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Multifrequency-Gray Method for Radiation Diffusion with Compton Scattering

ALAN M. WINSLOW*

Lawrence Livermore National Laboratory, Livermore, California 94550

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We describe an improved multifrequency-gray method for time-dependent nonequilibrium flux-limited radiation diffusion in a high temperature system, using a two-temperature model for electrons and ions and including energy exchange between photons and electrons by Compton scattering. Our gray equation has a nonsymmetric finite difference matrix that allows us to represent negative gray diffusion coefficients, which occur in the presence of a "greenhouse" effect, in a numerically stable manner. Numerical results are presented. © 1995 Academic Press, Inc.

I. INTRODUCTION

Radiation transport in a nonequilibrium high temperature system, such as is encountered in plasma physics or astrophysics, is often calculated by using multigroup radiation diffusion. When the energy in the radiation field is comparable to the material energy and interacts strongly with it, the radiation and material energy fields must be advanced in time simultaneously in order to permit time steps that are physically reasonable. A method currently in use for solving this coupled system of equations is the multifrequency-gray (MFG) method of H. L. Wilson [1] and B. Freeman [2]; see also [3]. In this paper we describe an improved version of the MFG method which has two new features: (a) energy exchange between photons and electrons by Compton scattering; (b) a stable numerical scheme for representing negative gray diffusion coefficients.

In the following sections we discuss the differential equations, the MFG method, the finite difference equations and numerical methods for their solution, and we present some typical results.

II. DIFFERENTIAL EQUATIONS

The frequency-dependent radiation diffusion equation, derived from the frequency-dependent radiation transport equation [4], is

$$\rho\frac{\partial}{\partial t}(E_\nu/\rho) + \nabla\cdot\mathbf{F}_\nu = c\rho\kappa_\nu(B_\nu - E_\nu) + \frac{\nu}{3}\frac{\partial E_\nu}{\partial \nu}\nabla\cdot\mathbf{w} + \nu\frac{\partial H_\nu}{\partial \nu} + S_\nu, \tag{1}$$

where ν is the frequency variable (in energy units), $E(\nu, \mathbf{r}, t)$ is the radiation energy density per unit energy, $\mathbf{F}_\nu$ is the radiation flux, ρ is the matter density, $\mathbf{w}$ is the matter velocity, B_ν is the Planck function $B(\nu, T) \equiv (\text{const})\nu^3/(e^{\nu/T} - 1)$ normalized to aT^4, T_e is the electron temperature, κ_ν is the reduced absorption opacity, a is the radiation constant, c is the speed of light, and S_ν is a source rate. We have used the subscript ν as an abbreviation for functional dependence on frequency; e.g., $E_\nu \equiv E(\nu, \mathbf{r}, t)$, where $\mathbf{r}$ is the position vector and t stands for time. The term containing $\mathbf{w}$ represents a frequency shift due to material motion. The function $H(\nu, T_e)$ represents Compton scattering in the Fokker–Planck approximation,

$$H(\nu, T_e) \equiv \frac{\sigma_0}{mc}\frac{8\pi}{h^3c^3}G(\nu, T_e),$$

where σ_0 is the macroscopic Thomson cross section, h is Planck's constant, and m is the electron mass. $G(\nu, T_e)$ is the Kompaneets expression [5] multiplied by Cooper's relativistic correction factor [6] $g(\nu, T_e)$ (see Appendix A):

$$G(\nu, T_e) \equiv g(\nu, T_e)\nu^4\left(T_e\frac{\partial f}{\partial \nu} + f + f^2\right).$$

Here $f(\nu)$ is the photon distribution function: $f(\nu) \equiv (h^3c^3/8\pi)E(\nu)/\nu^3$. The correction factor $g(\nu, T_e)$ extends the upper limit of accuracy of the Fokker–Planck approximation to temperatures of about 100 keV.

In the diffusion approximation, the flux is given by

$$\mathbf{F}_\nu = -c\lambda_\nu\nabla E_\nu, \tag{2}$$

where $c\lambda_\nu$ is the flux-limited diffusion coefficient [7].

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* Present address: 28 Castlewood Drive, Pleasanton, California 94566.

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Besides Eq. (1) for the radiation energy, we have two equations for T_e and the ion temperature T_i,

$$C_e \frac{\partial T_e}{\partial t} = -\nabla \cdot \mathbf{F}_e - \Pi_e \frac{\partial \mathcal{V}}{\partial t} - c \int_0^\infty \kappa_\nu (B_\nu - E_\nu)\, d\nu \\ - \frac{1}{\rho} \int_0^\infty \nu \frac{\partial H_\nu}{\partial \nu}\, d\nu - \Omega_{ei}(T_e - T_i) + S_e \qquad (3)$$

$$C_i \frac{\partial T_i}{\partial t} = -\nabla \cdot \mathbf{F}_i - \Pi_i \frac{\partial \mathcal{V}}{\partial t} + \Omega_{ei}(T_e - T_i) + S_i, \qquad (4)$$

where

$$C_e \equiv \frac{\partial \varepsilon_e}{\partial T_e}, \quad C_i \equiv \frac{\partial \varepsilon_i}{\partial T_i}, \quad \Pi_e \equiv p_e + \frac{\partial \varepsilon_e}{\partial \mathcal{V}}, \quad \Pi_i \equiv p_i + \frac{\partial \varepsilon_i}{\partial \mathcal{V}}.$$

Here $\mathcal{V}$ is the specific volume, ε_e and ε_i are the electron and ion specific energies, respectively, p_e, p_i are the electron and ion pressures, respectively, S_e and S_i are electron and ion specific energy sources, respectively, and Ω_{ei} is a function of T_e and T_i representing the Coulomb interaction of the electrons and ions which are each assumed to have Maxwellian velocity distributions [8]. The quantities $\mathbf{F}_e$ and $\mathbf{F}_i$ respectively represent electron and ion heat conduction fluxes,

$$\mathbf{F}_e \equiv -D_e \nabla T_e, \quad \mathbf{F}_i \equiv -D_i \nabla T_i,$$

where D_e, D_i are flux-limited conduction coefficients.

At high temperatures and densities, the radiation energy density is large and is strongly coupled to the electron energy which in turn is strongly coupled to the ion energy. Hence we need to advance all three energy fields in time simultaneously in order to be able to use a time step which is large compared to the characteristic emission or absorption time $(c\rho\kappa_\nu)^{-1}$ or the analogous Compton scattering time. For this purpose we use a modified MFG method as discussed in the next two sections.

III. THE GRAY RADIATION ENERGY EQUATION

We obtain an equation for the gray (total) radiation energy density E by integrating Eq. (1) over frequency:

$$\rho \frac{\partial (E/\rho)}{\partial t} = c \nabla \cdot \int_0^\infty \lambda_\nu \nabla E_\nu\, d\nu + \frac{\nabla \cdot \mathbf{w}}{3} \int_0^\infty \nu \frac{\partial E_\nu}{\partial \nu}\, d\nu \\ + c\rho \int_0^\infty \kappa_\nu (B_\nu - E_\nu)\, d\nu + \int_0^\infty \nu \frac{\partial H_\nu}{\partial \nu}\, d\nu + \int_0^\infty S_\nu\, d\nu. \qquad (5)$$

We convert the integrals over frequency in (5) to functions of E and T_e, as follows:

(a) *Emission.* Dividing and multiplying by the integral of B_ν over frequency, we get

$$\int \kappa_\nu(T_e) B_\nu(T_e)\, d\nu \equiv \left(\frac{\int \kappa_\nu(T_e) B_\nu(T_e)\, d\nu}{\int B_\nu(T_e)\, d\nu} \right) \int B_\nu(T_e)\, d\nu \qquad (6)$$

$$\approx \frac{\int \kappa_\nu(T_e) B_\nu(T_e)\, d\nu}{\int B_\nu(T_e)\, d\nu} a T_e^4 \equiv \kappa_p(T_e) a T_e^4.$$

The mean emission opacity κ_p is the usual Planck mean opacity. It is a function of T_e, using the latest available estimate of T_e.

(b) *Absorption.* Dividing and multiplying by the integral of E_ν over frequency, we get

$$\int \kappa_\nu E_\nu\, d\nu \equiv \left(\frac{\int \kappa_\nu E_\nu\, d\nu}{\int E_\nu\, d\nu} \right) \int E_\nu\, d\nu \approx \frac{\int \kappa_\nu E_\nu\, d\nu}{\int E_\nu\, d\nu} E \equiv \kappa_a E. \qquad (7)$$

The mean absorption opacity κ_a is a homogeneous functional of the spectral energy density E_ν, using the latest available estimate of E_ν.

(c) *Material motion.* Using the relation

$$\nabla \cdot \mathbf{w} = \frac{1}{\mathcal{V}} \frac{\partial \mathcal{V}}{\partial t}$$

and integrating by parts

$$\frac{1}{3} \int_0^\infty \nu \frac{\partial E_\nu}{\partial \nu}\, d\nu = -\frac{E}{3} = -p_r$$

where p_r is the radiation pressure, we get

$$\frac{1}{3} \nabla \cdot \mathbf{w} \int_0^\infty \nu \frac{\partial E_\nu}{\partial \nu}\, d\nu = -\rho p_r \frac{\partial \mathcal{V}}{\partial t}. \qquad (8)$$

(d) *Compton scattering.* Integrating the Compton scattering term, we obtain (see Appendix B)

$$\int_0^\infty \nu \frac{\partial H_\nu}{\partial \nu}\, d\nu = \frac{4\sigma_0}{mc} L(T_e - T_c) E \qquad (9)$$

which expresses energy exchange by Compton scattering between electrons and photons as the difference between "emission" and "absorption" terms. Here L is a dimensionless relativistic correction factor, and T_c, which we may call the "Compton temperature," depends on the radiation spectrum and is approximately one-fourth of the average spectral energy. For a Planckian spectrum, T_c equals T_r, the radiation temperature $(E/a)^{1/4}$. Equation (9) turns out to be a generalization of a well-known formula due to Hurwitz [9] and Weymann [10], derived in an entirely different manner, for the rate of Compton scattering energy exchange between an electron gas at temperature T_e and a Planckian radiation field of energy density E. It reduces to their formula when $L = 1$ and $T_c = T_r$.

(e) *Diffusion.* In one space dimension, we average by dividing and multiplying by the integral of the gradient of E_ν over frequency, obtaining

$$\begin{aligned}\frac{\mathbf{F}}{c} &= -\int \lambda_\nu \nabla E_\nu \, d\nu \equiv -\left(\frac{\int \lambda_\nu \nabla E_\nu \, d\nu}{\int \nabla E_\nu \, d\nu}\right) \int \nabla E_\nu \, d\nu \\ &\approx -\frac{\int \lambda_\nu \nabla E_\nu \, d\nu}{\int \nabla E_\nu \, d\nu} \nabla E \equiv -\lambda_G \nabla E,\end{aligned} \tag{10}$$

thus defining a gray mean free path λ_G as the ratio of two integrals containing the gradient of E_ν, the latest available spectrum.

In the equilibrium limit, where E_ν becomes equal to B_ν, a function of T_e, we have gradients of T_e in numerator and denominator which cancel and λ_G becomes the usual Rosseland mean free path λ_R, where

$$\lambda_R \equiv \int \lambda_\nu \frac{\partial B_\nu}{\partial T_e} d\nu \Big/ \int \frac{\partial B_\nu}{\partial T_e} d\nu.$$

This expression, which is positive, is valid also in the multidimensional case.

In the nonequilibrium case, λ_G is not well conditioned and may be negative, which leads to numerical instability but, as we show in Section X, is physically correct. To obtain an expression that is numerically stable and also valid multidimensionally, we do not use λ_G, but instead we integrate in frequency over the finite difference expression for $\mathbf{F}$. We assume that at the interface between two zones, the gradient of E_ν is approximated by a two-point expression having the form

$$\nabla E_\nu = \frac{E_\nu^+ - E_\nu^-}{\Delta x},$$

where + and − refer to the zones lying on each side of the zone interface and Δx represents an appropriate measure of the distance between zone centers. Then instead of (10) we write

$$\begin{aligned}\frac{\mathbf{F}}{c} &= -\int \lambda_\nu \nabla E_\nu \, d\nu = -\frac{1}{\Delta x} \int \lambda_\nu (E_\nu^+ - E_\nu^-) \, d\nu \\ &= -\left(\frac{\lambda^+ E^+ - \lambda^- E^-}{\Delta x}\right),\end{aligned} \tag{10a}$$

where

$$\begin{aligned}\lambda^+ &= \frac{\int \lambda_\nu E_\nu^+ \, d\nu}{\int E_\nu^+ \, d\nu}, \quad \lambda^- = \frac{\int \lambda_\nu E_\nu^- \, d\nu}{\int E_\nu^- \, d\nu}, \\ E^+ &= \int E_\nu^+ \, d\nu, \quad E^- = \int E_\nu^- \, d\nu.\end{aligned} \tag{10b}$$

The denominators of these expressions contain E_ν instead of ∇E_ν and, hence, are always positive. Using (10a) and (10b), with *two* spectrum-dependent diffusion coefficients at each zone interface, allows the gray energy to diffuse with or against the gradient of E, depending on the relative magnitudes of $\lambda^+ E^+$ and $\lambda^- E^-$. We thus achieve the same result as using a negative λ_G, but in a numerically stable way. Other users of the MFG method have resorted to incorrect ad hoc procedures such as forcing λ_G to be positive [11]. For discussion of the general case, see Section VII.

We can obtain a numerically stable differential form equivalent to Eq. (10a) by rewriting $\mathbf{F}$ in the form [12]

$$\frac{\mathbf{F}}{c} = -\nabla \int \lambda_\nu E_\nu \, d\nu + \int E_\nu \nabla \lambda_\nu \, d\nu = -\nabla(\bar{\lambda} E) + (\overline{\nabla \lambda}) E,$$

where

$$\bar{\lambda} = \int \lambda_\nu E_\nu \, d\nu \Big/ \int E_\nu \, d\nu$$

and

$$\overline{\nabla \lambda} = \int (\nabla \lambda_\nu) E_\nu \, d\nu \Big/ \int E_\nu \, d\nu.$$

The denominators of these expressions also contain E_ν, instead of ∇E_ν. We thus obtain

$$\mathbf{F} = -c\bar{\lambda} \nabla E + (\overline{\nabla \lambda} - \nabla \bar{\lambda}) cE. \tag{11}$$

The first term in Eq. (11) has a positive diffusion coefficient, but it may be dominated by the second term; if the latter is negative, we get the same result as using Eq. (10) with a negative diffusion coefficient. By using this form we avoid numerical instabilities but add an advection term to the gray energy equation. As E_ν approaches B_ν, this advection term disappears, λ_G approaches λ_R, and the expression for $\mathbf{F}$ given in (11) becomes the usual expression (10).

Substituting Eqs. (6) to (9) and (11) into Eq. (5), we get the gray energy equation

$$\begin{aligned}\rho \frac{\partial}{\partial t}(E/\rho) &= c\nabla \cdot (\bar{\lambda} \nabla E - (\overline{\nabla \lambda} - \nabla \bar{\lambda})E)) - \rho p_r \frac{d\mathcal{V}}{dt} \\ &\quad + c\rho(\kappa_p a T_e^4 - \kappa_a E) + \frac{4\sigma_0}{mc} L(T_e - T_c)E + S_r,\end{aligned} \tag{12}$$

where S_r is the integrated radiation source. Using (6), (7), and (9), we can eliminate the integrals over frequency from (3) and rewrite it in the form

$$
\begin{aligned}
C_e \frac{\partial T_e}{\partial t} = -\nabla \cdot \mathbf{F}_e - \Pi_e \frac{\partial \mathcal{V}}{\partial t} - c(\kappa_p a T_e^4 - \kappa_a E) \\
- \frac{4\sigma_0}{\rho m c} L(T_e - T_c) - \Omega_{ei}(T_e - T_i) + S_e.
\end{aligned} \tag{12a}
$$

Numerical solution of the coupled energy equations (12a), (4), and (12) is discussed in Section VIII.

IV. THE MULTIGROUP EQUATIONS

To form the multigroup diffusion equations, we choose a nonuniform frequency mesh ν_k ($k = 1, 2, ..., k_{\max}$), integrate Eq. (1) over each group k, and average. We get

$$
\begin{aligned}
\rho \frac{\partial}{\partial t}(E_k/\rho) + \nabla \cdot F_k = c\rho\kappa_k(B_k - E_k) \\
+ \frac{\nu_{k+1/2}}{3}\left(\frac{E_{k+1} - E_k}{\nu_{k+1} - \nu_k}\right)\nabla \cdot \mathbf{w} \\
+ \nu_k \left(\frac{G_{k+1/2} - G_{k-1/2}}{\nu_{k+1/2} - \nu_{k-1/2}}\right) + S_k \\
(k = 1, 2, ..., k_{\max})
\end{aligned} \tag{13}
$$

where

$$
\mathbf{F}_k = -c\lambda_k \nabla E_k.
$$

Here the coefficients κ_k and λ_k represent averages over the kth group. The calculation of $\nu_{k+1/2}$ and $G_{k+1/2}$ is discussed in Appendix A.

V. THE MULTIFREQUENCY-GRAY METHOD

The multifrequency-gray method consists of the following operations, carried out over each time step:

(a) solve the system of Eqs. (13) for E_k with T_e fixed;

(b) using T_e and the spectrum E_k just obtained, calculate the gray coefficients L, T_c, κ_p, κ_a, and $\lambda^{\pm}$, which govern the emission, absorption, and diffusion of gray radiation energy;

(c) solve the system of Eqs. (3), (4), (12) to obtain new values of E, T_e, and T_i.

By adding the redundant Eq. (12) we have split the system of equations (3), (4), (13) into two simpler systems:

(A) the $k_{\max}$ multigroup equations (13)

(B) the three energy equations (3), (4), (12).

No energy exchange takes place when solving the multigroup equations (A); they are used only to update the radiation energy spectrum, which is then used to calculate the gray coefficients for equations (B). We have found that when solving the multigroup equations (13), it is practical to uncouple them by treating the velocity and Compton scattering terms by operator splitting. The difference equations for Compton scattering are discussed in Appendix A.

Lund [13] has proposed iterating over steps (a) to (c) so that the solution will be fully implicit. This means that the integrals of B_ν and E_ν over frequency, which form the denominators of Eqs. (6), (7), and (10b), will equal aT_e^4 and E, respectively, as we assumed. Since for reasons of efficiency we do not iterate, our scheme is only semi-implicit. In regions where T_e or the spectrum E_k is changing rapidly, there may be some inconsistency between these integrals and their gray values, but it is usually small. The gray coefficients κ_a, λ^+, and λ^- are not sensitive to changes in T_e or the radiation spectrum E_ν because the spectral integrals appear in both numerator and denominator.

We solve these equations in finite difference form which we derive in the next three sections.

VI. FINITE DIFFERENCE FORM OF THE MULTIGROUP DIFFUSION EQUATIONS

Using a control volume approach to derive the finite difference equations, we integrate each of the $k_{\max}$ equations (13) over a zone volume δV and over the time step Δt. We omit the velocity and Compton terms which we treat by operator splitting. For the kth equation this gives us

$$
\begin{aligned}
\int \rho \frac{\partial}{\partial t}\left(\frac{E_k}{\rho}\right) dV = -\int \nabla \cdot \mathbf{F}_k \, dV \\
+ c \int \rho\kappa_k(B_k - E_k)\, dV + \int S_k \, dV.
\end{aligned} \tag{14}
$$

Using Gauss' theorem, the first integral on the right-hand side becomes a surface integral,

$$
-\int \nabla \cdot \mathbf{F}_k \, dV = -\int \mathbf{F}_k \cdot \hat{\mathbf{n}} \, dA = c \int \lambda_k \nabla E_k \cdot \hat{\mathbf{n}} \, dA,
$$

where $\hat{\mathbf{n}}$ is the unit outward normal vector at the zone surface. Discretization of this surface integral will depend on the shape of the zone, but in general it leads to an expression of the form [14] $w_{ij}^k(E_{i,k} - E_{j,k})$, where the subscripts i and j refer to adjacent zones. The coupling coefficient w_{ij}^k depends on geometrical factors and on the mean free path λ_{ij}^k evaluated at the edge between zones i and j. It is symmetric; i.e., $w_{ij}^k = w_{ji}^k$. In a 1D mesh or in a rectangular 2D mesh, $w_{ij}^k > 0$, but in a distorted mesh it is possible to have $w_{ij}^k < 0$. However, it can be shown that in general

$$\sum_i w^k_{ij} > 0, \tag{15}$$

summing over the neighboring zones i of zone j.

Discretizing the other terms, we obtain for zone j,

$$\begin{aligned} \delta V_j \cdot E_{j,k} - \delta V^n_j \cdot E^n_{j,k} = \Delta t \sum_i (w^k_{ij})^n (E_{i,k} - E_{j,k}) \\ + c\kappa^n_{j,k}\, \Delta t\, \delta m_j (B^n_{j,k} - E_{j,k}) \qquad \text{(16a)} \\ + S^n_{j,k}\, \Delta t\, \delta V_j \quad (k = 1, 2, ..., k_{\max}) \end{aligned}$$

as the finite difference form of Eqs. (13). Here δV is the zone volume, δm is the constant zone mass, and the sum is over the neighboring zones i of zone j. The superscript n refers to discretization in time: variables with superscript n are evaluated at the time t^n, the beginning of the time step; those without a superscript at time t^{n+1}, the end of the time step.

Equations (16a) can be rearranged into the form

$$\begin{aligned} \left(\delta V_j + c\kappa^n_{j,k}\, \Delta t\, \delta m_j + \Delta t \sum_i w^k_{ij}\right) E_{j,k} - \Delta t \sum_i w^k_{ij} E_{i,k} \\ = \delta V^n_j E^n_{j,k} + c\kappa^n_{j,k}\, \Delta t\, \delta m_j B^n_{j,k} + S^n_{j,k}\, \Delta t\, \delta V_j \qquad \text{(16b)} \\ (k = 1, 2, ..., k_{\max}), \end{aligned}$$

dropping the superscript n on the coupling coefficients for simplicity of notation. Because of (15), the diagonal elements of the matrices in (16b) are positive.

VII. FINITE DIFFERENCE FORM OF THE GRAY DIFFUSION OPERATOR

Since the gray energy density E is defined only as the solution of Eq. (12), it is not guaranteed to be equal to the integral of E_ν over frequency. To maintain consistency between the gray and multifrequency solutions, we need to difference the gray Eq. (12) in a manner that is consistent with the multigroup difference equations (16). If we try to difference (12), we face the problem of differencing the advection term in a manner consistent with the differencing of the $\lambda_k \nabla E_k$ terms in Eqs. (16), which do not contain gradients of λ_k. To avoid this problem, we derive the gray energy difference equation directly from the multigroup difference equations (16) by integrating them over frequency. This means that we integrate over frequency *after* spatially differencing the multigroup differential equations rather than before [15].

The sum in Eqs. (16) for zone j and frequency group k is

$$S^k_j = \sum_i w^k_{ij} (E_{i,k} - E_{j,k}) \tag{17}$$

summed over the neighboring zones i of zone j. Multiplying (17) by $\Delta\nu_k$, the width of group k, and summing over all frequency groups, we get

$$S_j = \sum_i (w_{ij,i} E_i - w_{ij,j} E_j), \tag{18}$$

where E_i and E_j represent the gray energy densities in zones i and j, respectively:

$$E_i \equiv \sum_k E_{i,k}\, \Delta\nu_k, \quad E_j \equiv \sum_k E_{i,k}\, \Delta\nu_k.$$

We have averaged the group coupling coefficients w^k_{ij} separately over $E_{i,k}$ and $E_{j,k}$ to form two gray coupling coefficients:

$$w_{ij,i} \equiv \sum_k w^k_{ij} E_{i,k}\, \Delta\nu_k \Big/ \sum_k E_{i,k}\, \Delta\nu_k$$

and

$$w_{ij,j} \equiv \sum_k w^k_{ij} E_{j,k}\, \Delta\nu_k \Big/ \sum_k E_{j,k}\, \Delta\nu_k$$

which have positive denominators. The third subscript on these gray coupling coefficients indicates the zone over whose spectrum we average.

Some basic properties of the gray diffusion matrix w_{ij} are:

(1) in general, $w_{ij,i} \neq w_{ij,j}$; i.e., it is nonsymmetric (although symmetric in its sparsity structure);

(2) it is conservative. Consider the flux F_{ij} from zone i to zone j:

$$F_{ij} = w_{ij,i} E_i - w_{ij,j} E_j \tag{19a}$$

Interchanging i and j, and using the fact that $w_{ij,k}$ is symmetric in the first two subscripts, we get

$$F_{ji} = w_{ij,j} E_j - w_{ij,i} E_i = -F_{ij};$$

(3) it is flux-limited, since flux limiting is incorporated in the coupling coefficients w^k_{ij} for each group;

(4) it permits gray energy to flow "uphill," i.e., from low to high energy density, depending on the relative magnitudes of $w_{ij,j}$ and $w_{ij,i}$. This is a fundamental property of non-Planckian gray radiation and gives rise to the "greenhouse" effect (see Section X). By using two positive coupling coefficients for each pair of coupled zones, we achieve the same result as using a single negative diffusion coefficient, but without the resulting numerical problems.

The degree of asymmetry of the gray diffusion matrix is problem-dependent. We can see this by writing the flux F_{ij}, from (19a), in the symmetric form

$$F_{ij} = \left(\frac{w_{ij,i}E_i - w_{ij,j}E_j}{E_i - E_j}\right)(E_i - E_j)$$
$$= \langle w_{ij}\rangle(E_i - E_j), \tag{19b}$$

where

$$\langle w_{ij}\rangle \equiv \frac{\sum_k w_{ij}^k(E_{i,k} - E_{j,k})\,\Delta\nu_k}{\sum_k (E_{i,k} - E_{j,k})\,\Delta\nu_k}.$$

In equilibrium regions, where E_ν approaches B_ν, $\langle w_{ij}\rangle$ clearly becomes proportional to the Rosseland mean free path λ_R in finite difference form, and we can use the symmetric form (19b) instead of (19a). Where there is a "greenhouse" effect, however, $\langle w_{ij}\rangle$ will be negative (see Section X) and we must use the nonsymmetric form (19a).

VIII. FINITE DIFFERENCE FORM OF THE COUPLED ENERGY EQUATIONS

Using Eqs. (6), (7), (8), and (18) and discretizing by integrating over Δt and δV, the energy differential equations (12a), (4), and (12) can be written in finite difference form for the jth zone (for simplicity of notation we have suppressed the subscript j) as follows:

$$C_e(T_e - T_e^n) = L_e(T_e)\,\Delta t - \Pi_e\,\Delta V - \Omega_{ei}\,\Delta t(T_e - T_i)$$
$$+ S_e\,\Delta t - \chi_{er}\,\Delta t \tag{20}$$

$$C_i(T_i - T_i^n) = L_i(T_i)\,\Delta t - \Pi_i\,\Delta V$$
$$+ \Omega_{ei}\,\Delta t(T_e - T_i) + S_i\,\Delta t \tag{21}$$

$$\delta V{\cdot}E - \delta V^n{\cdot}E^n = -p_r\,\Delta V + \Delta t \sum_i (w_{i,i}E_i - w_iE)$$
$$+ S_r\,\Delta t + \chi_{er}\,\Delta t\,\delta m, \tag{22}$$

where

$$\Delta V \equiv \delta V - \delta V^n, \quad w_{i,i} \equiv w_{ij,i}, \quad w_i \equiv w_{ij,j}$$

and C_e, C_i, P_e, P_i, W_{ei}, S_e, S_i, S_r, and p_r are all evaluated at time t^n. Here L_e and L_i are the electron and ion conduction terms, respectively, and χ_{er} is the electron–radiation coupling term:

$$\chi_{er} = c(\kappa_p a T_e^4 - \kappa_a E) + \frac{4\sigma_0}{\rho mc} L(T_e - T_c)E.$$

Substituting this into (22) we have

$$\left[\delta V\left(1 + \rho c\kappa_a\,\Delta t - \frac{4\sigma_0}{mc} L\,\Delta t(T_e - T_c)\right) + w_i\,\Delta t\right]$$
$$E - \Delta t \sum_i w_{i,i}E_i = \delta V^n E^n - p_r\,\Delta V + S_r\,\Delta t \tag{23}$$
$$+ c\kappa_p\,\Delta t\,\delta m\,aT_e^4.$$

Because of (15), we have $w_i > 0$, and the diagonal elements of the matrix will be positive if $T_e \leq T_c$. If $T_e > T_c$, then the diagonal elements will be positive if the time step Δt satisfies the restriction

$$\Delta t < \frac{1}{4\sigma_0 cL}\left(\frac{mc^2}{T_e - T_c}\right) \approx \frac{2 \times 10^{-8}}{\rho L(T_e - T_c)}\,\mathrm{s} \quad (T_e, T_c \text{ in kev})$$

In order to solve Eqs. (20) to (22), we use operator splitting and first calculate conduction only,

$$C_e(T_e^* - T_e^n) = L_e(T_e^*)\,\Delta t$$

$$C_i(T_i^* - T_i^n) = L_i(T_i^*)\,\Delta t,$$

thus advancing the electron and ion temperatures to T_e^* and T_i^*, respectively and reducing (20) and (21) to

$$C_e(T_e - T_e^*) = -\Pi_e\,\Delta V - \Omega_{ei}\,\Delta t(T_e - T_i)$$
$$+ S_e\,\Delta t - \chi_{er}\,\Delta t \tag{24}$$

$$C_i(T_i - T_i^*) = -\Pi_i\,\Delta V + \Omega_{ei}\,\Delta t(T_e - T_i) + S_i\,\Delta t. \tag{25}$$

Next we formally eliminate the electron–ion coupling term. Defining the dimensionless electron–ion coupling parameters

$$x \equiv \frac{\Omega_{ei}\,\Delta t}{C_i + \Omega_{ei}\,\Delta t}, \quad y \equiv \frac{\Omega_{ei}\,\Delta t}{C_e + \Omega_{ei}\,\Delta t}$$

and making use of the identities

$$C_eC_i + (C_e + C_i)\Omega_{ei}\,\Delta t \equiv (C_i + \Omega_{ei}\,\Delta t)(C_e + xC_i)$$
$$\equiv (C_e + \Omega_{ei}\,\Delta t)(C_i + yC_e),$$

we can rewrite Eqs. (24) and (25) with Ω_{ei} hidden, but with altered specific heats and source terms

$$C_e^*(T_e - T_e^{**}) = -\Pi_e^*\,\Delta V + S_e^*\,\Delta t - \chi_{er}\,\Delta t \tag{26}$$

$$C_i^*(T_i - T_i^{**}) = -\Pi_i^*\,\Delta V + S_i^*\,\Delta t - y\chi_{er}\,\Delta t, \tag{27}$$

where the starred variables C_e^*, P_e^*, S_e^*, etc. represent mixed electron–ion quantities having the form

$$f_e^* \equiv f_e + x f_i, \quad f_i^* \equiv f_i + y f_e$$

and the mixed electron and ion temperatures T_e^{**} and T_i^{**} are defined by

$$C_e^* T_e^{**} \equiv C_e T_e^* + x C_i T_i^*, \quad C_i^* T_i^{**} \equiv C_i T_i^* + y C_e T_e^*$$

In the limit of zero electron–ion coupling ($x = y = 0$), the star superscripts disappear, while in the limit of infinitely strong coupling ($x = y = 1$), the electron and ion energy equations reduce to one equation for the total material energy.

We linearize χ_{er} in T_e and E by using the approximations:

$$\begin{aligned} T_e^4 &\equiv (T_e^n + \Delta T_e)^4 = (T_e^n)^4 + 4(T_e^n)^3 \Delta T_e \left(1 + \frac{3}{2}\frac{\Delta T_e}{T_e^n} + \cdots\right) \\ &\approx 4(T_e^n)^3 T_e - 3(T_e^n)^4, \end{aligned}$$

provided $\Delta T_e \ll T_e^n$, and

$$\begin{aligned} T_e E &\equiv (T_e^n + \Delta T_e)(E^n + \Delta E) \\ &= (T_e E^n + E T_e^n - T_e^n E^n)\left(1 + \frac{\Delta T_e}{T_e^n}\frac{\Delta E}{E^n}\Big/\left(1 + \frac{\Delta T_e}{T_e^n}\frac{\Delta E}{E^n}\right)\right) \\ &\approx T_e E^n + E T_e^n - T_e^n E^n, \end{aligned}$$

provided $\Delta T_e \ll T_e^n$ or $\Delta E \ll E^n$. Using the linearized form of χ_{er} in Eqs. (22) and (26), we formally solve (26) for T_e and substitute into (22), yielding an equation that can be solved for E, as discussed in the next section. We then solve (26) for T_e and finally (27) for T_i.

IX. NUMERICAL SOLUTION OF FINITE DIFFERENCE EQUATIONS

(a) *Multigroup equations.* Each of the $k_{\max}$ multigroup difference equations (16) has the form $A_k \mathbf{x}_k = \mathbf{b}_k$, where A_k is the vector of the unknown E_k's, and $\mathbf{b}_k$ is a known vector. For 1D problems, the matrix A_k is tridiagonal and is easily solved by Gaussian elimination in the "back substitution" form. For 2D problems we use the incomplete-Cholesky conjugate gradient (iccg) method as advocated by Kershaw [16].

Since the E_k's are formally decoupled in (16), these equations are well-suited to solution by parallel processing.

(b) *Gray equation.* After eliminating T_e, Eq. (22) is a nonsymmetric equation for E of the form $A\mathbf{x} = \mathbf{b}$, where $\mathbf{x}$ is the vector of unknown E's. In 1D, the nonsymmetric gray finite difference matrix A is tridiagonal and its lack of symmetry is not a barrier to its solution by Gaussian elimination ("back substitution"). However, in 2D, iterative schemes which require A to be symmetric, such as conjugate gradient methods, cannot be used. This restriction applies also to the method of Concus, Golub, and O'Leary [17] for nonsymmetric matrices because their method requires that the symmetric part of A $(=(A + A^{T})/2)$ be positive definite. It can be shown that A does not have this property.

Currently we solve (22) by a first-order iterative scheme. The equation for $\mathbf{x}^{m+1}$, the $(m + 1)^{\text{th}}$ iterate, can be written

$$\mathbf{x}^{m+1} = \mathbf{x}^m + M^{-1}(b - A\mathbf{x}^m) = \mathbf{x}^m + \mathbf{z}^{m+1}, \tag{28}$$

where

$$M\mathbf{z}^{m+1} = \mathbf{r}^m \tag{29}$$

and the residual at the m^{th} iteration $\mathbf{r}^m$ is given by

$$\mathbf{r}^m = \mathbf{b} - A\mathbf{x}^m.$$

We can write (28) in the form

$$\mathbf{x}^{m+1} = (I - M^{-1}A)\mathbf{x}^m + M^{-1}\mathbf{b} \tag{30}$$

and we see that the convergence rate will depend on the eigenvalues of the matrix $I - M^{-1}A$; rapid convergence requires that $M^{-1}A$ be close to the unit matrix I.

Two preconditioning matrices M have been used successfully:

(1) incomplete LDU factorization. $M_I = LDU$, where the three matrices LDU are respectively lower triangular, diagonal, and upper triangular, chosen so that $M_{ij} = A_{ij}$, where $A_{ij} \neq 0$; otherwise we set $M_{ij} = 0$, thus forcing M_I to have the same sparsity pattern as A. This is the analogue of the incomplete Cholesky factorization for symmetric matrices (see [14] for details). In constructing M_I we take advantage of the fact that A is symmetric in structure. The inverse $M_I^{-1} = U^{-1}D^{-1}L^{-1}$ is easily obtained recursively.

(2) symmetrization. We define M_S to be the matrix of the symmetrized problem; i.e., in (22) we replace the diffusion matrix elements $w_{ij,j}$ and $w_{ij,i}$ by $w_{ij} = (w_{ij,j} + w_{ij,i})/2$. Since M_S is symmetric and positive definite, we can then solve Eq. (29) by the iccg method (inner iteration), update $\mathbf{r}^m$ (outer iteration), and solve (29) again until convergence.

When it converges, using M_I is usually faster than using M_S. However, convergence sometimes fails when using M_I, whereas iteration with M_S so far has always converged.

Because Eq. (30) is only first-order, solving it generally takes more iterations (usually by a factor of 5 to 15) than solving a group equation. In a problem with many groups (we typically use 20 to 50) this is not a large cost.

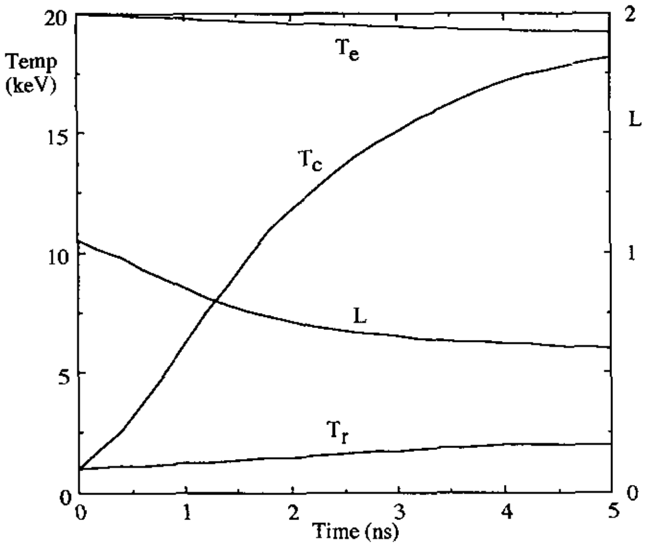

FIG. 1. Equilibration by Compton scattering only.

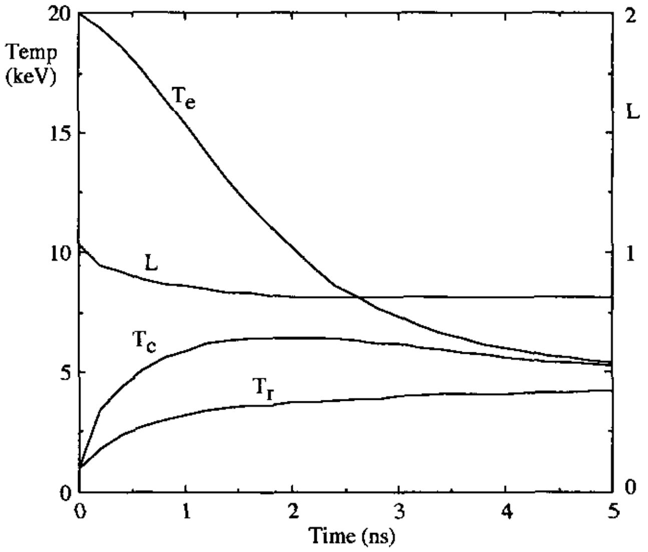

FIG. 2. Equilibration by Compton scattering, emission, and absorption.

X. NUMERICAL RESULTS

A. *Energy Exchange in an Infinite Medium with an Initial Planck Spectrum*

The heating or cooling of a photon gas, initially in a Planck distribution, demonstrates energy exchange in an infinite medium. In the following two problems we have used ionized hydrogen at a density of 1 gm/cm^3. In Figure 1 we show graphs of T_e, T_c, T_r versus time with energy exchange by Compton scattering only (keeping only the third term on the right-hand side of (1)). Here $T_c = T_r$ initially, since we begin with a Planck spectrum. The photons gain energy from the electrons and reach equilibrium when $T_c = T_e$ but $T_r < T_e$, since there are not sufficient photons (in the absence of emission processes) and equilibration occurs with a Bose–Einstein spectrum.

In Fig. 2 we show the results of another calculation in which emission and absorption also took place. Equilibrium is reached at a later time (not shown), and we then have a Planck spectrum with $T_e = T_r = T_c$.

B. *Diffusion of a Non-Planckian Spectrum and the Greenhouse Effect*

A non-Planckian spectrum can easily be produced by spherical divergence of a Planck spectrum. We consider an aluminum sphere of radius $a = 1$ cm, density 2.78 g/cm^3, separated from a concentric spherical aluminum shell of inner radius 51 cm by a region of He^4 gas at density 0.0001 g/cm^3. Let the initial temperature of the sphere be $T_e = T_i = 2$ keV and of the outer two regions 0.01 keV. For simplicity we ignore hydrodynamics. The radiation emitted from the sphere maintains its Planckian spectral shape as it crosses the He^4 because the mean free path there is on the order of 1000 cm. However, when $R \gg a$, the energy density E is reduced proportionally to R^{-2}, where R is the distance from the center of the sphere, so that we have a "dilute" Planck spectrum whose color temperature is approximately 0.2 keV but whose energy density temperature T_r is about 0.1 keV, an energy density dilution factor of $(0.2/0.1)^4 = 16$. The arriving photons are absorbed in the aluminum shell and reradiated as softer photons which have much shorter mean free paths and thus less ability to escape. The gray energy density E inside the aluminum shell becomes greater than E in the neighboring gas and, since the gray energy flux is directed outward, the gray diffusion coefficient must be negative. This problem is a good test of our gray diffusion equation.

A graph of T_e and T_r versus radius at $t = 2$ ns is shown in Fig. 3. A narrow temperature maximum just inside the alumi-

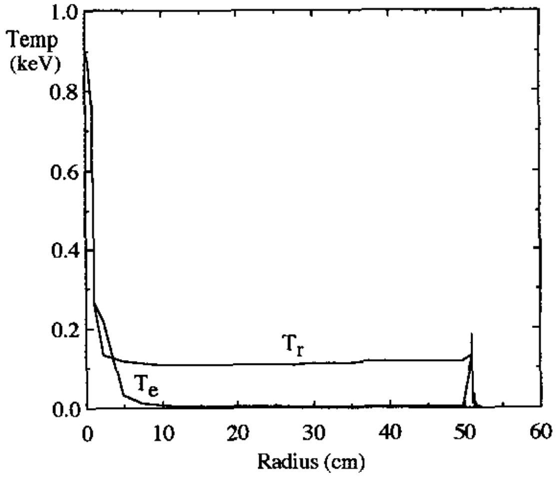

FIG. 3. T_e, T_r vs radius at $t = 2$ ns.

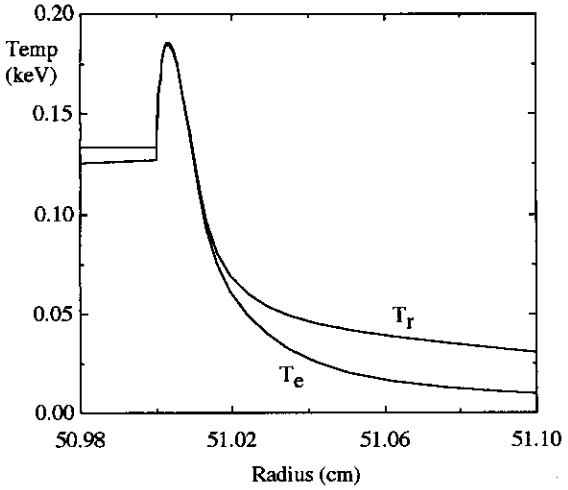

FIG. 4. T_e, T_r in shell vs radius at $t = 2$ ns.

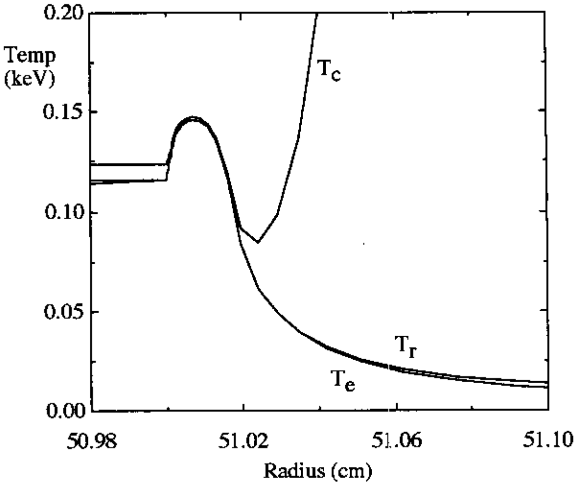

FIG. 6. T_e, T_r, T_c in shell vs radius at $t = 5$ ns.

num shell, due to the greenhouse effect, appears in Fig. 3 and is shown enlarged at $t = 2$, 3, and 5 ns in Figs. 4 to 6. Graded fine zoning, of the order of a mean free path in thickness, was used at the inner surface of the shell in order to calculate this effect. We also show T_c versus radius in Figs. 5 and 6. As the inner surface of the shell reaches equilibrium, T_c decreases and approaches T_e and T_r.

XI. CONCLUSIONS

We have demonstrated an improved form of the multifrequency-gray method for radiation diffusion in one or two space dimensions which includes: (a) Compton scattering energy exchange; (b) a nonsymmetric gray equation which can handle the physically realizable situation where the symmetric gray diffusion coefficient becomes negative.

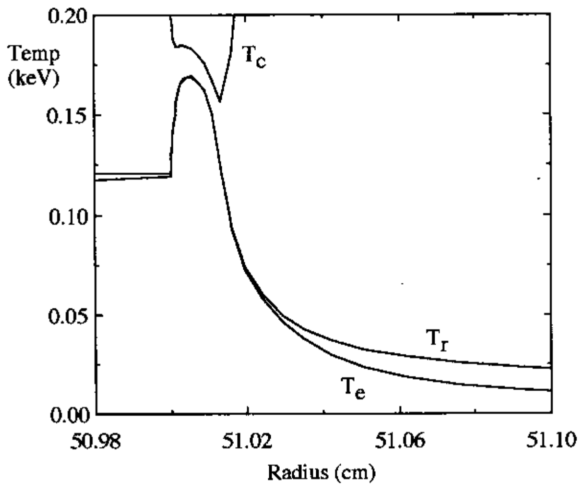

FIG. 5. T_e, T_r, T_c in shell vs radius at $t = 3$ ns.

The accuracy of this method has been assessed in a few cases by comparison with the results of an implicit Monte Carlo calculation, especially for the greenhouse case. The agreement was generally good. Another accuracy test that can be made is to compare the integral of energy over the multifrequency groups with the gray energy. Using physically reasonable timesteps, these agree within a few percent.

We are continuing to investigate faster iterative methods for the solution of the gray equation.

APPENDIX A: MULTIGROUP TREATMENT OF COMPTON SCATTERING IN THE FOKKER–PLANCK APPROXIMATION

In the Fokker–Planck approximation, the rate of change of the photon distribution function $f(\nu, t)$ due to Compton scattering is given by

$$\nu^2 \frac{\partial f}{\partial t} = \frac{\sigma_0}{mc} \frac{\partial G}{\partial \nu}, \tag{A.1}$$

where

$$G(\nu, T_e) \equiv g(\nu, T_e)\nu^4 \left(T_e \frac{\partial f}{\partial \nu} + f + f^2\right). \tag{A.2}$$

The relativistic correction of Cooper [6] has the form

$$g(\nu, T_e) = (1 + a_1\nu + a_2\nu^2)^{-1}[1 + \beta(T_e)(1 + a_3\nu)^{-1}], \tag{A.3}$$

where $\beta(T_e) \equiv \frac{5}{2}u + \frac{15}{2}u^2(1 - u)$, $u \equiv T_e/mc^2$, and a_1, a_2, and a_3 are positive constants.

Using a non-uniform frequency mesh ν_k ($k = 1, 2, \ldots, k_{\max}$) in energy space, we difference Eq. (A.1) in the form

$$\nu_k^2(f_k - f_k^n) = \Delta t \frac{\sigma_0}{mc}\left(\frac{G_{k+1/2} - G_{k-1/2}^n}{\nu_{k+1/2} - \nu_{k-1/2}}\right), \tag{A.4}$$

where

$$G_{k+1/2} \equiv g_{k+1/2}\nu_{k+1/2}^4\left[T_e\left(\frac{f_{k+1} - f_k}{\nu_{k+1} - \nu_k}\right) + f_{k+1/2}(1 + f_{k+1/2}^n)\right]. \tag{A.5}$$

Here $\nu_{k+1/2} \equiv (\nu_k + \nu_{k+1})/2$ and $f_{k+1/2} \equiv \delta_{k+1/2}f_k + (1 - \delta_{k+1/2})f_{k+1}$. The variable interpolator δ of Chang and Cooper [18] is obtained from the equilibrium spectrum and is recalculated each time step as the temperature changes. Its use permits a relatively coarse ν_k mesh.

Recently simpler differencing methods for (A.1) have been developed which better preserve positivity of the solution. They are based on the transformation (discovered independently by Youngs [19] and Larsen *et al.* [20]):

$$T\frac{\partial f}{\partial \nu} + f + f^2 = (1 + f)^2 \frac{\partial}{\partial e^{\nu/T}}\left(\frac{fe^{\nu/T}}{1 + f}\right). \tag{A.6}$$

Using (A.6), we can write (A.1) in the form

$$\nu^2\frac{\partial f}{\partial t} = \frac{\partial}{\partial \nu}\left[D(\nu, T_e)\frac{\partial}{\partial e^{\nu/T_e}}\left(\frac{fe^{\nu/T_e}}{1 + f}\right)\right], \tag{A.7}$$

where

$$D(\nu, T_e) \equiv g(\nu, T_e)\nu^4(1 + f)^2. \tag{A.8}$$

Differencing schemes for (A.7) using (A.8) are given by Youngs [19], Larsen *et al.* [20], and Shestakov *et al.* [21].

APPENDIX B: DERIVATION OF GRAY EXPRESSION FOR COMPTON SCATTERING ENERGY EXCHANGE [22]

The rate of change of the radiation energy density E due to Compton scattering is given by integrating Eq. (A.1) over frequency:

$$\left(\frac{dE}{dt}\right)_c = \frac{\sigma_0}{mc}\frac{8\pi}{h^3c^3}\int_0^\infty \nu\frac{\partial G}{\partial \nu}\,d\nu. \tag{B.1}$$

Multiplying and dividing the right-hand side of (B.1) by E, we obtain

$$\left(\frac{dE}{dt}\right)_c = \frac{\sigma_0}{mc}\left(\int_0^\infty \nu\frac{\partial G}{\partial \nu}\,d\nu \bigg/ \int_0^\infty \nu^3 f\,d\nu\right)E. \tag{B.2}$$

Temporarily ignoring the relativistic correction (setting $g = 1$), we integrate the numerator by parts twice,

$$\begin{aligned}\int_0^\infty \nu\frac{\partial G}{\partial \nu}\,d\nu &= -\int_0^\infty G\,d\nu = -T_e\int_0^\infty \nu^4\frac{\partial f}{\partial \nu}\,d\nu \\ &\quad - \int_0^\infty \nu^4 f(1 + f)\,d\nu \\ &= 4T_e\int_0^\infty \nu^3 f\,d\nu - \int_0^\infty \nu^4 f(1 + f)\,d\nu,\end{aligned} \tag{B.3}$$

where we have assumed that νG and $\nu^4 f$ vanish at both limits. Defining a mean energy of the radiation field which we call the "Compton temperature" T_c,

$$T_c \equiv \int_0^\infty \nu^4 f(1 + f)\,d\nu \bigg/ 4\int_0^\infty \nu^3 f\,d\nu; \tag{B.4}$$

then using (B.3) and (B.4), (B.2) becomes

$$\left(\frac{dE}{dt}\right)_c = \frac{4\sigma_0}{mc}(T_e - T_c)E. \tag{B.5}$$

If we now restore $g(\nu, T_e)$ to G and repeat the above integration by parts, T_c becomes

$$T_c \equiv \int_0^\infty g\nu^4 f(1 + f)\,d\nu \bigg/ \int_0^\infty f\frac{\partial}{\partial \nu}(g\nu^4)\,d\nu \tag{B.6}$$

and Eq. (B.5) becomes

$$\left(\frac{dE}{dt}\right)_c = \frac{4\sigma_0}{mc}L(T_e - T_c)E, \tag{B.7}$$

where L is a dimensionless relativistic correction factor:

TABLE I

Relativistic Correction Factor L_p for a Planck Spectrum

T_r (keV) / T_e (keV)	5.11	10.22	25.5	51.1	102.2
0.001	0.836	0.721	0.510	0.346	0.213
	0.835	0.721	0.513	0.344	0.202
5.11	—	0.735	0.512	0.345	0.212
	0.850	0.731	0.518	0.346	0.203
10.22	0.864	—	0.515	0.345	0.210
	0.864	0.741	0.522	0.348	0.204
25.5	0.910	0.767	—	0.345	0.210
	0.910	0.772	0.537	0.355	0.206
51.1	0.997	0.823	0.556	—	0.207
	0.990	0.827	0.561	0.366	0.210
102.2	1.149	0.924	0.584	0.369	—
	1.159	0.943	0.614	0.389	0.218

Note. Upper values are from Reference [23]. Lower values are calculated.

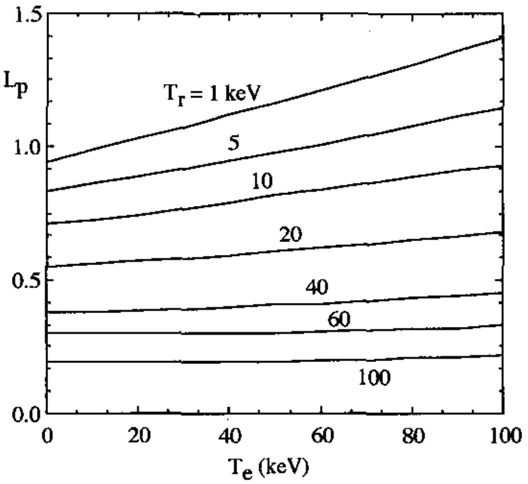

FIG. 7. Planck relativistic correction factor L_p vs T_e for various values of T_r.

$$L \equiv \int_0^\infty f \frac{\partial}{\partial \nu}(g\nu^4)\,d\nu \Big/ 4\int_0^\infty \nu^3 f\,d\nu. \tag{B.8}$$

Except for the stimulated emission term proportional to f^2, T_c may be regarded as the "color" temperature, or average frequency, of the spectrum. For certain spectra, it takes on special values. For a Planck spectrum, where $f = (e^{\nu/\theta} - 1)^{-1}$, or for a spectrum in equilibrium under Compton scattering ($G = 0$), where $f = (Ce^{\nu/\theta} - 1)^{-1}$ ($C > 1$), we find from Eq. (B.6) that $T_c = \theta$. In general we find that T_c lies between T_e and $T_r \equiv (E/a)^{1/4}$.

For a Planck spectrum in the nonrelativistic limit, Eq. (B.7) becomes

$$\left(\frac{dE}{dt}\right)_c = \frac{4\sigma_0}{mc}(T_e - T_r)aT_r^4, \tag{B.9}$$

a result first obtained by Hurwitz [9] and later by Weymann [10].

Calculation of L for a Planck spectrum from the Klein–Nishina cross section has been carried out by Warham [23]. His results provide a useful test of Cooper's function $g(\nu, T_e)$ given in Appendix A. With T_e and ν in kilo electron volts, Cooper's values for the three constants, obtained from a fit to the energy transfer rate as calculated by Stone and Nelson [24], are $a_1 = 0.009$, $a_2 = 4.2 \times 10^{-6}$, and $a_3 = 0.02$. Somewhat better values of a_1 and a_2 can be obtained as follows. For $T_e = 0$, $g(\nu, 0)$ is proportional to the so-called Klein–Nishina absorption cross section [25]. An expansion in powers of ν shows that, for low ν, $g(\nu, 0) = 1 - 4.2(\nu/mc^2) + \ldots$ so that $a_1 = 0.00822$ in our units. Also, $\nu g(\nu, 0)$ has a maximum when $\nu = mc^2$, which leads to $a_2 = (1/mc^2)^2 = 3.83 \times 10^{-6}$.

Using Eq. (B.8) and the revised values of the constants, we have calculated L_p (i.e., L for a Planck spectrum) using 99 frequency groups from 0.5 to 5000 keV for electron and radiation temperatures up to 102 keV. The results are shown in Table I and Fig. 7. The difference from Warham's results is less than 2% for T_e, $T_r < 50$ keV, and about 5% for T_e or $T_r = 100$ keV.

ACKNOWLEDGMENTS

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