JOURNAL OF COMPUTATIONAL PHYSICS 29, 283–288 (1978)

Note

Time-Dependent Ionization

A numerical method is described which allows the calculation of the time-dependent ionization structure of a plasma heated and ionized by a given input radiation field. The method is sufficiently general to be applicable also to other many-state-problems, in which the time-dependent occupation of one state depends only linearly on the occupation of all other states, as long as the total number of states remains finite and the total number of particles is a known quantity at all times.

INTRODUCTION

In many astrophysical problems the accurate calculation of the physical state of a radiatively heated and ionized gas is very important as a link between observed emission and absorption line strength and deduced parameters such as densities, temperatures, etc.

For local thermodynamical equilibrium LTE this link is provided by the Boltzmann and Saha equations together with a radiation transfer theory. However, under astrophysical circumstances, LTE conditions are often not satisfied. Frequently, the impinging radiation field is only weakly determined by the local properties of the gas and may be regarded as an "external" field. In this situation the photon to particle ratio becomes an essential quantity which determines the behavior of the gas.

As long as the timescale for changing the photon to particle ratio is long compared to the timescales for ionization and recombination, the abundance of any particular atom or ion of a given element is described by a system of linear, inhomogeneous, temperature-dependent equations. Generally the temperature is unknown and must be calculated simultaneously from an additional energy balance equation. These interconnected, simultaneous equations are solved in an iterative manner. Because of the nonlinearity of the problem the global existence of a unique solution cannot be demonstrated. However, for most practical cases, experience has shown that locally unique, numerically stable solutions exist.

In many interesting cases, the timescale for establishing the ionization and energy equilibrium exceeds the timescale with which the photon to particle ratio changes. In this case the set of simple balance equations is replaced by a corresponding set of differential equations. We describe in this paper a new method that allows us to solve these equations for the abundances and temperatures of the various constituents of the gas.

0021-9991/78/0292–0283$02.00/0

THE EQUATIONS

The density D_{zi} of the ith ionization stage of the element with nuclear charge z can be described by

$$\begin{aligned}\dot{D}_{zi}(t) = {} & I_{zi-1}(N_e(t), T_e(t)) \cdot D_{zi-1}(t) + R_{zi+1}(N_e(t), T_e(t)) \cdot D_{zi+1}(t) \\ & - (I_{zi}(N_e(t), T_e(t)) + R_{zi}(N_e(t), T_e(t))) \cdot D_{zi}(t), \qquad (1)\end{aligned}$$

with T_e: electron temperature, N_e: electron density, I_{zi}: ionization rate of ions with nuclear charge z from ionization stage i to ionization stage $i + 1$, R_{zi}: corresponding recombination rate. For our application, the relevant atomic processes are: ground-state collisional and photo-ionization, radiative recombination and dielectronic recombination. These processes and the assumptions under which Eqs. (1) or similar types of equations are valid are described in detail by Dalgarno and McCray [1].

Together with Eqs. (1) the condition

$$\sum_{i=1}^{z+1} D_{zi}(t) = N \cdot H_z\,, \qquad (1')$$

with N: total density of heavy particles, H_z: relative abundance of element z, must be satisfied for each element.

The electron density N_e is given by

$$N_e(t) = \sum_z \sum_{i=1}^{z+1} (i - 1) \cdot D_{zi}(t). \qquad (2)$$

The electron temperature T_e and the temperature of heavy particles T_i, here called ion temperature, can be described in their time evolution by

$$\begin{aligned}\dot{T}_e(t) = {} & \frac{2}{3K \cdot N_e(t)} \sum_z \sum_{i=1}^{z+1} (G_{zi} - L_{zi}(T_e(t), N_e(t))) \cdot D_{zi} \\ & + 0.08 \frac{N}{N_e(t)} T_e^{3/2} \cdot (T_i - T_e), \qquad (3)\end{aligned}$$

$$\dot{T}_i(t) = 0.08 \frac{N_e(t)}{N} \cdot T_e^{3/2} \cdot (T_e - T_i). \qquad (4)$$

In Eq. (3), G_{zi} denotes the energy gain rate of the electron gas which in our example will be due to photo-ionization. It competes with the loss processes L_{zi}, which in our case are radiative recombination, dielectronic recombination, collisional ionization, collisional excitation, and free-free-radiation. Because of the interconnection of temperature and ion densities by ionization and recombination and by energy gain and loss the whole system of (1), (1′), (2), and (3) is strongly nonlinear.

Whenever the timesclae for the adjustement of electron and ion temperature is larger than the timescale for changing the photon to particle ratio, Eq. (4) for the ion temperature has to be taken into account additionally. "Ion temperature" here is the temperature of both neutral atoms and ions, which for the conditions here will always be equal.

SOLUTION PROCEDURE

In solving the system of ordinary, nonlinear, first-order differential equations 1), (1′), (2), (3), and (4) numerically, the following problems are encountered:

Eqs. (1) and (1′) by themselves form a stiff system.

For a given z, the largest D_{zi} may be some hundred (!) orders of magnitude different from the smallest one. During one calculation (e.g. cooling from 10^7 K to 10^2 K) the initially largest D_{zi} can become the finally smallest one and vice versa. The coefficients I_{zi} and R_{zi} are different by many orders of magnitude for sufficiently different i. Choosing the integration step-width from the largest derivative, the computing time would become unacceptably long. On the other hand, too large steps could produce unphysical solutions as negative D_{zi} or, near the steady-state solution $\dot{D}_{zi} = 0$ for the ion densities, the equilibirum may be reached only after some unreal oscillations.

To overcome these difficulties, we choose a solution scheme with the following properties:

(a) For very small time-steps Δt it is a procedure of first order in Δt to solve the initial-value problem (1), (1′) and (2) with initial values $D_{zi}(0) = D^0_{zi}$.

(b) For very large Δt the steady-state solution $\dot{D}_{zi}(t) = 0$ is reached in *one* calculation step independent of the initial values.

(c) Equation (1′) is exactly fullfilled except for rounding errors. The *absolute* error in every single D_{zi} is only given by the machine rounding error. The relative error of an individual D_{zi} is then

$$\rho_{zi} = \alpha \cdot \rho_m \cdot \left| \frac{N \cdot H_z}{D_{zi}} - 1 \right|$$

with $\alpha \leqslant 10$, ρ_m: machine rounding error. It may become very large for very small D_{zi}, but then the ion densities themselves are too small to have any physical relevance.

The scheme actually used has the following simple structure: The linearized equations (1)

$$(D^{n+1}_{zi} - D^n_{zi})/\Delta t = I_{zi-1} \cdot D^n_{zi-1} - (I_{zi} + R_{zi}) \cdot D^n_{zi} + R_{zi+1} \cdot D^n_{zi+1} \quad (n\text{: iteration index})$$

(n: iteration index) can be written implicitly

$$(D^{n+1}_{zi} - D^n_{zi})/\Delta t = I_{zi-1} \cdot D^{n+1}_{zi-1} - (I_{zi} + R_{zi}) \cdot D^{n+1}_{zi} + R_{zi+1} \cdot D^{n+1}_{zi+1}$$

and solved for D_{zi}^n

$$D_{zi}^n = -\Delta t \cdot I_{zi-1} \cdot D_{zi-1}^{n+1} + (1 + \Delta t \cdot (I_{zi} + R_{zi})) \cdot D_{zi}^{n+1} - \Delta t \cdot R_{zi+1} \cdot D_{zi+1}^{n+1} \,. \tag{$\hat{1}$}$$

Together with

$$\sum_{i=1}^{z+1} D_{zi}^{n+1} = N \cdot H_z \tag{$\hat{1}'$}$$

the first z equations form for a given z a linear inhomogeneous system for the $z + 1$ quantities D_{zi}^{n+1}, having a very simple structure:

$$\begin{bmatrix} 1 + \Delta t \cdot I_{z1} & -\Delta t \cdot R_{z2} & 0 & \cdots & \cdots & 0 \\ -\Delta t \cdot I_{z1} & 1 + \Delta t \cdot (I_{z2} + R_{z2}) & -\Delta t \cdot R_{z3} & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & -\Delta t \cdot I_{zz-1} & 1 + \Delta t \cdot (I_{zz} + R_{zz}) & -\Delta t \cdot R_{zz+1} \\ 1 & \cdots & \cdots & 1 & 1 & 1 \end{bmatrix}$$

$$\cdot \begin{bmatrix} D_{z1}^{n+1} \\ D_{z2}^{n+1} \\ \vdots \\ D_{zz}^{n+1} \\ D_{n+1}^{n+1} \end{bmatrix} = \begin{bmatrix} D_{z1}^{n} \\ D_{z2}^{n} \\ \vdots \\ D_{zz}^{n} \\ NH_z \end{bmatrix} .$$

Because of the simplicity of the matrix structure the time to solve the equations is smaller than the time to calculate the individual matrix elements. It is very easy to see that (1) and (1′) yield the stationary solution for the D_{n+1}^{zi} independent of the D_{zi}^n, if Δt is sufficiently large, as physically required. In addition to Eqs. ($\hat{1}$) and ($\hat{1}'$) and the trivial equation (2), Eqs. (3) and possibly (4) have to be integrated. Due to the stiffness of the whole system a low-order scheme seems preferable. Equations (3) and (4) are therefore linearized and explicitly solved. It turns out that this simple approach yields sufficiently accurate results for all practical applications. The integration stepwidth is calculated from

$$\Delta t^{n+1} = s \cdot \left| \frac{T_e^{n-1}}{T_e^n} - 1 \right| ,$$

where s is a given limit. Choosing for s a typical value of 0.01, even after 400 integration steps the error in T_e is only a few percent. Especially for the D_{zi} it is more reasonable to look at the error in the time for reaching a particular ionization structure than to examine the values of D_{zi} after a given time. Here, too, we find an error of only a few percent for $s = 0.01$ and 400 steps.

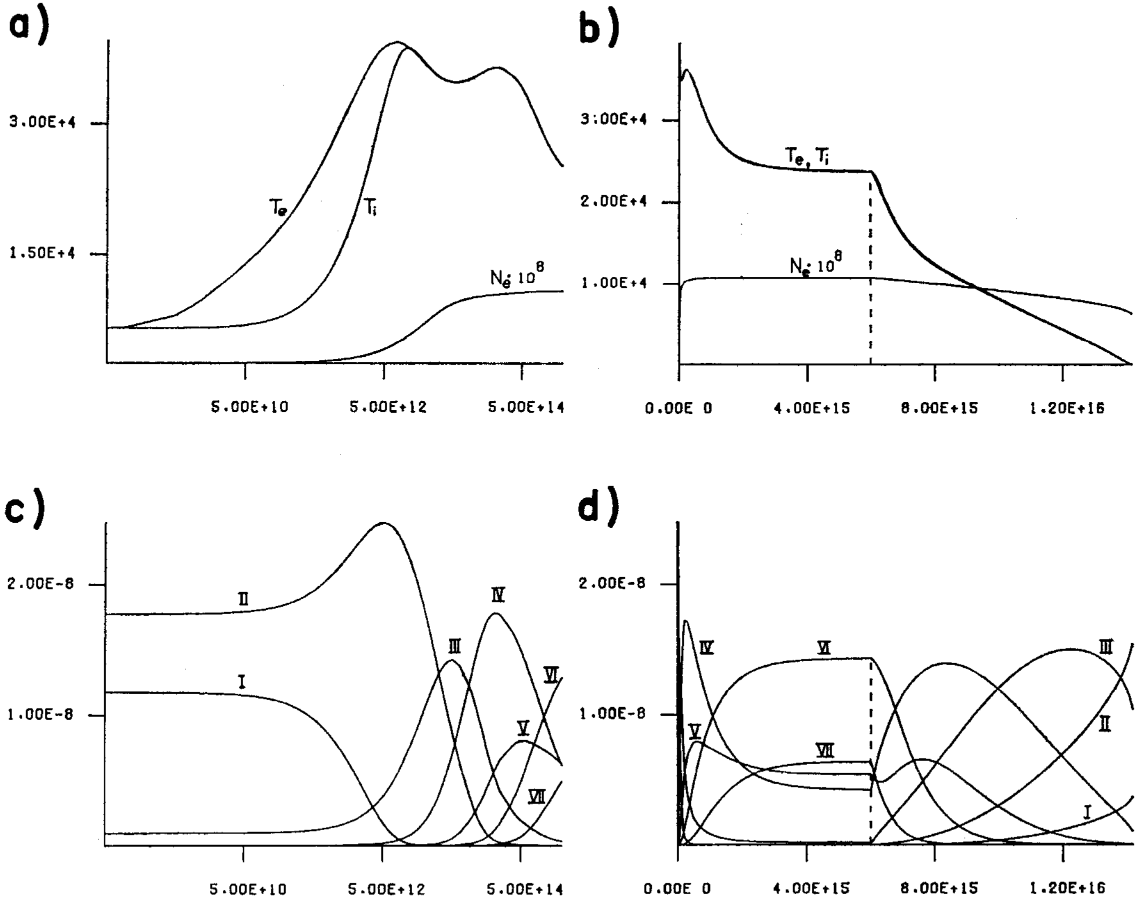

FIG. 1. (a, b) Electron temperature T_e, ion temperature T_i, electron density N_e as functions of time. (c, d) Densities of the carbon ionization stages CI, CII, CIII, CIV, CV as functions of time. (a) and (c) are a blow up of the initial phase shown in (b) and (d) on a logarithmic timescale.

EXAMPLE FOR APPLICATION

To illustrate the method described above, a short example is given: We consider a tenuous gas with $N = 10^{-4}$ cm^{-3} exposed to thermal bremsstrahlung photons. The bremsstrahlung temperature is kept constant at $T_R = 10^7$ K. This determines the spectral shape of the impinging radiation. The bremsstrahlung intensity is adjusted in such a way that an initial equilibrium temperature of $T_e = T_i = 6{,}550$ K is obtained. In this equilibrium (defined by $\dot{T}_e = \dot{T}_i = 0$, $\dot{D}_{zi} = 0$ for all z, i) the ratio of ionized to neutral hydrogen is 0.25. Starting from this arbitrarily chosen initial state we assume the bremsstrahlung *intensity* to be suddenly increased by a factor 10^4. The gas reacts by increasing the ion and electron temperature and the ionization state in a characteristic manner. After 6×10^{15} sec when a new equilibrium is reached, the photon intensity is reduced again by a factor 10^4 to its original value. However, as illustrated in Fig. 1, the gas does not return to the initial equilibrium. This results from the very different timescales of recombination and cooling in our example.

ACKNOWLEDGMENTS

The author is very much indebted to M. Grewing for many helpful discussions and critically reading the manuscript. This work has been supported by the Deutsche Forschungsgemeinschaft through a grant to the Sonderforschungsbereich Radioastronomie.

REFERENCE

1. A. DALGARNO AND R. A. MCCRAY, *Ann. Rev. Astron. Astrophys.* **10** (1972).

RECEIVED: September 20, 1977; REVISED: November 30, 1977

PAUL-ROLF PREUSSNER
Institut für Astrophysik
Universität Bonn
Federal Republic of Germany