FEBRUARY 1980

PPPL - 1648

TIME RATE COLLISION MATRIX

BY

M. I. STOENESCU

AND

T. M. SMITH

PLASMA PHYSICS

LABORATORY

TIME RATE COLLISION MATRIX

TABLE OF CONTENTS

	Abstract	ii
1.	Introduction	i
2.	Binary collisions	2
3.	Collisional transformation of particle sets <i>in the velocity space</i>	10
4.	Representation of particle kinetics based on velocity distribution functions	12
5.	Matrix formulation of the collisional time rate of change of the velocity distribution function	14
6.	Thermalization and randomization rates	19
7.	Relaxation time and energy exchange	20
8.	Sample computations	22
9.	Concluding remarks	24
	Acknowledgements	25
	List of Figures and Figures	26

TIME RATE COLLISION MATRIX

Abstract

The collision integral terms in Boltzmann equation are reformulated numerically leading to the substitution of the multiple integrals with a multiplicative matrix of the two colliding species velocity distribution functions which varies with the differential collision cross section. A matrix of lower rank may be constructed when one of the distribution functions is specified, in which case the matrix elements represent kinetic transition probabilities in the velocity space and the multiplication of the "time rate collision matrix" with the unknown velocity distribution function expresses the time rate of change of the distribution. The collision matrix may be used to describe the time evolution of systems in nonequilibrium conditions, to evaluate the rate of momentum and energy transfer between given species, or to generate validity criteria for linearized kinetic equations.

1. Introduction

The solution of the general kinetic equation expressing the particle conservation in the 'phase' space, known as Boltzmann equation, is a problem of a rather complex nature, due to the structure of the terms in the differential equation, to the limited knowledge of the boundary conditions, to the numerical instability of such an integration for standard techniques, and to the tediousness of evaluating the error of the results.

Integrations of Boltzmann equation for extreme cases where some type of interactions (long range or short range) are predominant, are presented in the literature, and prove, to require a high level of computational effort.

However, the importance for various applicative fields, of the Boltzmann equation solution for physical systems consisting of regions of different nature (collisionless and collisional), calls for a continuing effort in this direction.

The present paper addresses the problem of restructuring the integral terms of Boltzmann equation such as to reduce the computational volume of multistep integrations, to make them appropriate to a built-in mechanism of numerical stabilization and to cast them in a form which makes their physical interpretation more accessible.

2. Binary Collisions

Binary collisions are described by the momentum and energy conservation equations of the two colliding particles:

$$m\vec{v} + m_n\vec{v}_n = m\vec{v}' + m_n\vec{v}'_n \quad (1)$$

$$\mu g^2/2 = \mu g'^2/2 + \epsilon \quad (2)$$

where $\vec{v}, \vec{v}_n$ are the particle velocities before collision, $\vec{v}', \vec{v}'_n$ are the particle velocities after collision, μ is the reduced mass:

$$\mu = mm_n/(m + m_n) \quad (3)$$

g and g' are the magnitude of the relative velocities $\vec{g}$ and $\vec{g}'$ before and after collision:

$$\vec{g} = \vec{v} - \vec{v}_n \quad (4)$$

$$\vec{g}' = \vec{v}' - \vec{v}'_n \quad (5)$$

and ϵ is the kinetic energy lost in the collision process. If $\epsilon = 0$, the magnitude of the relative speed is invariant, $g = g'$, and the collision is called elastic.

Equations (1) and (2) constitute 4 scalar equations for the $4 \times 3 = 12$ components of the collision velocities $\vec{v}, \vec{v}_n, \vec{v}', \vec{v}'_n$. These equations determine completely the collision, namely 2 out of the 4 velocities, if additional information is provided for the relative position of the two particles at any time t at which they are not interacting, which is equivalent

lent with providing information on the direction of the relative velocity $\vec{g}$ determined by the b, β colliding variables indicated on Figure 1, where b is the shock parameter and β the corresponding azimuthal angle. The force of action law:

$$\chi = \chi(b, g) \quad (6)$$

or, in differential form

$$b \, db = b \left(\frac{\partial b}{\partial \beta} \right) g \frac{1}{\sin \chi} \sin \chi \, d\chi \equiv \sigma \sin \chi \, d\chi \quad (7)$$

where the differential cross section σ is defined as:

$$\sigma \equiv \frac{b}{\sin \chi} \left(\frac{\partial b}{\partial \chi} \right) g \quad (8)$$

establishes the $\chi(b)$ correlation for any relative speed g . The angles χ and β specify the direction of the scattered velocity $\vec{g}'$ with respect to $\vec{g}$:

$$\vec{u}(\chi, \beta) = \frac{\vec{g}'}{g} \equiv \sin \chi \frac{\vec{g}_1}{g} + \cos \chi \frac{\vec{g}}{g} \quad (9)$$

where the second equality results from the definition of the vector $\vec{g}_1(g, \chi, \beta)$ which is perpendicular to $\vec{g}$ in the plane $(\vec{g}, \vec{g}')$ and has the magnitude g as shown on Figure 2.

In conclusion the binary collision is described by equations (1), (2) and (9) which represent six equations determining the post collision velocities $\vec{v}_1'$ and $\vec{v}_2'$ for given $\vec{v}_1, \vec{v}_2$, and $\frac{\vec{g}'}{g}(\chi, \beta)$.

The expressions of the post collision velocities, after rearranging

equations (1), (5) and (9) are:

$$\vec{V}' = (M + M_n \frac{g'}{g} \cos \chi) \vec{V} + M_n (1 - \frac{g'}{g} \cos \chi) \vec{V}_n + M_n \frac{g'}{g} \sin \chi \vec{g} \quad (10)$$

$$\vec{V}'_n = M(1 - \frac{g'}{g} \cos \chi) \vec{V} + (M_n + M \frac{g'}{g} \cos \chi) \vec{V}_n - M \frac{g'}{g} \sin \chi \vec{g} \quad (11)$$

where $\vec{g}$ is expressed by equation (9) and where the following notations are used:

$$M \equiv m/(m + m_n) \quad (12)$$

$$M_n \equiv m_n/(m + m_n) \quad (13)$$

If the vectors $\vec{V}$, $\vec{V}_n$ are represented in polar coordinates $\vec{V}(v, \theta, \phi)$ and $\vec{V}_n(v_n, \theta_n, \phi_n)$ then the scattered velocities $\vec{V}'(v', \theta', \phi')$ and $\vec{V}'_n(v'_n, \theta'_n, \phi'_n)$ have the following components:

$$\begin{aligned} v'^2 = & (M^2 + M_n^2 \frac{g'^2}{g^2} + 2M M_n \frac{g'}{g} \cos \chi) v^2 + M_n^2 (1 - 2 \frac{g'}{g} \cos \chi + \frac{g'^2}{g^2}) v_n^2 \\ & + 2M_n [(M_n - M) \frac{g'}{g} \cos \chi - M_n \frac{g'^2}{g^2} + M] v v_n [\cos \theta \cos \theta_n + \\ & \sin \theta \sin \theta_n \cos (\phi - \phi_n)] \\ & + 2M_n \frac{g'}{g} \sin \chi v g [\sin \theta \cos \phi (\sin \phi_g \sin \beta - \cos \phi_g \\ & \times \cos \phi_g \cos \beta) \\ & - \sin \theta \sin \phi (\cos \phi_g \sin \beta + \cos \theta_g \sin \phi_g \cos \beta) \\ & + \cos \theta \sin \phi_g \cos \beta] \end{aligned} \quad (14)$$

$$\cos \theta' = \frac{1}{v'} \left[(M_1 + M_n \frac{g'}{g} \cos \chi) v \cos \theta + M_n (1 - \frac{g^2}{g} \cos \chi) v_n \cos \theta_n + \right. \\ \left. + M_n \frac{g'}{g} \sin \chi g \sin \theta_g \cos \beta \right] \quad (15)$$

$$\cos \phi' = \frac{1}{v' \sin \theta'} \left[M + M_n \frac{g'}{g} \cos \chi \right] v \sin \theta \cos \phi + M_n (1 - \frac{g'}{g} \cos \chi) \times \\ \times v_n \sin \theta_n \cos \phi_n + M_n \frac{g'}{g} \sin \chi (g \sin \theta \sin \phi_g - g \cos \theta \cos \phi_g \cos \phi_g) \quad (16)$$

where:

$$g_x = g \sin \theta_g \cos \phi_g = v \sin \theta \cos \phi - v_n \sin \theta_n \cos \phi_n \quad (17)$$

$$g_y = g \sin \theta_g \sin \phi_g = v \sin \theta \sin \phi - v_n \sin \theta_n + \sin \phi_n \quad (18)$$

$$g_z = g \cos \theta_g = v \cos \theta - v_n \cos \theta_n \quad (19)$$

$$g = [v^2 + v_n^2 - 2v v_n (\cos \theta \cos \theta_n + \sin \theta \sin \theta_n \cos (\phi - \phi_n))]^{1/2} \\ = (v^2 + v_n^2 - 2v v_n \cos \xi)^{1/2} \quad (20)$$

$$v_n'^2 = \frac{2}{m_n} \left(\frac{1}{2} m v^2 + \frac{1}{2} m_n v_n^2 - \frac{1}{2} m v^2 \right) \quad (21)$$

$$\cos \theta'_n = \frac{1}{m_n v'_n} (m v \cos \theta + m_n v_n \cos \theta_n - m v' \cos \theta') \quad (22)$$

And is the vector $\vec{v}$ is referred to a general frame and the vector $\vec{v}_n$ is referred to $\vec{v}$ through polar coordinates, $\vec{v} (v \theta \phi)$, $\vec{v}_n (v_n \xi \eta)$, then the scattered velocities have the following components which are equivalent with expressions (14) - (16):

$$\begin{aligned}
 v'^2 = & [1 + M_n^2 \left(\frac{g'^2}{g^2} - 1\right) + 2M M_n \left(\frac{g'}{g} \cos\chi - 1\right)] v^2 + \\
 & + M_n^2 \left[\left(\frac{g'^2}{g^2} - 1\right) - 2 \left(\frac{g'}{g} \cos\chi - 1\right)\right] v_n^2 + \\
 & + 2M_n [(M_n - M) \left(\frac{g'}{g} \cos\chi - 1\right) - M_n \left(\frac{g'^2}{g^2} - 1\right)] v v_n \cos\xi \\
 & + 2M \frac{g'}{g} \sin\chi v v_n \sin\xi \cos\beta \quad (23)
 \end{aligned}$$

$$\begin{aligned}
 \cos\theta' = & \frac{1}{v'} \{M v \cos\theta + M_n (v_n \sin\xi \cos\eta \sin\theta + v_n \cos\xi \cos\theta) \\
 & + M \frac{g'}{g} \cos\chi (v \cos\theta - v_n \sin\xi \cos\eta \sin\theta - v_n \cos\xi \cos\theta) \\
 & + M_n \frac{g'}{g} \sin\chi [v_n \sin\xi \cos\beta \cos\theta - g \sin\beta \sin\eta \sin\theta \\
 & + (v - v_n \cos\xi) \cos\beta \cos\eta \sin\theta]\} \quad (24)
 \end{aligned}$$

$$\begin{aligned}
 \cos\phi' = & \frac{1}{v' \sin\theta'} \{ (M + M_n \frac{g'}{g} \cos\chi) v \sin\theta \cos\phi \\
 & + M_n (1 - \frac{g'}{g} \cos\chi) v_n \sin\theta_n \cos\phi_n + M_n \frac{g'}{g} \sin\chi g \\
 & \times [\sin\beta \cos\eta \sin\phi + \cos\beta (\frac{v}{g} - \frac{v_n}{g} \cos\xi) (\sin\eta \sin\phi \\
 & - \cos\eta \cos\theta \cos\phi) + \cos\beta \frac{v^2}{g} \sin\xi \sin\theta \cos\phi \\
 & + \sin\beta \sin\eta \cos\theta \cos\phi]\} \quad (25)
 \end{aligned}$$

The limit of variation of colliding particle speed, in particular the limit of variation of v' when $\vec{v}_n(v_n, \xi)$ and $\vec{\Omega}(\chi, \beta)$ vary may be found according to the following considerations.

As observed on Figure 2 the minimum v' with respect to β occurs for $\beta = \pi$ and the maximum for $\beta = 0$ for which $\vec{v}$, $\vec{v}_n$, $\vec{v}'$, $\vec{v}'_n$ are coplanar. It is easy to see that the maximum v' with respect to β and χ takes place when the scattered $\vec{g}'$ is along and in the same direction as the center of mass velocity $\vec{V}$, where:

$$\vec{V} = M \vec{v} + M_n \vec{v}_n \quad (26)$$

and has the magnitude =

$$V = (M^2 v^2 + M_n^2 v_n^2 + 2M M_n v v_n \cos \xi)^{1/2} \quad (27)$$

in which case

$$(v'_n)_{\chi\beta} = V + M_n g' \quad (28)$$

where $g'(g\xi)$ results from (2) and $g(v, v_n, \xi)$ results from (20), and the minimum v' with respect to β and χ takes place when $\vec{g}'$ is along and in the opposite direction of $\vec{V}$ in which case

$$(v'_n)_{\chi\beta} = |V - M_n g'| \quad (29)$$

The extremum of v' with respect to β , χ and ξ depends on the behavior of the functions $V + M_n g'$ and $|V - M_n g'|$ when ξ varies. The following intersections with the $\cos \xi$ axis and location of maxima and minima determine this behavior as observed on Figure 3; it is

assumed that the collision is elastic which conserves the relative speed $g' = g$:

$V = 0$ for:

$$\cos \xi_1 = - \frac{M_v^2 + M_n^2 v_n^2}{2 M M_n v v_n} \equiv c_1 \quad (< 0) \quad (30)$$

$M_n g = 0$ for:

$$\cos \xi_2 = \frac{v}{2 v_n} + \frac{v_n}{2 v} \equiv c_2 \quad (> 0) \quad (31)$$

Extremum of $V = M_n g$ for:

$$\cos \xi_3 = \frac{1}{2} \left(1 - \frac{M_n}{M} \frac{v_n}{v} \right) \equiv c_3 \quad (> c_1; \text{ usually } < 0) \quad (32)$$

If $c_3 > -1$ this extremum is a maximum and the value of the function is:

$$(v_M')_{\chi B \xi} = \left(v^2 + \frac{M_n}{M} v_n^2 \right)^{1/2} \quad (\cos \xi_3 = c_3) \quad (33)$$

If $c_3 < -1$ the function reaches its maximum at $\cos \xi_3' = -1$ and the maximum is:

$$(v_M')_{\chi B \xi} = (M_n - M) v + 2 M_n v \quad (\cos \xi_3' = -1) \quad (34)$$

Extremum of $|V - M_n g|$ for:

$$\cos \xi_4 = \frac{1}{2} \left(1 - \frac{M}{M_n} \right) \frac{v}{v_n} \equiv c_4 \quad (> 0) \quad (35)$$

If $c_4 \leq 1$ this extremum is a minimum and the value of the function is:

$$\langle v' \rangle_m = 0 \quad (36)$$

If $c_4 > 1$ the function reaches its minimum at $\cos \xi_4' = +1$ and the

$$\langle v' \rangle_m = \langle M_n - M \rangle v - 2M_n v \quad (\cos \xi_4' = +1) \quad (37)$$

3. Collisional transformation of particle sets in the velocity space

As shown previously collisions transform point by point the velocity space $(\vec{v}, \vec{v}_n)$ into the velocity space $(\vec{v}', \vec{v}'_n)$; thus also an ensemble of points enclosed in a $d\vec{v}d\vec{v}_n$ into an ensemble of points enclosed in a determined $d\vec{v}'d\vec{v}'_n$. It may be shown that collisions conserve a pair of colliding particles velocity space volume element:

$$d\vec{v}d\vec{v}_n = d\vec{v}'d\vec{v}'_n \quad (18)$$

for each $(\chi\beta)$ value. The total velocity space volume enclosing all particles of a system is conserved through collisions.

One may set up the limit of variation of $\vec{v}_n$ for each $(\chi\beta)$ such as to have scattered particles scanning either given $d\vec{v}'$ and any $d\vec{v}'_n$ or given both $d\vec{v}'$ and $d\vec{v}'_n$. Due to the $(\chi\beta)$ variation the elements $d\vec{v}'d\vec{v}'_n$ are multiply scanned.

A general case of mapping of a set of variables into another set is represented on Figure 4. When one space is scanned by two independent variables xy along a rectangular grid, a second space is scanned by a pair of new variables $u \equiv u(x,y)$, $v \equiv v(x,y)$ along a curvilinear grid whose curves correspond to displacements for constant x , $(du)_x = \frac{\partial u}{\partial y} dy$, or constant y , $(du)_y = \frac{\partial u}{\partial x} dx$, as represented by the AHOK elements in the two (xy) , (uv) spaces. Similarly an inverse change of variables, from (uv) to (xy) leads to the correspondence of rectangular elements in the (uv) space and constant u , constant v elements in the (xy) space.

One may avoid the inverse transformation by numerically scanning the (xy) space along rectangular coordinates under a given constraint, for example by scanning along the dotted segments parallel to oy which are determined by the condition of having (u,v) projections inside a given rectangular dudv example TNSO. The result is equivalent with a reverse change of variables from dudv to $\frac{D(uv)}{D(xy)} dx dy$.

4. Representation of particles based on the velocity distribution function.

The definition of the velocity distribution function leads to the following kinetic functions:

Particle density:

$$n \equiv \int f d\vec{v} \quad (39)$$

Flux of particles of given velocity along a direction of unit vector $\vec{e}$:

$$d\vec{\Gamma}(\vec{v}) \equiv f d\vec{v} \vec{v} \cdot \vec{e} \quad (40)$$

Flux of particles through a moving target:

$$d\vec{\Gamma}_{relative} = f d\vec{v} g \int dS \vec{e}_g \quad (\vec{g} \parallel \vec{e}_g) \quad (41)$$

Flux of particles of any velocity along a direction $\vec{e}$:

$$\vec{\Gamma} \equiv \int f \vec{v} \cdot \vec{e} d\vec{v} \quad (42)$$

Number of collisions of monokinetic test particles with one field particle in one second:

$$N = \int f(\vec{v}) d\vec{v} a \int b db d\delta \quad (43)$$

Number of collisions of monokinetic test particles with monokinetic field particles of a unit volume, in a unit time:

$$f(\vec{v}) d\vec{v} f_n(\vec{v}_n) d\vec{v}_n g \int b db d\beta \equiv f(\vec{v}) d\vec{v} f_n(\vec{v}_n) d\vec{v}_n g \int d\vec{\Omega} \quad (44)$$

where

$$d\vec{\Omega} \equiv \sin\chi d\chi d\beta \quad (45)$$

Collision frequency or number of collisions of monokinetic test particles with all the field particles of a unit volume in a unit time:

$$\nu(\vec{v}) \equiv f(\vec{v}) d\vec{v} \int f_n(\vec{v}_n) g \sigma d\vec{v}_n d\vec{\Omega} \quad (46)$$

The number of collisions of monokinetic test particles with monokinetic field particles of a unit volume in a unit time is given in expression (44). The particles which occupy a volume $d\vec{v}d\vec{v}_n$ will occupy after one collision a volume $d\vec{v}'d\vec{v}_n'$ which according to (38) is equal to $d\vec{v}d\vec{v}_n$. Based on the collision reversibility property, particles existing at some moment in $d\vec{v}'d\vec{v}_n'$ will scatter back into $d\vec{v}d\vec{v}_n$ for reverse collision parameters, with a similar rate:

$$f(\vec{v}') d\vec{v}' f_n(\vec{v}_n') d\vec{v}_n' g' \sigma d\vec{\Omega}' \quad (47)$$

In conclusion, observing that $g' = g$ and $d\vec{\Omega}' = d\vec{\Omega}$, the net time rate of change of the $f(\vec{v}) d\vec{v}$ particles is:

$$\begin{aligned} \frac{\partial f}{\partial t} d\vec{v} &= f(\vec{v}') f_n(\vec{v}_n') d\vec{v}' d\vec{v}_n' g' \sigma d\vec{\Omega}' \\ &\quad - f(\vec{v}) f_n(\vec{v}_n) d\vec{v} d\vec{v}_n g \sigma d\vec{\Omega} \\ &= d\vec{v} [f(\vec{v}') f_n(\vec{v}_n') - f(\vec{v}) f_n(\vec{v}_n)] g \sigma d\vec{v}_n d\vec{\Omega} \end{aligned} \quad (48)$$

5. Numerical evaluation of the collision time rate
of change of the velocity distribution function
(collision integral in Boltzmann equation).

Equation (48) may be solved numerically. The variables $\vec{v}$, $\vec{v}_n$, $\vec{\Omega}$ are independent while the variables $\vec{v}'(\vec{v}, \vec{v}_n, \vec{\Omega})$, $\vec{v}'_n(\vec{v}, \vec{v}_n, \vec{\Omega})$ and their domain of variation are determined by the collisional laws expressed in equations (14) - (25).

The variables $\vec{v}$ and $\vec{v}'$ describe the same species and they represent thus variables associated with the same physical space which is scanned twice, once by $\vec{v}$ in $\frac{\partial f}{\partial t}(\vec{v})$ and a second time by $\vec{v}'$ in $f(\vec{v}')$. Two independent numerical grids $\vec{v}_{kjl} \equiv \vec{v}(v_k, \theta_j, \phi_l)$ and $\vec{v}^*_{kjl} \equiv \vec{v}^*(v_k^*, \theta_j^*, \phi_l^*)$ are assigned to the scanning of $\vec{v}$ respectively $\vec{v}'$ and a third grid $\vec{v}^0_{kjl} \equiv \vec{v}^0(v_k^0, \theta_j^0, \phi_l^0)$ is assigned to $\vec{v}'$ for each given $\vec{v}$ and it indicates thus, within numerical limitations, the boundary of the domain $\vec{v}'$ (given $\vec{v}$, variable $\vec{v}_n, \vec{\Omega}$). The grid $\vec{v}^*_{kjl}$ is used to collect all the $\vec{v}^0_{kjl}$ (given $\vec{v}_{kjl}, \dots$) this time for all $\vec{v}_{kjl}$.

For convenience the following discussion is limited to axially symmetric distribution functions, which does not restrict the generality of the numerical approach. Consequently the azimuthal variable index "l" is omitted, / time a function is independent of ϕ_l and $\vec{v}_{kjl}$ becomes $\vec{v}_{kj} (v_k, \theta_j, \phi_l = \text{any given value, for example } 0)$.

In the numerical equivalent of equation (48) which is described hereafter the function $f(\vec{v}_{kj})$ is specified at the $\vec{v}_{kj}$ nodes and propagated in time through $\frac{\partial f}{\partial t}(\vec{v}_{kj})$ at the same $\vec{v}_{kj}$ nodes. The function $f' \equiv f(\vec{v}')$ is defined at values $\vec{v}'(\vec{v}_{kj}, \dots)$ which do not coincide necessarily with any of the $\vec{v}_{kj}$ and is therefore extrapolated as function of known $f(\vec{v}_{kj})$. The results of various extrapolations are shown below.

The numerical expression of the integral (48) may be rearranged as follows:

$$\begin{aligned}
 \frac{\partial f(\vec{v})}{\partial t} &\equiv \left\{ f[\vec{v}^1(\vec{v}, \vec{v}_n, \vec{\Omega})] f_n[\vec{v}_n^1(\vec{v}, \vec{v}_n, \vec{\Omega})] - f(\vec{v}) f_n(\vec{v}_n) \right\} \\
 &\quad \times g(\vec{v}, \vec{v}_n) \sigma(\vec{v}, \vec{v}_n, \vec{\Omega}) d\vec{v}_n d\vec{\Omega} \\
 &\approx \lim_{\Delta \vec{v}_n \rightarrow 0} \lim_{\Delta \vec{\Omega} \rightarrow 0} \sum_{\vec{v}_n} \sum_{\vec{\Omega}} \left\{ f[\vec{v}^0(\vec{v}, \vec{v}_n, \vec{\Omega})] f_n[\vec{v}_n^0(\vec{v}, \vec{v}_n, \vec{\Omega})] - f(\vec{v}) f_n(\vec{v}_n) \right\} \\
 &\quad \times g(\vec{v}, \vec{v}_n) \sigma(\vec{v}, \vec{v}_n, \vec{\Omega}) v_n^2 \Delta v_n \Delta \cos \theta_n \Delta \phi_n \Delta \cos \chi_n \Delta \delta \\
 &= \lim \left\{ \sum_{\vec{v}^0} f(\vec{v}^0) \sum_{\vec{v}_n^0} f_n(\vec{v}_n^0) \sum_{\vec{v}_n \text{ res } \vec{v}^0} \sum_{\vec{v}_n} g v_n^2 \sum_{\vec{\Omega} \text{ res } \vec{v}^0} \sigma \right. \\
 &\quad \left. - f(\vec{v}) \sum_{\vec{v}_n} [g v_n^2 f_n(\vec{v}_n) \sum_{\vec{\Omega}} \sigma] \right\} \Pi_{\Delta} \\
 &= \lim \left\{ \sum_{\vec{v}^*} \delta_{\vec{v}^* \vec{v}^0} f(\vec{v}^*) \sum_{\vec{v}_n^*} \delta_{\vec{v}_n^* \vec{v}_n^0} f_n(\vec{v}_n^*) \right. \\
 &\quad \left. \times \sum_{\vec{v}_n \text{ res } \vec{v}^0} \sum_{\vec{v}_n} g v_n^2 \sum_{\vec{\Omega} \text{ res } \vec{v}^0} \sigma - f(\vec{v}) \sum_{\vec{v}_n} [g v_n^2 f_n(\vec{v}_n) \sum_{\vec{\Omega}} \sigma] \right\} \Pi_{\Delta} \\
 &= \lim \sum_{\vec{v}^*} f(\vec{v}^*) \left\{ \delta_{\vec{v}^* \vec{v}^0} \sum_{\vec{v}_n^*} \delta_{\vec{v}_n^* \vec{v}_n^0} f_n(\vec{v}_n^*) \right. \\
 &\quad \left. \times \sum_{\vec{v}_n \text{ res } \vec{v}^0} \sum_{\vec{v}_n} g v_n^2 \sum_{\vec{\Omega} \text{ res } \vec{v}^0} \sigma - \delta_{\vec{v}^* \vec{v}} \sum_{\vec{v}_n} [g v_n^2 f_n(\vec{v}_n) \sum_{\vec{\Omega}} \sigma] \right\} \Pi_{\Delta} \\
 &= \lim \sum_{\vec{v}^*} f(\vec{v}^*) \left[\sum_{\vec{v}_n^*} \tilde{T}^+(\vec{v}, \vec{v}^*, \vec{v}_n^*) f_n(\vec{v}_n^*) - \delta_{\vec{v}^* \vec{v}} R(\vec{v}) \right] \\
 &= \lim \sum_{\vec{v}^*} f(\vec{v}^*) \left[\tilde{K}^+(\vec{v}, \vec{v}^*) - \delta_{\vec{v}^* \vec{v}} R(\vec{v}) \right] \\
 &= \lim \sum_{\vec{v}^*} f(\vec{v}^*) \tilde{K}(\vec{v}, \vec{v}^*)
 \end{aligned}
 \tag{49}$$

where:

$$\pi_{\Delta} \equiv \Delta v_n \Delta(\cos \theta_n) \Delta \phi_n \Delta(\cos \chi) \Delta \beta \quad (50)$$

$$T^+(\vec{v}, \vec{v}^*, \vec{v}_n^{\rightarrow 0}) \equiv \delta_{\vec{v}^* \vec{v}}^{\rightarrow 0} \delta_{\vec{v}_n^* \vec{v}_n}^{\rightarrow 0} \sum_{\vec{v}_n \text{ res } \vec{v}_n^{\rightarrow 0}} g v_n^2 \sum_{\vec{\Omega} \text{ res } \vec{v}_n^{\rightarrow 0}} \sigma \Pi_{\Delta} \quad (51)$$

$$R(\vec{v}) \equiv \sum_{\vec{v}_n} g v_n^2 f_n(\vec{v}_n) \sum_{\vec{\Omega}} \sigma \Pi_{\Delta} \quad (52)$$

$$\tilde{K}^+(\vec{v}, \vec{v}^*) \equiv \delta_{\vec{v}^* \vec{v}}^{\rightarrow 0} \sum_{\vec{v}_n \text{ res } \vec{v}} g v_n^2 f_n(\vec{v}_n) \sum_{\vec{\Omega} \text{ res } \vec{v}^{\rightarrow 0}} \sigma \Pi_{\Delta} \quad (53)$$

$$\tilde{K}(\vec{v}, \vec{v}^*) \equiv K^+(\vec{v}, \vec{v}^*) - \delta_{\vec{v}^* \vec{v}}^{\rightarrow 0} R(\vec{v}) \quad (54)$$

The first equality indicates that $\vec{v}^{\rightarrow 0}, \vec{v}_n^{\rightarrow 0}$ are approximated by the nearest velocities $\vec{v}^{\rightarrow 0}, \vec{v}_n^{\rightarrow 0}$ belonging to the set $\vec{v}, \vec{v}_n$. The second equality results from the fact that upon scanning the discrete set of values of the variables $\vec{v}_n, \vec{\Omega}$ there is a variable frequency of occurrence of any pair $\vec{v}_n^{\rightarrow 0}, \vec{v}_n^{\rightarrow 0}$. For each subset $\vec{v}_n, \vec{\Omega}$ which leads to a specified $\vec{v}_n^{\rightarrow 0}, \vec{v}_n^{\rightarrow 0}$ and therefore to a given $f(\vec{v}_n^{\rightarrow 0}) f_n(\vec{v}_n^{\rightarrow 0})$ there corresponds in general a different value of the product $g \sigma v_n^2$ and one may thus factor out $f(\vec{v}_n^{\rightarrow 0}) f_n(\vec{v}_n^{\rightarrow 0})$ from the terms in the restricted sums

$$\sum_{\vec{v}_n \text{ res } \vec{v}_n^{\rightarrow 0}} \sum_{\vec{\Omega} \text{ res } \vec{v}_n^{\rightarrow 0}}$$

The third equation transforms conceptually the dependent variables $\vec{v}^{\rightarrow 0}, \vec{v}_n^{\rightarrow 0}$ into independent variables $\vec{v}^*, \vec{v}_n^*$ without performing any additional operation, but by assigning $\vec{v}^*, \vec{v}_n^*$ to an arbitrary space. The product of delta functions delineate the boundaries of those domains in the

$\vec{v}^*$, $\vec{v}_n^*$ space in which $\vec{v}^0$, $\vec{v}_n^0$ are defined. The fourth equality factors out $f(\vec{v}^*)$ from that term in $\sum_{\vec{v}^*}$ for which $\vec{v}^* = \vec{v}^1$ and from the negative term. The fifth and sixth equalities define the coupling functions T^+ and K^+ and the seventh defines the coefficients K evaluated for a known f_n .

An alternate method of approximating $f(\vec{v}^1)$ is based on a two-dimensional linear extrapolation as shown on Figure 5:

$$f(\vec{v}^1) = f^{int}(\vec{v}_{kj}^0, \vec{v}_{k+1,j}^0, \vec{v}_{k+1,j+1}^0, \vec{v}_{k,j+1}^0) \quad (55)$$

where $\vec{v}^1$ is situated in the bin kj characterized by the velocity $\vec{v}_{kj}^0$ of the upper left corner. The expression of the interpolated function for an m^{th} $\vec{v}^1$ scattered in the bin kj is:

$$\begin{aligned} f^{int} = & \eta_{kj}^{vm} \eta_{kj}^{\theta m} f_{k+1,j+1} + \eta_{kj}^{vm} (1 - \eta_{kj}^{\theta m}) f_{k+1,j} \\ & + (1 - \eta_{kj}^{vm}) \eta_{kj}^{\theta m} f_{k,j+1} + (1 - \eta_{kj}^{vm}) (1 - \eta_{kj}^{\theta m}) f_{kj} \end{aligned} \quad (56)$$

$$\eta_{kj}^{\theta m} \equiv \frac{\theta_{kj,m}^1 - \theta_{kj}^0}{\theta_{k,j+1}^0 - \theta_{kj}^0} \quad (57)$$

$$\eta_{kj}^{vm} \equiv \frac{v_{kj,m}^1 - v_{kj}^0}{v_{k+1,j}^0 - v_{kj}^0} \quad (58)$$

The function f^{int} substitutes $f(\vec{v}^0)$ in the third equality of expression (49) which, for a known f_n becomes:

$$\begin{aligned}
 \frac{\partial f}{\partial t}(\vec{v}) &= \lim_{\Delta \rightarrow 0} \sum_{k,j} f(\vec{v}_{kj}^0) \left[\sum_{(\vec{v}_n^0)} \text{res}_{\vec{v}_{kj}^0} (1-\eta_{kj}^v) (1-\eta_{kj}^\theta) f_n^v v_n^2 g_\sigma \right. \\
 &+ \sum_{(\vec{v}_n^0)} \text{res}_{\vec{v}_{k,j-1}^0} (1-\eta_{k,j-1}^v) \eta_{k,j-1}^\theta f_n^v v_n^2 g_\sigma \\
 &+ \sum_{(\vec{v}_n^0)} \text{res}_{\vec{v}_{k-1,j-1}^0} \eta_{k-1,j-1}^v \eta_{k-1,j-1}^\theta f_n^v v_n^2 g_\sigma \\
 &+ \left. \sum_{(\vec{v}_n^0)} \text{res}_{\vec{v}_{k-1,j}^0} \eta_{k-1,j}^v (1-\eta_{k-1,j}^\theta) f_n^v v_n^2 g_\sigma \right] \\
 &- f(\vec{v}) \sum_{\vec{v}_n} g v_n^2 f_n \sum_{\vec{\Omega}} \pi_\Delta \\
 &= \left\{ \sum_{k,j} f(\vec{v}_{kj}^0) \tilde{K}^+(\vec{v}\vec{v}^0) - f(\vec{v}) R(\vec{v}) \right\} \\
 &= \sum_{\vec{v}^*} f(\vec{v}^*) \left[\delta_{\vec{v}^* \vec{v}^0} K^+(\vec{v}\vec{v}^0) - \delta_{\vec{v}^* \vec{v}} R(\vec{v}) \right] \\
 &= \sum_{\vec{v}^*} f(\vec{v}^*) \tilde{K}(\vec{v}\vec{v}^*) \tag{59}
 \end{aligned}$$

where by convention $\vec{v}_{kj}$ represents a vector of coordinates v_k, θ_j and any $\sum_{k,j}$ represents a summation over v_k^0, θ_j^0 , and the restricted sums of the form "res $\vec{v}_{\alpha,\beta}^0$ " stand for scattering transitions from the velocity element $\vec{v}^0 = \vec{v}^0 + \Delta \vec{v}^0, \theta^0 = \theta^0 + \Delta \theta^0, \phi^0 = 0 - 2\pi$ to the element $\vec{v} = \vec{v} + \Delta \vec{v}, \theta = \theta + \Delta \theta, \phi = 0 - \Delta \phi$.

6. Thermalization and Randomization rates

The effect of elastic collisions on a velocity distribution function is to bring it closer to an equilibrium distribution function. The departure of the steady state from equilibrium and the rate at which the steady state is reached depend on the relative magnitude of the rate of thermalizing collisions compared to disturbing effects as for example inhomogeneities triggered by boundary exchange.

The collision matrix described in the previous paragraph represents a multiplicative operator of the distribution function which determines the equilibration rate of a given species while colliding with a second species.

One may separate the angular redistribution from the speed redistribution by defining a randomization rate which is the rate of change of the distribution function due to particles scattered within a $v - v + \Delta v$ shell:

$$R_{\text{rand}}(v\theta) \equiv \left[\frac{\partial f}{\partial t}(v\theta) \right]_{v \leq v^* \leq v + \Delta v} = \sum_{\theta^*, v \leq v^* \leq v + \Delta v} f(\vec{v}^*) [K^+(\vec{v}\vec{v}^*) - \delta_{v^*v} \sum_n \int_{\Omega} \text{res}_{v \leq v^* \leq v + \Delta v} v_n^2 f_n g \sigma] \quad (60)$$

and a thermalization rate which is the rate of change of the distribution function due to particles scattered within a $\theta - \theta + \Delta\theta$ slice:

$$R_{\text{therm}}(v\theta) = \left[\frac{\partial f}{\partial t}(v\theta) \right]_{\theta \leq \theta^* \leq \theta + \Delta\theta} = \sum_{v^*, \theta \leq \theta^* \leq \theta + \Delta\theta} f(\vec{v}^*) [\tilde{K}^+(\vec{v}\vec{v}^*) - \delta_{\theta^*\theta} \sum_n \int_{\Omega} \text{res}_{\theta \leq \theta^* \leq \theta + \Delta\theta} v_n^2 f_n g \sigma] \quad (61)$$

7. Relaxation time and energy exchange

A relaxation time is defined for quasi-equilibrium distribution functions through the following relation:

$$\frac{\partial T}{\partial t} = \frac{T - T_n}{\tau_{rel}} \quad (62)$$

where T is the temperature of the test species, T_n is the temperature of the field species and τ_{rel} the relaxation time.

One may define a relaxation time for a general distribution function through a similar relation in which T represents the average kinetic energy of particles.

The matrix formulation (49) of the collision integral enables the evaluation of relaxation times of quasimonokinetic subgroups of particles. The energy of a monoenergetic group of particles is:

$$W(v)\Delta v \equiv \sum_{\theta\phi} f(\vec{v}) \frac{mv^2}{2} \Delta \vec{v} \quad (63)$$

and the time rate of change of $W(v)$ results from expression (49):

$$\begin{aligned} \frac{\partial W}{\partial t} \Delta v &= \sum_{\theta\phi} \frac{\partial f}{\partial t} \frac{mv^2}{2} \Delta \vec{v} \\ &= \frac{mv^2}{2} \sum_{\theta\phi} \sum_{\vec{v}^*} \tilde{K}(\vec{v}\vec{v}^*) f(\vec{v}^*) \Delta \vec{v} \\ &\equiv \sum_{\vec{v}^*} \tilde{W}(\vec{v}\vec{v}^*) f(\vec{v}^*) \Delta v \end{aligned} \quad (64)$$

where

$$\tilde{W}(\vec{v}\vec{v}^*) \equiv \frac{mv^2}{2} \sum_{\theta\phi} \tilde{K}(\vec{v}\vec{v}^*) v^2 \Delta \cos \theta \Delta \phi = 2\pi \frac{mv^4}{2} \Delta \cos \theta \sum_{\theta} \tilde{K}(\vec{v}\vec{v}^*) \quad (65)$$

The "relaxation time $t_{v,rel}$ " of monoenergetic particles is defined as follows:

$$\begin{aligned} \frac{1}{\sum_{\theta\phi} f(\vec{v}) \Delta\vec{v}} \frac{\partial W}{\partial t} \Delta v &= \frac{1}{\sum_{\theta\phi} f(\vec{v}) \Delta\vec{v}} \sum_{\vec{v}^*} \tilde{W}(\vec{v}\vec{v}^*) f(\vec{v}^*) \Delta v \\ &\equiv \frac{\frac{mv^2}{2} - \frac{3}{2} kT_n}{t_{v,rel}} \end{aligned} \quad (56)$$

where $t_{v,rel}$ is a function of speed. Using equation (52) to define a relaxation time of a nonthermal species and substituting T with the average kinetic energy leads to the following expression:

$$\tau_{rel} \equiv \frac{\frac{1}{n} \sum_v W(v) \Delta v - kT_n}{\frac{1}{n} \sum_v \sum_{\vec{v}^*} \tilde{W}(\vec{v}\vec{v}^*) f(\vec{v}^*) \Delta v} \quad (57)$$

8. Sample computations

The sample computations represent examples of elements of the elements of the time rate matrix defined in expression (59), evaluated for an axially symmetric distribution function for which a matrix element $\hat{K}^+(v, \theta, v^* = v, \theta^*)$ and its associated elements $\hat{K}_a^+(v, \theta, v^* = v \pm \Delta v, \theta^*)$ represent the probability of electrons to be scattered by the neutral species from the torus $(v^* = v - \frac{1}{2}\Delta v) - (v^* = v + \frac{1}{2}\Delta v)$, $(\theta^* - \frac{1}{2}\Delta\theta^*) - (\theta^* + \frac{1}{2}\Delta\theta^*)$ into a cone around (v, θ) whose size remains unspecified in the $\hat{K}$ element evaluation. The associated elements are generated by the linear extrapolation method of f versus f^* and the $\hat{K}^+(v, \theta, v^* = v \pm n\Delta v, \theta^*) = 0$ for $n \neq 0, 1$ are zero due to the clustering of the $v'(v)$ around v for elastic scattering such that $|v' - v| \ll \Delta v^*$. By definition, the time rate of change of the velocity distribution function is expressed as follows:

$$\begin{aligned} \frac{\partial f}{\partial t}(v, \theta) = & \sum_{\theta^*} \hat{K}^+(v, \theta, v^* = v, \theta^*) f(v, \theta^*) \\ & + \sum_{\theta^*} \hat{K}_a^+(v, \theta, v^* = v - \Delta v, \theta^*) f(v - \Delta v, \theta^*) \\ & + \sum_{\theta^*} \hat{K}_a^+(v, \theta, v^* = v + \Delta v, \theta^*) f(v + \Delta v, \theta^*) \\ & - R(\vec{v}) f(v, \theta) \end{aligned}$$

The magnitude of the matrix elements is determined by the physical

functions: the differential cross section $\sigma(q, \chi)$ and the normalized density of scattered electrons $N(\vec{v}, v', \theta')$, and by the geometrical properties of the $(\vec{v}, \vec{v}', \vec{q})$ space. The domain of variables is illustrated on Figure 6. For each $\vec{v}_n$ the summation over χ, β is done over the surface Z cut into the sphere S_2 by the cones $C_{\theta^*}, C_{\Delta\theta^*}$, along the segments $b(\theta, \chi)$ of intersection of the azimuthal circles $\chi = \text{constant}$ and the surface Z . Such intersections exist for a limited range of $\chi_{\min} - \chi_{\max}$ of χ and thus the matrix elements contain information on a truncated $\sigma(\chi)$ function. If v_n is small and $\theta = 0$ or π the χ range is the smallest, namely, equal to $\Delta\theta^*$ as seen on Figure 7. The functions $b(\theta, \chi), \chi_{\min}(\theta), \chi_{\max}(\theta)$ may be determined geometrically. They represent a useful information in the curve decomposition of the experimental determination of the cross section.

Figures 8 and 9 represent examples of $\tilde{K}$ matrix elements for electrons colliding elastically with cesium and hydrogen, respectively. The differences in shape are largely due to differences in cross sections, as seen from Figure 10. For reasons of simplicity of writing, the matrix elements defined in expressions (49) or (59) are proportional with the velocity space volume element $\Delta\vec{v}^*$ and thus only $\tilde{K}/\Delta\vec{v}^*$ have physically meaningful values which should converge in the limit of small $\Delta\vec{v}^*$.

Figure 11 represents an example of energy transfer rate between electrons of $v = (v \pm v)$ and the hydrogen species evaluated as described in expression (64) for maxwellian distribution functions.

9. Concluding remarks

The formalism described above is based on the representation of the velocity distribution function as a step function $f(\vec{v}_\alpha)$ of a discrete vector variable $\vec{v}_\alpha$, characterizing an ensemble of particles assumed to be grouped in monokinetic subensembles. Depending upon the physical problem treated the domain and stepsize of the vector variable $\vec{v}_\alpha$ need to be adjusted in order to achieve the desired accuracy on one side of the density and energy density evaluation on the other side, of the time rate of change of the distribution function. The error limitation in the second case is attributed to the representation of the function $f(\vec{v}_\alpha)$ on a discrete grid of the variable $\vec{v}_\alpha$ which introduces the need for interpolating, $f(\vec{v} \neq \vec{v}_\alpha)$ as function of known $f(\vec{v}_\alpha)$'s.

The essence of the present work is to define and evaluate transition probabilities in the velocity space and to introduce the matrix functions $\tilde{K}(\vec{v} \vec{v}^*)$ which describe the rate of scattering of particles from a domain around $\vec{v}^*$ into a domain around $\vec{v}$ when they interact with an entire second species. For convenience the matrix $\tilde{K}(\vec{v} \vec{v}^* \theta^*)$ corresponding to a two dimensional function $f(v \theta)$ is exemplified and describes the rate of scattering of particles from a spherical ring $(v^* = v^* + \Delta v^*, \theta^* = \theta^* + \Delta \theta^*, \phi^* = 0 - 2\pi)$ into an element $(v = v + \Delta v, \theta = \theta + \Delta \theta, \phi = \phi + \Delta \phi)$. The matrix $\tilde{K}$ reduces the Boltzmann integro-differential equation for $f(\vec{v})$ to a regular differential equation and the propagation of $f(\vec{v})$ in a space-time space becomes a matter of regular numerical algebra. This equation sets the grounds for the kinetics of general non-equilibrium problems.

ACKNOWLEDGEMENTS

Are addressed to:

Lars E. Hernquist for writing the computer codes which generate collision matrices, to Ralph A. Nichols for the numerous runs leading to converged solutions and to both for their helpful discussions;

And to:

The U. S. Department of Energy for the funding under the Contract Number F-11-1-2798 which made this work possible;

And to:

Bobbie Cruser, for her speedy and competent typing assistance.

LIST OF FIGURES

1. Binary Collision Variables
2. Conditions for Extremum v'
3. Schematic Representation of v' Extrema
4. Numerical Change of Variables
5. Two Dimensional Extrapolation of f
6. Variables in the K Matrix Elements
7. Variables When $v_n \ll v$
8. Elastic Collision Matrix Elements for Electrons Colliding with Cesium
9. Elastic Collision Matrix Elements for Electrons Colliding with Hydrogen
10. Electron-Atom Elastic Differential Cross Sections
11. Electron-Atom Energy Transfer for Elastic Collisions

$$\sigma(g, \chi) = \frac{b}{\sin \chi} \frac{\partial b}{\partial \chi}$$

Figure 1a
Binary Collision Variables

Figure 2

Conditions for Extremum v'

Figure 3

Schematic Representation of v' Extremum

Figure 4
Numerical change of variables, schematic

Figure 5
Two-dimensional extrapolation of f

Figure 6

Variables in the K matrix elements

Figure 7

Variables in the K matrix elements when $v_n \ll v$

Figure 8
Elastic Collision Matrix Elements for Electrons Colliding with Cesium

Figure 9
Elastic Collision Matrix Elements for Electrons Colliding with Hydrogen

Figure 10

Electron-atom elastic differential cross section

Figure 11

Energy transfer rate between electrons of $v \sim vt$ and the hydrogen species