eq. [15]).

Let us consider how one may modify a simple redistribution function obeying equation (16) so that it satisfies equation (15) instead. DW85 did this by choosing the usual expression for $\nu > \nu'$ and obtaining the result for $\nu < \nu'$ by the detailed balance relation (see discussion in DW85 after their eq. [22]). In our notation, this may be written as

$$R_{\rm DW}(\nu,\nu') = \begin{cases} R^*(\nu,\nu'), & \nu > \nu', \\ R^*(\nu',\nu)(\nu/\nu')^2 \exp[h(\nu'-\nu)/kT], & \nu < \nu'. \end{cases}$$
(17)

While this choice clearly will lead to thermal equilibrium in the appropriate limit, it does have the undesirable property of creating a discontinuity in slope in the redistribution function at $\nu = \nu'$, even when one does not exist in R^* .

In this paper we use a different method of correction. Again starting with an R^* that satisfies the approximate detailed balance relation (eq. [16]), we define the "corrected" redistribution function R_c , which is related to the original R^* through a "diagonal similarity transformation,"

$$R_{c}(\nu,\nu') = U(\nu)R^{*}(\nu,\nu')U^{-1}(\nu'), \quad \text{or} \quad R^{*}(\nu,\nu') = U^{-1}(\nu)R_{c}(\nu,\nu')U(\nu'), \quad (18)$$

$$U(\nu) = \nu e^{-(1/2)h\nu/kT}.$$
(19)

It is easily verified that this corrected redistribution function satisfies the detailed balance relation (eq. [15]). We prefer this method to that of DW85, because it introduces no new discontinuities of slope at $\nu = \nu'$ and is more amenable to the kind of analytic manipulations employed in this paper.

4. CORRECTED FOKKER-PLANCK EQUATION

The correction procedure given in equation (18) can be used in any formulation of the redistribution problem. For this paper, however, we apply it to the Fokker-Planck equation (eq. [8]). In Appendix A, we show that the $R(\nu,\nu')$ implied by equation (8) satisfies the symmetry condition (eq. [16]), so equation (18) may be used to define a corrected redistribution function. Using this, we straightforwardly derive our new corrected F-P equation that obeys detailed balance, namely,

$$\frac{1}{c\chi}\frac{\partial J}{\partial t} = \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\left\{D\left[\frac{\partial J}{\partial\nu} + \left(\frac{h}{kT} - \frac{2}{\nu}\right)J + \frac{c^2J^2}{2kT\nu^2}\right]\right\}.$$
(20)

(See Appendix B for the mathematical details of this derivation.)

We now identify the physical significance of the terms in the inner set of brackets of this corrected F-P equation. The first term, $\partial J / \partial \nu$, is easily understood, since it is the same diffusion term as in the uncorrected version given in equation (8). The last term, involving

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the square of J, clearly describes the stimulated scattering; let us ignore this term for the moment, since we want to make comparisons with other F-P equations that have also ignored this process; we will return to it in § 5.

There are two remaining terms, hJ/kT and $-J/2\nu$. The first of these is precisely the Basko recoil term, as in equation (14). This may seem remarkable, since the F-P equation in its uncorrected form in equation (8) does not include recoil at all. However, there is a simple physical explanation for this seeming coincidence. In the theory of Brownian motion, which is also described by a F-P equation, Einstein found that thermal equilibrium required a certain relation between the coefficients of "diffusion" and "drift" (other terms for drift are "mobility" or "dynamical friction"). In the present case, the uncorrected version given in equation (8) describes only the "diffusion" part of the process. Imposing detailed balance through our correction procedure has automatically generated the proper "drift" term, here given by the recoil term.

The remaining term $-J/2\nu$ can be explained as follows. With just the diffusion term and the Basko recoil term, as in equation (14), the equilibrium solution (setting the bracket to zero) would give $J \propto \exp(-h\nu/kT)$. In fact, Basko (1981), following Field (1959), claimed that his treatment of recoil led to thermal equilibrium because the equilibrium solution of his equation was proportional to $\exp(-h\nu/kT)$. However, to be rigorously thermal (without stimulated processes), J should be proportional to the Wien law, $\nu^2 \exp(-h\nu/kT)$, not just $\exp(-h\nu/kT)$. The extra term $-2J/\nu$ in the F-P equation given in equation (20) is just what is needed to account for the missing factor of ν^2 . In many applications this additional slowly varying factor may be unimportant. However, since the goal here is to account for thermal equilibrium as precisely as possible, this term should be included as a matter of principle.

5. RELATION TO THE KOMPANEETS EQUATION

For further investigation of the corrected form of equation (20), especially the stimulated scattering process, it is useful to write it in terms of the photon occupation number *n*:

$$\frac{1}{c\chi}\frac{\partial n}{\partial t} = \frac{\Delta\nu_{\rm D}^2}{2}\frac{1}{\nu^2}\frac{\partial}{\partial\nu}\left\{\nu^2 D\left[\frac{\partial n}{\partial\nu} + \frac{h}{kT}n(1+n)\right]\right\}.$$
(21)

This is reminiscent of the Kompaneets equation (Kompaneets 1957; Rybicki & Lightman 1979), which can be written

$$\frac{1}{N_e \sigma_{\rm T} c} \frac{\partial n}{\partial t} = \frac{kT}{m_e c^2} \frac{1}{\nu^2} \frac{\partial}{\partial \nu} \left\{ \nu^4 \left[\frac{\partial n}{\partial \nu} + \frac{h}{kT} n(1+n) \right] \right\},\tag{22}$$

where N_e is the electron density and σ_T is the Thomson cross section.

Some of the desirable general properties of the new equation follow exactly as in the Kompaneets case. It satisfies photon conservation exactly, due to the form of the right-hand side being $1/\nu^2$ times a frequency derivative. It satisfies detailed balance by construction; a result of this is that it has the correct thermal equilibrium solution. We can see this by setting the right-hand side to zero, which leads to the condition

$$\frac{\partial n}{\partial \nu} + \frac{h}{kT}n(1+n) = 0.$$
(23)

The general solution to this differential equation can be written

$$n = \frac{1}{e^{(h\nu - \mu)/kT} - 1},$$
(24)

where μ is a constant. This is a thermal Bose-Einstein distribution with chemical potential μ , which is the correct thermal distribution for photons obeying a conservation law. We note that the general properties of photon conservation and detailed balance are independent of the particular form of $D(\nu)$.

The similarity between the corrected RD94 equation (eq. [21]) and the Kompaneets equation (eq. [22]) can be emphasized further by using the definition in equation (7) and choosing the RD94 value (eq. [13]) for the diffusion coefficient $D(\nu)$. Then equation (21) can be written

$$\frac{1}{c}\frac{\partial n}{\partial t} = \frac{kT}{m_a c^2} \frac{1}{\nu^2} \frac{\partial}{\partial \nu} \left\{ \nu^2 \nu_0^2 \alpha \left[\frac{\partial n}{\partial \nu} + \frac{h}{kT} n(1+n) \right] \right\},\tag{25}$$

where $m = m_a$ is the atomic mass and α is the line absorption coefficient,

$$\alpha_L(\nu) = \chi \varphi(\nu). \tag{26}$$

We now make a minor modification of equation (25) by replacing ν_0^2 by ν^2 . This is a very slight change, since $\alpha(\nu)$ is significant only in a narrow region around the line center, so the distinction between ν and ν_0 is slight. Such a replacement is not unusual for line problems; it is quite typical when deriving line redistribution functions, and is even found in the definition of the Doppler width, equation (7).

One may also regard the above modification as equivalent to a slightly different diffusion coefficient $D(\nu)$, and, as noted above, the important properties of photon conservation and detailed balance are independent of $D(\nu)$. With this modification, equation (25) becomes

$$\frac{1}{c}\frac{\partial n}{\partial t} = \frac{kT}{m_a c^2} \frac{1}{\nu^2} \frac{\partial}{\partial \nu} \left\{ \nu^4 \alpha \left[\frac{\partial n}{\partial \nu} + \frac{h}{kT} n(1+n) \right] \right\}.$$
(27)

Remarkably, equation (27) is precisely the same as the Kompaneets equation if we take *m* to be the electron mass m_e and α to be the Thomson scattering coefficient, $\alpha_T = N_e \sigma_T$. Thus, equation (27) provides a *unification* of the F-P equation for resonance-line scattering and the Kompaneets equation. One only needs to substitute the appropriate scattering coefficient and mass of the scatterer.

It should be noted that this unification is even valid if one chooses to use one of the forms in equations (11) or (12) for $D(\nu)$ instead of that in equation (13). In either case, this simply involves replacing α by $\alpha + C\alpha''$ in equation (27), where C is a constant. This will still be completely consistent with the Kompaneets equation, because α for Thomson scattering is independent of frequency. However, for the remainder of this paper we will continue to use the corrected F-P equation in the simple form of equation (27).

6. ENERGY EXCHANGE FORMULA

Equation (27) can be used to derive an energy exchange formula between the radiative energy and kinetic energy of the atoms. The energy density of the radiation field is

$$U = \frac{8\pi h}{c^3} \int \nu^3 n \, d\nu. \tag{28}$$

Differentiating with respect to time and using equation (27), followed by an integration by parts, yields the rate of change of the radiation energy density,

$$\frac{\partial U}{\partial t} = -\frac{8\pi hkT}{m_a c^4} \int \nu^4 \alpha_L(\nu) \left[\frac{\partial n}{\partial \nu} + \frac{h}{kT}n(1+n)\right] d\nu, \tag{29}$$

which is the negative of the heating rate for the gas.

Equation (29) is the general formula for energy exchange within our F-P formulation. The presence of the frequency derivative in the integral makes the formula difficult to interpret, but it may be put into a more revealing form by defining at each frequency an appropriate temperature of the radiation field by comparison to a thermal Bose-Einstein distribution with temperature T and chemical potential μ :

$$n_{\rm th} = \frac{1}{e^{(h\nu-\mu)/kT} - 1}$$
, for which $n'_{\rm th} = -\frac{h}{kT}n(1+n)$. (30)

Given the values at frequency ν of an arbitrary radiation field $n(\nu)$ and its slope $n'(\nu)$, by using equation (30) one may define the local "radiation temperature" $T_R(\nu)$ for an arbitrary radiation field by

$$T_{R}(\nu) = -\frac{h}{k} \frac{n(1+n)}{n'}.$$
(31)

With this definition, equation (29) becomes

$$\frac{\partial U}{\partial t} = -\frac{8\pi\hbar^2}{m_a c^4} \int \nu^4 \alpha_L(\nu) n(1+n) \left[1 - \frac{T}{T_R(\nu)}\right] d\nu.$$
(32)

In order to interpret this equation, let us consider the special case in which the radiation field is smooth and slowly varying in the neighborhood of the line center at ν_0 , so that both it and its derivative can be considered to be constant. Then the delta-function character of $\alpha_L(\nu)$ implies

$$\frac{\partial U}{\partial t} = -\frac{8\pi h k T \chi \nu_0^4}{m_a c^4} n_0 (1+n_0) \left(1-\frac{T}{T_{R0}}\right),\tag{33}$$

where the subscript "0" indicates evaluation at ν_0 .

This may be put into another form by defining the rate of scattering per unit volume:

$$P = 4\pi \int \alpha_L (1+n) J \, d\nu = \frac{8\pi\chi}{c^2} \nu_0^2 n_0 (1+n_0), \tag{34}$$

where we have again used the delta-function character of $\alpha_L(\nu)$. Note that stimulated scatterings are included in this rate. Then our energy exchange formula takes the simpler form

$$\frac{\partial U}{\partial t} = -P\left(\frac{h\nu_0}{m_a c^2}\right)h\nu_0\left(1 - \frac{T}{T_{R0}}\right).$$
(35)

(We remark that the general energy exchange formula given in eq. [32] could be written in this same simplified form, provided one uses for the radiation temperature a suitable mean value, frequency-averaged over the line.)

The factor $1 - T/T_{R0}$ in the formula given in equation (35) shows how the energy exchange between the radiation and the matter depends on their relative temperatures. In particular, energy always flows from the hotter to the colder system; no energy exchange occurs when the radiation and matter temperatures are the same. These fundamental principles of thermodynamics are guaranteed by the detailed balance built into our equations.

The factor $1 - T/T_{R0}$ is particularly important for situations with large optical depth in the resonance line. In these cases, the Wouthuysen-Field effect (Wouthuysen 1952; Field 1959) becomes relevant. According to this effect, the scattering within the line changes the local radiation field in such a way that the radiation temperature within the line is brought close to the gas temperature. Therefore, the factor $1 - T/T_{R0}$ becomes very small and so greatly reduces the flow of energy between the radiation and the gas to a value much less than one what might estimate from simple arguments based on the radiation temperature of any incident radiation. We are now in a position to compare our energy exchange formulas to those of Madau et al. (1997, hereafter MMR97) and Chen & Miralda-Escudé (2004, hereafter CM04).

6.1. Comparison with MMR97

In deriving their energy exchange formula, MMR97 assumed (implicitly) the near-constancy of the radiation field near the line center, so it should be compared with our equation (35). Some translation is necessary, since their rates are defined per atom instead of per unit volume. Making that adjustment, the MMR97 formula (their eq. [30]) is, in our notation,

$$\frac{\partial U}{\partial t} = -\tilde{P}\left(\frac{h\nu_0}{m_a c^2}\right)h\nu_0. \tag{36}$$

The rate \tilde{P} is the same as our rate P, as defined in equation (34), except that it omits the stimulated scattering factor 1 + n.

The omission of stimulated scattering is minor, but more importantly, the MMR97 formula does not contain the factor $1 - T/T_{R0}$, which, as we have seen, describes how the energy exchange depends on the relative temperatures of the matter and radiation. The MMR97 result will be valid only when the radiation temperature is much greater than the matter temperature so that the recoil effect dominates the counterbalancing diffusive effect of the thermal electrons.

In Appendix B of their paper, MMR97 outlined a derivation of their energy exchange formula from a Fokker-Planck equation that contained the Basko recoil term. In that derivation they eventually dropped the diffusion term and kept only the recoil terms. They clearly recognized that because of this their formula would only apply for photons of much higher energies than the thermal energies of the atoms.

MMR97 were reluctant to include the diffusion term, because they argued that only terms of order v/c had been included and that one needed to include terms up to $(v/c)^2$ in order to get the reverse flow of energy from the atoms to the radiation. However, the present approach using detailed balance automatically provides the correct description of the reverse flow, as evidenced by the correct thermal equilibrium.

6.2. Comparison with CM04

Another approach to energy exchange was given by CM04, who used the F-P equation with the Basko recoil term as given in equation (14) to find the energy exchange rate in a particular cosmological context. By using this equation, CM04 assumed (as MMR97 did not) that this equation could be relied on to describe the reverse flow of energy.

CM04 used numerical solutions to equation (14) to evaluate the energy transfer and did not derive a general formula such as our equation (35), but we may do so now. In a sense the present derivation is merely extending the derivation outlined by MMR97 in their Appendix B, except that here the diffusion term is included.

Multiplication of equation (14) by $h\nu$ and integrating over ν gives, after integration by parts and other straightforward manipulations,

$$\frac{\partial U}{\partial t} = -\frac{4\pi hkT}{m_a c^2} \int \nu_0^2 \alpha_L(\nu) \left(\frac{\partial J}{\partial \nu} + \frac{hJ}{kT}\right) d\nu.$$
(37)

In order to compare this with our result from equation (32), we define a new "radiation temperature" T_{CM} by the relation

$$T_{\rm CM} = -\frac{h}{k} \frac{J}{J'}.$$
(38)

This differs from the definition in equation (30) by ignoring stimulated emission and also by the factor ν^2 in the relation between *n* and *J*. It is equivalent to assuming that a thermal radiation field is proportional simply to $\exp(-h\nu/kT)$.

Under the same assumptions as made for equation (35), we obtain the following energy exchange formula:

$$\frac{\partial U}{\partial t} = -\tilde{P}\left(\frac{h\nu_0}{m_a c^2}\right)h\nu_0\left(1 - \frac{T}{T_{\rm CM0}}\right) \qquad (CM04). \tag{39}$$

We call this the "CM04 formula" because it is a natural consequence of their approach, even though they did not derive it explicitly. The CM04 formula differs from our equation (35) by the replacement of T_{R0} by T_{CM0} (and the fact that \tilde{P} does not include stimulated scatterings).

The most noteworthy feature of the CM04 formula is that it shares with equation (35) the desirable property of taking into account the relationship between matter and radiation temperature (although with an slightly approximate radiation temperature). In particular, the approach of CM04 does take into account the suppression of energy transfer for lines of high optical depth, in accordance with the Wouthuysen-Field effect. This clearly explains why CM04 found much lower energy exchange rates than did MMR97.

Let us make some estimate of the difference between the radiation temperatures T_R and T_{CM} . Stimulated emission is usually fairly negligible for resonance-line transfer, so let us ignore it for the moment. Then one can easily show that

$$T_{\rm CM} = \frac{T_R}{1 - 2kT_R/h\nu}.\tag{40}$$

As an practical example, in problems involving hydrogen Ly α , gas temperatures are typically below $\sim 10^4$ K, since anything much higher leads to the rapid ionization of hydrogen. The equivalent temperature for the Ly α transition is $\sim 10^5$ K, so by equation (40) the two radiation temperatures T_R and T_{CM} may differ by up to $\sim 20\%$. However, for lower radiation temperatures, they will differ proportionally less, and the CM04 radiation temperature T_{CM} may be a reasonable approximation to the more accurate T_R . For very sensitive applications, however, it would be prudent to use the accurate form.

7. DISCUSSION

A new form for the Fokker-Planck equation describing resonant line scattering has been derived that incorporates detailed balance and stimulated scattering. When put into the form of equation (27), the new equation shows a surprising unification with the Kompaneets equation.

The new F-P equation has been used to derive expressions for the rate of energy transfer between the radiation and the thermal gas, incorporating both recoil and the proper reverse flow of energy from the gas to the radiation. We have compared our energy exchange result to those used by MMR97 and CM04.

In their paper MMR97 noted that their energy exchange formula would be limited to cases in which the radiation temperature greatly exceeds the gas temperature. We have verified this explicitly by deriving the general dependence on the radiation and gas temperatures, as seen, for example, in the factor $1 - T/T_{R0}$ in our equation (35). This factor is thermodynamically required and also will be absolutely crucial in cases of resonance-line scattering of high optical depth, where the Wouthuysen-Field effect can play a pivotal role.

We have also derived an approximate explicit energy transfer formula by closely following the work of CM04, which is based on the F-P equation (eq. [14]). The resulting energy exchange formula given in equation (39) (which we call the CM04 formula) does approximately incorporate detailed balance and does approximately account for the relative radiation and gas temperatures. The CM04 formula should give acceptable results in most cases of interest. This demonstrates that the CM04 approach to energy transfer is clearly superior to the more limited formula of MMR97.

However, although the F-P equation given in equation (14) and the associated CM04 energy exchange formula would seem to provide adequate results for most situations, there may be other reasons for preferring our new formulation of the F-P equation, given in equation (27). From a purely theoretical point of view, it treats the thermodynamics in a more precise manner and has the aesthetically pleasing property of being unified in form with the Kompaneets equation. There may also be practical reasons for using our more accurate formulation. For example, in determining the spin temperature of the 21 cm line in cosmological contexts, one needs to consider the delicate balance of different processes, and here a thermodynamically correct description of Ly α scattering could prove to be a crucial element. We plan to investigate this in the near future.

The results of the present paper suggest some avenues for possible future work. The unification of the resonance-line and electronscattering F-P equations discussed in § 5 strongly suggests that one might develop a single derivation of both equations, based on expansions of the transfer equations with redistribution functions that take all physical effects explicitly into account. Done carefully, this could resolve the somewhat unfortunate ambiguity of what the proper value of $D(\nu)$ should be.

One limitation of the present paper is its assumption of a homogeneous and isotropic radiation field $J(\nu)$, a limitation shared by the Kompaneets equation. It would be desirable to derive a F-P equation for resonance scattering with a spatially dependent and anisotropic radiation field, $I(\nu, \mathbf{r}, \mathbf{n})$, that was dependent on position \mathbf{r} and direction \mathbf{n} . This would be useful for cases in which the incident irradiation is anisotropic or in cases in which the medium itself is inhomogeneous.

There is one way to obtain an approximate equation for anisotropic radiation fields, one that is commonly used with the Kompaneets equation. Neglecting stimulated emission, we write

$$\frac{1}{c}\frac{\partial I}{\partial t} + \boldsymbol{n} \cdot \nabla I = -\chi \phi I + \chi \phi J + \chi \frac{\Delta \nu_{\rm D}^2}{2} \frac{\partial}{\partial \nu} \left\{ D \left[\frac{\partial J}{\partial \nu} + \left(\frac{h}{kT} - \frac{2}{\nu} \right) J \right] \right\}. \tag{41}$$

This is equivalent to assuming that the extinction part of the scattering is treated with the directional intensity, but the emission part is treated as if the radiation field were isotropic, as in equation (20). Since scattered radiation is not too far from being isotropic, and becomes more so after many scatterings, this is often an acceptable approximation. We note that when the radiation field is homogeneous and isotropic, equation (41) reduces to equation (20) when integrated over all solid angles.

However, equation (41) does have some definite defects. If one wanted to include stimulated scattering, the extinction term would have to depend on angle in some as yet unknown way; this defect is not too serious, since stimulated scattering is not likely to be important for any resonance lines. A more serious defect is that the equation does not include the correlation of the frequency diffusion and shift on the scattering angle, an effect that we know is very strong from the form of the angle-dependent redistribution function $R_{II}(\nu, n; \nu', n')$ (Hummer 1962).

RESONANCE-LINE SCATTERING

Therefore, for theoretical reasons, as well as practical ones, it would be desirable to derive a Fokker-Planck equation for resonance scattering with a fully anisotropic radiation field. This could be done using the same correction procedure of the present paper, but applied to the angle-dependent results of RD94, as in their equation (A16). Such a derivation is currently under investigation. The author would like to thank Avi Loeb and Avery Meiksin for helpful discussions and comments.

APPENDIX A

SYMMETRY OF THE FOKKER-PLANCK REDISTRIBUTION FUNCTION

The redistribution function from which the RD94 Fokker-Planck equation, given in equation (8), was derived satisfies the symmetry $R(\nu, \nu') = R(\nu', \nu)$. However, because approximations have been made, it is not obvious that the F-P redistribution function R defined implicitly through equation (8) must necessarily satisfy this same symmetry. To investigate this it is useful to consider the following double integral:

$$\int \int G(\nu)R(\nu,\nu')F(\nu')\,d\nu\,d\nu'.$$
(A1)

This quantity is bilinear in the two functions $F(\nu)$ and $G(\nu)$, which are completely arbitrary, except that they and their derivatives are assumed to vanish sufficiently rapidly at the limits of integration $(0,\infty)$.

We write the basic RD94 F-P result from equation (6) for an arbitrary function $F(\nu)$,

$$\int R(\nu,\nu')F(\nu')\,d\nu' = \varphi(\nu)F(\nu) + \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\left[D(\nu)\frac{\partial F(\nu)}{\partial\nu}\right].\tag{A2}$$

Using this for the integral over ν' in equation (A1), we have

$$\int \int G(\nu)R(\nu,\nu')F(\nu')\,d\nu\,d\nu' = \int G(\nu)\left\{\varphi(\nu)F(\nu) + \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\left[D(\nu)\frac{\partial F(\nu)}{\partial\nu}\right]\right\}d\nu. \tag{A3}$$

Integrating by parts twice, assuming zero contributions at the limits, gives

$$\int \int G(\nu')R(\nu',\nu)F(\nu)\,d\nu\,d\nu' = \int \left\{\varphi(\nu)G(\nu) + \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\left[D(\nu)\frac{\partial G(\nu)}{\partial\nu}\right]\right\}F(\nu)\,d\nu,\tag{A4}$$

where we have interchanged $\nu \leftrightarrow \nu'$ in the double integral on the left-hand side. Interchanging $F \leftrightarrow G$ yields

$$\int \int G(\nu)R(\nu',\nu)F(\nu')\,d\nu\,d\nu' = \int G(\nu)\left\{\varphi(\nu)F(\nu) + \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\left[D(\nu)\frac{\partial F(\nu)}{\partial\nu}\right]\right\}d\nu.\tag{A5}$$

Subtracting this equation from equation (A3) gives

$$\int \int G(\nu)[R(\nu,\nu') - R(\nu',\nu)]F(\nu')\,d\nu\,d\nu' = 0.$$
(A6)

This relation is true for arbitrary $G(\nu)$ and $F(\nu)$, which implies

$$R(\nu,\nu') = R(\nu',\nu); \tag{A7}$$

that is, the RD94 F-P approximation maintains the exact symmetry of the redistribution function on which it was based.

APPENDIX B

DERIVATION OF THE "CORRECTED" FOKKER-PLANCK EOUATION

Since $R(\nu,\nu')$ is symmetric, we may write the following for an arbitrary function $G(\nu)$:

$$\int G(\nu')R(\nu',\nu)\,d\nu' = \varphi(\nu)G(\nu) + \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\left[D(\nu)\frac{\partial G(\nu)}{\partial\nu}\right].\tag{B1}$$

The symmetry also allows us to use equation (18) to give "corrected" versions of equations (A2) and (B1), namely,

$$\int R_c(\nu,\nu')F(\nu')\,d\nu' = \varphi F + \frac{\Delta\nu_{\rm D}^2}{2}U\frac{\partial}{\partial\nu}\left[D\frac{\partial}{\partial\nu}\left(U^{-1}F\right)\right],\tag{B2}$$

$$\int G(\nu')R_c(\nu',\nu)\,d\nu' = \varphi G + \frac{\Delta\nu_{\rm D}^2}{2}\,U^{-1}\frac{\partial}{\partial\nu}\left[D\frac{\partial}{\partial\nu}(UG)\right] \tag{B3}$$

for arbitrary functions $F(\nu)$ and $G(\nu)$.

On the basis of the preceding, we now derive a corrected F-P transfer equation. Stimulated emission can be easily incorporated into this derivation by starting with the full equation,

$$\frac{1}{c\chi}\frac{\partial J}{\partial t} = \int [1+n(\nu)]R_c(\nu,\nu')J(\nu') - [1+n(\nu')]R_c(\nu',\nu)J(\nu)\,d\nu'.$$
(B4)

The integrals over ν' can be performed using equation (B2) with F = J and equation (B3) with G = 1 + n, which gives

$$\frac{1}{c\chi}\frac{\partial J}{\partial t} = \frac{\Delta\nu_{\rm D}^2}{2} \left((1+n)U\frac{\partial}{\partial\nu} \left[D\frac{\partial}{\partial\nu} \left(U^{-1}J \right) \right] - U^{-1}J\frac{\partial}{\partial\nu} \left\{ D\frac{\partial}{\partial\nu} \left[(1+n)U \right] \right\} \right). \tag{B5}$$

The right-hand side can be written as a frequency derivative,

$$\frac{1}{c\chi}\frac{\partial J}{\partial t} = \frac{\Delta\nu_{\rm D}^2}{2}\frac{\partial}{\partial\nu}\bigg\{(1+n)UD\frac{\partial}{\partial\nu}\left(U^{-1}J\right) - U^{-1}JD\frac{\partial}{\partial\nu}[(1+n)U]\bigg\}.$$
(B6)

Substituting $n = c^2 J/2\nu^2$ and using equation (19), we find, after some straightforward manipulations, the "corrected" equation (20) in terms of the mean intensity.

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