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A Nonlinear Transport Problem of Monochromatic Photons in Resonance with a Gas

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Abstract. A transport problem arising from the dynamics of a gas in a radiation field, recently modelled in kinetic theory, is formulated and the trend to equilibrium of the gas-photon system is studied. A computational technique matching relevant mathematical aspects of differential quadrature and spectral methods is applied. The numerical results are then compared with those of other models known in literature.

INTRODUCTION

Aim of the present paper is to provide a numerical analysis of a nonlinear transport problem arising in the dynamics of a gas imbedded in a monochromatic radiation field. The gas particles are endowed with two levels of internal energy, the fundamental and the excited one. Besides the elastic collisions, the gas particles may experience inelastic interactions, passing from an energy level to the other. Absorption, stimulated and spontaneous emission processes are taken into account in the interaction between photons and gas particles.

In this paper, the set of moment equations, namely the macroscopic conservation equations, derived from the kinetic equations given in Ref. [1], is considered under the assumption that the characteristic relaxation time of elastic collisions is much smaller than the one relevant to inelastic and gas-radiation interaction.

An initial boundary value problem in a slab is formulated for the nonlinear system of the moment equations and radiative transfer equation, with the aim of studying the trend to equilibrium of the gas-photon system. In unbounded domains such a trend has been shown in Ref. [2].

A numerical technique, proposed in Ref. [3], based on the spectral approximation of the solution expanded in terms of Legendre polynomials, transforms the original set of partial differential equations into a set of ordinary differential equations to be numerically solved with pertinent initial conditions. Numerical results are then given and compared with those obtained for the same physical problem, treated in Refs. [4], [5], [6] by means of simplified versions of the moment equations.

GOVERNING EQUATIONS

Consider, in slab geometry, a gas with particles endowed with two internal energy levels in presence of a monochromatic radiation field. With reference to papers [2], [4], the closed set of moment equations of the gas system is derived in a dimensionless and rescaled form:

$$\frac{\partial n^f}{\partial t} = -u \frac{\partial n^f}{\partial x} - n^f \frac{\partial u}{\partial x} + [\vartheta_1 n^f + \vartheta_2 n^e][n^e - n^f \exp(\frac{-1}{T})] + \eta[4\pi n^e + (n^e - n^f)J] \quad (1)$$

$$\frac{\partial n^e}{\partial t} = -u \frac{\partial n^e}{\partial x} - n^e \frac{\partial u}{\partial x} - [\vartheta_1 n^f + \vartheta_2 n^e][n^e - n^f \exp(\frac{-1}{T})] + \eta[4\pi n^e + (n^e - n^f)J] \quad (2)$$

$$\frac{du}{dt} = -u \frac{\partial u}{\partial x} - \sigma \frac{\partial T}{\partial x} - \sigma T \frac{\partial}{\partial x} \log(n^f + n^e) \quad (3)$$

$$\begin{aligned} \frac{\partial T}{\partial t} = & -u \frac{\partial T}{\partial x} - \frac{2}{3} T \frac{\partial u}{\partial x} + \\ & + \frac{2}{3(n^f + n^e)} [n^e - n^f \exp(\frac{-1}{T})] [\vartheta_1 n^f + \vartheta_2 n^e]. \end{aligned} \quad (4)$$

Besides the moment equations, the model includes the radiative transfer equation:

$$\frac{\partial I}{\partial t} = -\mu \frac{\partial I}{\partial x} + n^e + I(n^e - n^f). \quad (5)$$

The dimensionless state variables (n^f, n^e, u, T, I) are, respectively, the number density of gas molecules with internal energy at the fundamental (f) and excited (e) level, the mean velocity of the gas, the absolute temperature and the radiation intensity of the monochromatic field of photons. The parameters $\eta, \vartheta_i, i = 1, 2$, and σ are given by

$$\eta = \frac{I_r}{n_r c h \nu}, \quad \vartheta_i = \frac{\gamma_i}{\beta c h \nu}, \quad \sigma = \frac{h \nu}{m c^2}, \quad (6)$$

where n_r, I_r are given reference values of the total number density of the gas particles and the radiation intensity, respectively. In particular, according to paper [4], let $I_r = \frac{\alpha}{\beta}$, α, β being the so-called Einstein coefficients which account for absorption and emission rates. Moreover, $h \nu$ is the photon energy, c the speed of light, and γ_1, γ_2 are the inelastic frequencies of the atom-atom collisions, which are positive constants under the assumption of Maxwellian molecules interaction law.

Note that n^f, n^e, u and T depend on $t \in R_+$, and $x \in R$, whereas I depends also on $\mu = \cos \theta$, $\theta \in [0, 2\pi]$ being the angle between the x -axis and the velocity of photons. In addition J is the integrated radiation intensity, defined as

$$J(t, x) = 2\pi \int_{-1}^1 I(t, x, \mu) d\mu. \quad (7)$$

Observe that the presence of J in Eqs. (1), (2) implies that the model equations actually constitute an integro-differential system and thus differ from the ones of papers [2], [4] and [5], where the Eddington approximation [7] has been used. As shown in paper [1], Eqs. (1-5) admit an equilibrium solution given by

$$\frac{n^e}{n^f} = \exp(\frac{-1}{T}), \quad I = \frac{1}{\exp(\frac{1}{T}) - 1}, \quad (8)$$

which corresponds to the thermodynamical equilibrium of the system.

INITIAL-BOUNDARY VALUE PROBLEM

An initial-boundary value problem, in line with the one studied in the above mentioned papers [4], [5] and there solved for a simplified version of model (1-5), can now be formulated in the slab $[-1, 1]$ for the gas-photon system governed by Eqs. (1-5), with assigned conditions as follows.

■ Initial conditions

$$t = 0, \forall x \in [-1, 1]: \quad n^f(x) = n_0^f \quad (9)$$

$$n^e(x) = n_0^e = n_0^f \exp(\frac{-1}{T_0}) \quad (10)$$

$$u(x) = 0 \quad (11)$$

$$T(x) = T_0 \quad (12)$$

$$I(x, \mu) = I_0 = \frac{4\pi}{\exp(\frac{1}{T_0}) - 1}, \quad \mu \in [-1, 1]. \quad (13)$$

These data correspond to the following physical situation. At $t = 0$, the gas, with number densities n_0^f and n_0^e , is in absolute equilibrium at a temperature T_0 ; the boundaries of the slab are perfectly reflecting walls for the gas-particles and perfectly reflecting mirrors for the radiation field, so that this one is in equilibrium with the gas at the intensity I_0 . In data (9-13) the expressions of n^e and I_0 are in agreement with the hypothesis of absolute equilibrium.

■ *Boundary conditions*

$$\forall t > 0: \quad u(x = -1) = u(x = 1) = 0 \quad (14)$$

$$\frac{\partial T}{\partial x}(x = -1) = 0 \quad (15)$$

$$T(x = 1) = T^* = \frac{1}{\log(1 + \frac{1}{I^*})} \quad (16)$$

$$I(x = -1, \mu > 0) = 0, \quad I(x = 1, \mu < 0) = I^*. \quad (17)$$

These data correspond to the following. For $t = 0^+$ the mirrors are removed and successively the gas, $\forall t > 0$, is subjected to a radiation intensity $I^*(\mu)$, $\forall \mu < 0$, on the wall at $x = 1$, and to zero radiation intensity, $\forall \mu > 0$, on the other wall at $x = -1$; conversely, $\forall t > 0$, the gas-particles can never cross the walls, as stated by (14).

More in detail, conditions (15),(16) express that the the wall at $x = -1$ is thermically insulated, since no radiation source is present at $x = -1$ as stated in (17), whereas the wall at $x = 1$ is accomodated at the temperature T^* in equilibrium with the radiation source of intensity I^* present at $x = 1$.

Such a physical problem has its origin in paper [8] and has been considered in book [6], as well.

APPROXIMATION METHOD

The method here proposed to construct an approximated solution to the initial-boundary value problem (1-5), (9-17) adapts the differential quadrature technique, recently reviewed in [9], to spectral methods, for what attains the truncated series expansion of the solution in the basis of Legendre orthogonal polynomials. In order to apply the method, it is convenient first to rewrite system (1-5) in vector form.

Let \mathbf{g} denote the state variable (n^f, n^e, u, T, I) ; the system of Eqs. (1-5), recalling definition (7) of the integrated radiation intensity J , can be rewritten as

$$\frac{\partial \mathbf{g}}{\partial t} = \mathbf{G}(t, x, J, \mathbf{g}, \frac{\partial \mathbf{g}}{\partial x}) \quad (18)$$

with initial data

$$\mathbf{g}(0) = \left(n_0^f, n_0^e \exp\left(\frac{-1}{T_0}\right), 0, T_0, \frac{1}{\exp\left(\frac{1}{T_0}\right) - 1} \right). \quad (19)$$

The approximated solution to Eq. (18) has the spectral representation

$$\mathbf{g}(x, t) \simeq \sum_{m=0}^M \mathbf{c}_m(t) L_m(x), \quad (20)$$

where $L_m(x)$, $m = 1 \dots M$, are the orthogonal Legendre polynomials of degree m , and the vectors $\mathbf{c}_m(t) = (c_m^f, c_m^e, c_m^u, c_m^T, c_m^k)$ are the expansion coefficients, given by

$$\mathbf{c}_m(t) = \frac{2m+1}{2} \int_{-1}^1 L_m(x) \mathbf{g}(x, t) dx, \quad m = 0, \dots, M. \quad (21)$$

The x - dimension of the slab, namely the interval $[-1, 1]$, is discretized with $(N - 1)$ sub-intervals by N equally spaced nodes x_i , $i = 1, \dots, N$. Note that the number N of the nodes does not depend on the maximum degree M of the Legendre polynomials. The space derivative of the state variable \mathbf{g} is approximated in the nodes by

$$\frac{\partial \mathbf{g}_i}{\partial x} = \frac{\partial \mathbf{g}}{\partial x}(x_i, t) \simeq \sum_{m=0}^M \frac{dL_m}{dx}(x_i) \mathbf{c}_m(t) = \sum_{m=0}^M a_{im} \mathbf{c}_m(t), \quad (22)$$

where a_{im} define a $[N \times (M + 1)]$ matrix \mathcal{A} given by

$$\mathcal{A} = \{a_{im}\} = \left\{ \frac{dL_m}{dx}(x_i) \right\}, \quad (23)$$

which can be computed once for all. Hence, Eq. (18), by taking into account Eqs. (21-23), is transformed into the set of ordinary differential equations

$$\frac{d\mathbf{g}_i}{dt} = \mathbf{G}_i(t, \mathbf{g}_1, \dots, \mathbf{g}_N, J_1, \dots, J_N, \mathbf{c}_0(t), \dots, \mathbf{c}_M(t), x_i, \mathcal{A}), \quad i = 1, \dots, N \quad (24)$$

where $\mathbf{g}_i = \mathbf{g}(x_i, t)$ and $J_i = J(x_i, t)$. The time depending coefficients $\mathbf{c}_0(t), \dots, \mathbf{c}_M(t)$ must be computed at each time step through their definition (21). The initial data for system (24) are supplied by condition (19) discretized in each node. On the other hand, the boundary conditions (14-17) will be naturally included in the initial value problem, according to a procedure which will be shown in the next section.

COMPUTATIONAL SCHEME

The procedure outlined above is now applied to problem (1-5), (9-17), leading to the formulation of five ordinary differential systems with pertinent initial data. As it will be shown, the number of equations of each system depend on the assigned boundary conditions.

◇ **Equations for the number densities n^f and n^e .**

$$\begin{aligned} \frac{dn_i^f}{dt} = & -u_i \sum_{m=0}^M c_m^f a_{im} - n_i^f \sum_{m=0}^M c_m^u a_{im} + \\ & + [\vartheta_1 n_i^f + \vartheta_2 n_i^e] [n_i^e - n_i^f \exp(\frac{-1}{T_i})] + \eta [4\pi n_i^e + (n_i^e - n_i^f) J_i] \end{aligned} \quad (25)$$

$$\begin{aligned} \frac{dn_i^e}{dt} = & -u_i \sum_{m=0}^M c_m^e a_{im} - n_i^e \sum_{m=0}^M c_m^u a_{im} + \\ & - [\vartheta_1 n_i^f + \vartheta_2 n_i^e] [n_i^e - n_i^f \exp(\frac{-1}{T_i})] - \eta [4\pi n_i^e + (n_i^e - n_i^f) J_i]. \end{aligned} \quad (26)$$

The initial data to be joined to Eqs. (25), (26), taking into account conditions (9-10), are

$$n_i^f(0) = n_0^f, \quad n_i^e(0) = n_0^e = n_0^f \exp(\frac{-1}{T_0}). \quad (27)$$

Since no boundary conditions are prescribed for Eqs. (1-2), the index i actually ranges from 1 to N .

◇ **Equation for the mean velocity u .**

$$\frac{du_i}{dt} = -u_i \sum_{m=0}^M c_m^u a_{im} - \sigma \left[\sum_{m=0}^M c_m^T a_{im} + \frac{T_i}{n_i^f + n_i^e} \sum_{m=0}^M (c_m^f + c_m^e) a_{im} \right]. \quad (28)$$

The initial data to be joined to this equation are $u_i(0) = 0$. Since the boundary conditions (14) are applied to the first node $x_1 = -1$ and to the last one $x_N = 1$, solutions u_1 and u_N are directly given by $u_1(t) = 0$, $u_N(t) = 0$, $\forall t > 0$. Thus the index i in Eqs.(28) ranges, this time, from 2 to $N - 1$.

◇ **Equation for the temperature T .**

$$\begin{aligned} \frac{dT_i}{dt} = & -u_i \sum_{m=0}^M c_m^T a_{im} - \frac{2}{3} T_i \sum_{m=0}^M c_m^u a_{im} + \\ & + \frac{2}{3(n_i^f + n_i^e)} [n_i^e - n_i^f \exp(\frac{-1}{T_i})] [\vartheta_1 n_i^f + \vartheta_2 n_i^e], \end{aligned} \quad (29)$$

with initial data $T_i(0) = T_0$. Since the boundary condition (16) is applied to the last node $x_N = 1$, it is immediate to write

$$T_N(t) = T^* = \frac{1}{\log(1 + \frac{1}{T^*})}, \quad \forall t > 0, \quad (30)$$

so that the index i varies from 1 to $N - 1$, only. Conversely, boundary condition (15), which is of Neumann type, has no direct influence on the number of solutions to be computed, because it needs to be treated in a different way.

By taking into account the derivative expansion (22), we can write

$$\frac{dT_1}{dx} = \sum_{m=0}^M c_m^T a_{1m} = \sum_{m=0}^{M-1} c_m^T a_{1m} + c_M^T a_{1M} = 0 \quad \Rightarrow \quad c_M^T = -\frac{1}{a_{1M}} \sum_{m=0}^{M-1} c_m^T a_{1m}. \quad (31)$$

Let us underline that, in this case, the boundary condition implies that the unknown coefficients to be computed are only c_0^T, \dots, c_{M-1}^T . In addition, note that formula (31) has been arranged in such a way, since in the Legendre basis one has $a_{1M} \neq 0$.

◊ **Equation for the radiation intensity.**

First of all let us discretize the variable θ , $\theta \in [0, 2\pi]$, in an even number K of equally spaced angles θ^k , $k = 1, \dots, K$. In order to avoid particles grazing the walls, namely particles moving in the direction of the y -axis, the discretization of θ must be performed in such a way that the variables $\mu^k = \cos \theta^k$ never vanish. Accordingly the radiation intensity field will be discretized by $I(x, t, \mu^k) = I^k(x, t)$, $k = 1, \dots, K$. Then the form of Eq. (5), in each node x_i , is

$$\frac{dI_i^k}{dt} = -\mu^k \sum_{m=0}^M c_m^k a_{im} + n_i^e + I_i^k (n_i^e - n_i^f). \quad (32)$$

The initial data (13) assume the form

$$I_i^k(t=0) = I_0 = \frac{1}{\exp(\frac{1}{T_0}) - 1}. \quad (33)$$

For what concerns the boundary conditions (17), let us first introduce two sets of indexes $S_+ \subset \mathbf{N}$ and $S_- \subset \mathbf{N}$ such that

$$\begin{aligned} k \in S_+ &\Rightarrow \mu_k > 0, & k &= 1, \dots, \frac{K}{2} \\ k \in S_- &\Rightarrow \mu_k < 0, & k &= \frac{K}{2} + 1, \dots, K. \end{aligned}$$

Thus it is immediate to write

$$\forall t > 0, \quad k \in S_+ : \quad I_1^k(t) = 0; \quad k \in S_- : \quad I_N^k(t) = I^*. \quad (34)$$

The index i in Eqs. (32) runs from 2 to N when $k \in S_+$ and from 1 to $N - 1$ when $k \in S_-$. Consequently the number of equations (32) is $K(N - 1)$.

The knowledge in each node of $I_i^k(t)$ allows to compute, by a numerical quadrature on the variable μ , the integrated radiation intensity in each node as

$$J(x_i, t) = J_i(t) = 2\pi \int_{-1}^1 I(x_i, t, \mu) d\mu, \quad (35)$$

which appears in Eqs. (25), (26).

NUMERICAL RESULTS

Numerical results have been obtained using a 4th-order Runge-Kutta routine to integrate Eqs. (25), (26), (28), (29), and (32). Computation of the integral terms (35), concerning the radiation intensity, have been performed via a Gauss-Legendre formula, based on the same discretization points, as those in Eq. (32).

The purposes of this section consist both in validating the proposed numerical method, through the qualitative evolution of the system described in Ref. [8], and in comparing the quantitative results of the present model with those obtained

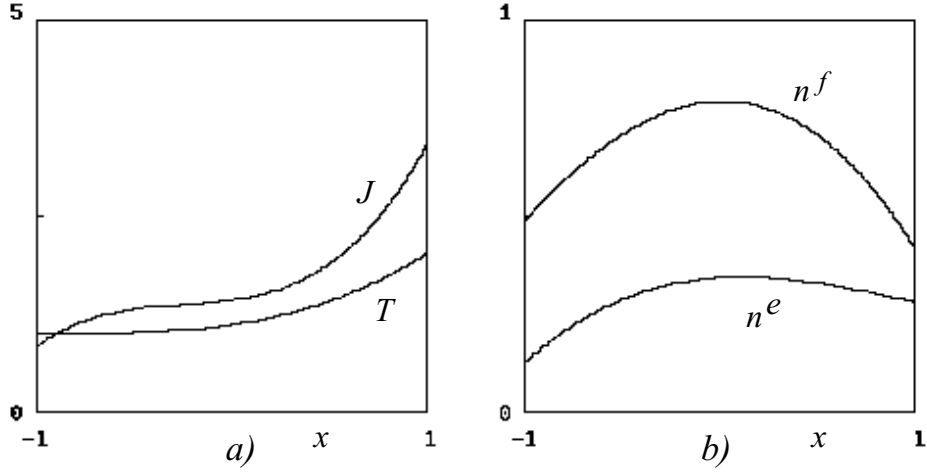


FIGURE 1. a) Profiles of T, J and b) profiles of n^f, n^e versus x , at $t = .5$, for $T_0 = 1$

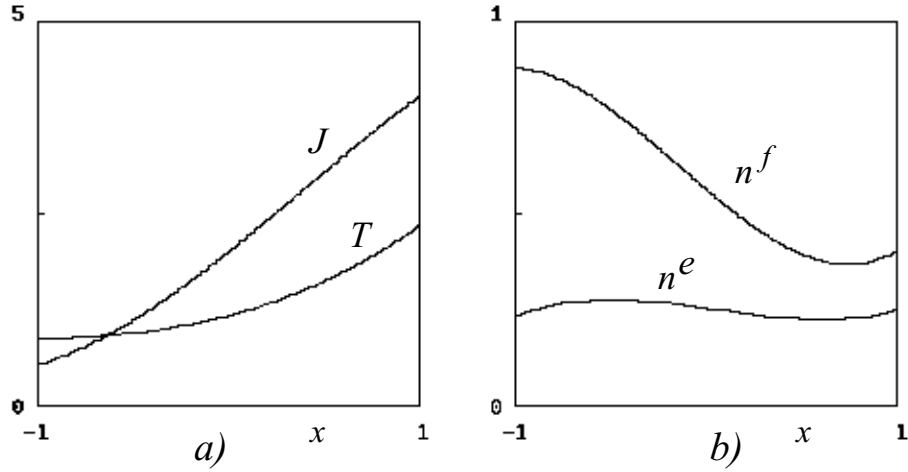


FIGURE 2. a) Profiles of T, J and b) profiles of n^f, n^e versus x , at $t = 1.45$, for $T_0 = 1$

in previous studies. As proven in Ref. [5], and shown in Ref. [8], the initial boundary value problem formulated in this paper presents an evolution towards a stationary equilibrium state for all the relevant macroscopic observables, i.e. n^f , n^e , T and J . In particular, when the stationary state is reached, temperature and integrated radiation intensity have an increasing monotone profile from the left boundary at $x = -1$ to the right one at $x = 1$.

Conversely, the maximum values of n^f and n^e , due to a small negative mean gas velocity, shift from the right to the left boundary and when total density has its maximum at $x = -1$, then the process becomes stationary and u vanishes again.

Such a behaviour is well represented by Fig. 1a and Fig. 2a for temperature T and intensity J and by Fig. 1b and Fig. 2b for numerical densities of the two populations n^f, n^e .

In particular, Figs. 1 are printed at time $t = 0.5$ (transient behaviour), while Figs. 2 show the stationary state at $t = 1.45$. The initial data used to obtain both Figs. 1 and Figs. 2 are: $n^f = 0.7, T_0 = 1$.

Relaxation to equilibrium is a bit faster when T_0 is higher (and, consequently, I_0 is smaller) and the profiles reach a slightly different shape.

This situation is shown by Fig. 3a, printed at $t = 1.2$ for $T_0 = 1.5$.

The initial datum on n^f does not affect the rapidity of relaxation.

All figures have been obtained for the same value $I^* = 2$ at the boundary $x = 1$.

As mentioned before, in paper [5] a simplified version of macroscopic equations has been used to solve the same

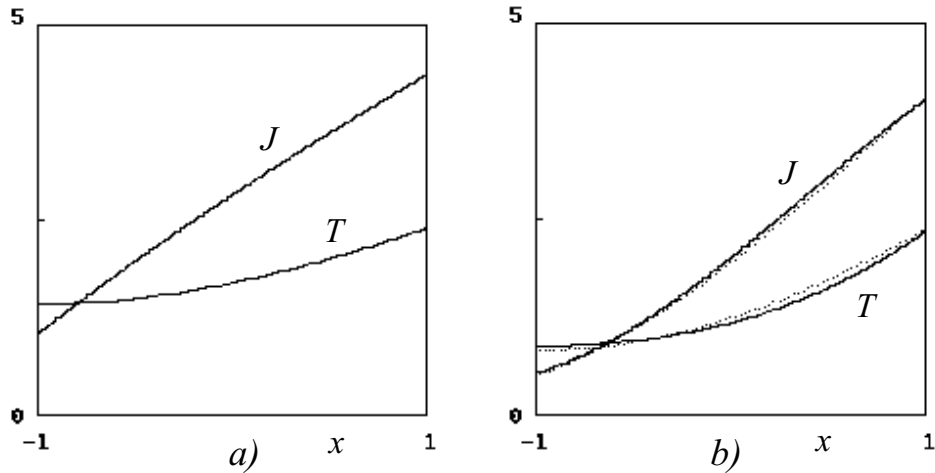


FIGURE 3. a) Profiles of T, J versus x , at $t = 1.2$, for $T_0 = 1.5$; b) this model (solid line) compared with that of [5] (dot line)

physical problem. Such a version did not consider the equation for the gas mean velocity (i.e. $u = 0 \forall t, x$) and that for n^e , since it was supposed that for each $x \in [-1, 1]$, $n^e = n_0 - n^f$, being $n_0 = n_0^f + n_0^e$. In paper [5] the results of that model were compared with those obtained in book [6], at least for the radiation intensity, since Chandrasekhar model did not consider an evolution equation for the temperature. In Fig. 3b, for the same data as in Figs. 2, we report the stationary profiles of T and J , for the present model (solid lines) and for that of [5] (dot lines).

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