Particle Transport
in Inelastically Scattering Media

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Abstract. We consider the Boltzmann transport equation for point test particles in a background of polyatomic field particles in thermal equilibrium, under the action of an external constant force field, and in the Lorentz gas limit. The internal degrees of freedom of field particles are described by a discrete set of quantum energy levels. The asymptotic limit when elastic scattering becomes dominant is performed by means of a first order Chapman-Enskog expansion, after discussing the main properties of the collision operator. For the proper hydrodynamic quantity (a partial energy-dependent density) the limiting equation is a suitable drift-diffusion approximation, with additional inelastic scattering terms linking together different energies.

INTRODUCTION

As well known in classical kinetic theory [1], a quite interesting situation arises in a two-component gas mixture when one of the components has very small density, so that collisions of particles of this species (test particles) with each other can be neglected in comparison with collisions with particles of the other species (field particles), and the latter collisions, in turn, can be neglected in comparison with collisions of field particles with each other. If this occurs, then the evolution of field particles is not influenced by test particles, while the behavior of the latter is driven by the state of a fixed background of field particles. When a field particle distribution function is given (in particular, a Maxwellian, if the background species is in equilibrium), the test particle distribution function is governed by a single linear integro-differential Boltzmann equation. Examples are offered by neutron transport in a medium, electron transport in ionized gases, and by radiative transfer through planetary or stellar atmosphere [2]. A very famous and important particular case in this field is the so called Lorentz gas, both as a significant limiting situation, and as an useful simplified model in order to clarify analytically the main features of transport theory. It corresponds to vanishingly small ratio between test particle and field particle masses.

In recent years, an extended kinetic theory has been introduced in the literature in order to account for nonconservative encounters between particles, besides elastic scattering. Considered nonconservative effects, important for applications, include inelastic scattering, interaction with the self-consistent radiation field, bimolecular chemical reaction [3-6]. In particular, particles are endowed with an internal quantum structure, and polyatomic molecules may be described in a semiclassical way in terms of a mixture of monoatomic gases. Aim of this paper is to move similar first steps in the linear frame of transport theory, by allowing, to the polyatomic target particles, an arbitrary number $L$ of internal energy levels $E_i$, ordered in an increasing sequence with $E_1 = 0$. In addition, in order to make our model equation suitable for a wider class of transport problems, test particles are subjected to the action of a constant and uniform force field per unit mass $F$. The considered problem shares several features with electron transport in semiconductors, where inelastic processes also play an important role [7-10], even though significant differences arise, from both physical and mathematical point of view [11]. Field particles are assumed to constitute a background in thermal equilibrium, with no drift and with temperature $T$. Densities at different levels $N_i$ are related by the Boltzmann factors

$$N_i = N_1 \exp(-E_i/KT) = q_i N_1$$

$$i = 1, \ldots, L$$

(1)
where \( K \) is the Boltzmann constant. We will stick here to the Lorentz gas approximation, and let the field particle mass \( M \) tend to infinity, so that the background Maxwellian distribution collapses actually to a Dirac delta function. Scattering with a test particle may trigger a transition from a quantum state \( i \) to a different state \( j \), in which case part of the overall kinetic energy of the colliding partners is transformed into internal energy, or vice-versa (inelastic scattering). When no transition occurs \( (j = i) \), we have the standard elastic scattering. The general interaction between test and field particles is \( A + B_i \rightleftharpoons A + B_j \), \( i, j = 1, \cdots, L \), where we may always take \( j \geq i \). The direct transition in which field particle \( B_i \) gets transformed into \( B_j \) is described in terms of a differential collision frequency \( \nu_{ij} \), supposed here isotropic for simplicity, with the collision frequency \( \nu_{ji} \) for the inverse interaction related to \( \nu_{ij} \) by the microreversibility condition [12]. The energy differences \( E_j - E_i \) are taken to be incommensurable [13].

The evolution of the distribution function \( f(x, v, t) \) of gas atoms \( A \) (the kinetic variable \( v \) stands for the molecular velocity) follows from a quite complicated (though linear) integro-differential equation. As usual, one of the crucial points is the derivation of hydrodynamic equations as asymptotic limit when a suitable dimensionless mean free path (Knudsen number) tends to zero, since they provide self-consistent balance equations at a macroscopic scale useful for practical applications. A rigorous Chapman-Enskog approach [14] has already been employed in the absence of force and in the simplest case \( L = 2 \) [11,15]. In the present work we analyze the extended transport equation with external force and derive formally the hydrodynamic approximation by a standard [1] first order Chapman-Enskog expansion when elastic scattering is the dominant process in the evolution. This goal is achieved in the third section, after examining the main properties of the kinetic equation in the next one. Under our assumptions all steps can be performed analytically, and the compatibility condition which necessarily arises in the procedure takes a very simple explicit form. The limiting equation contains collision contributions, due to the inelastic collision term (the non-dominant one), and drift-diffusion terms due to the streaming operator, including standard diffusion in the physical space, isotropic diffusion in the velocity space, plus cross interaction terms involving mixed space-velocity derivatives.

**THE TRANSPORT EQUATION AND ITS MAIN PROPERTIES**

The evolution problem for the test particle distribution function \( f(x, v, t) \) in the physical conditions described above may be cast as [16]

\[
\frac{\partial f}{\partial t} = -\mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} - \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{v}} + J[f]
\]

with

\[
J_{ij}[f] = - \left[ N_i \Gamma(v - \delta_{ij}) \nu_{ij}^0(v) + N_j \frac{\nu_{ij}^+}{v} \nu_{ij}^0(v) \right] f(v \Omega)
+ \frac{N_i}{4\pi} \frac{\nu_{ij}^+}{v} \nu_{ij}^0(v) \int f(v_{ij}^+ \Omega') d\Omega'
+ \frac{N_j}{4\pi} \Gamma(v - \delta_{ij}) \nu_{ij}^0(v) \int f(v_{ij}^- \Omega') d\Omega',
\]

and is characterized by the usual streaming and collision operators, the latter being constituted by all elementary collision integrals \( J_{ij} \), which represent elastic \( (j = i) \) and inelastic \( (j > i) \) scattering. The variable \( v \) has been split as \( v \Omega \), with \( v = |v| \) and \( |\Omega| = 1 \), and the direction \( \Omega \) will be described in terms of colatitudinal and longitudinal variables \( \theta \) and \( \varphi \), so that the velocity space is referred to a polar coordinate system \( (v, \theta, \varphi) \) and to the associated orthonormal basis \( (\Omega, e_\theta, e_\varphi) \). Integrations extend on the unit sphere \( S^2 \), \( \nu_{ij}^0(v) = 4\pi \nu_{ij}^0(v) \) stands for the total (angle integrated) microscopic collision frequency, the unit step function \( \Gamma \) accounts for the threshold in the endothermic interaction, and dependence on \( x \) and \( t \) is implicitly understood in collision terms. The other symbols used in (3) are defined as:

\[
\delta^2_{ij} = \frac{2(E_j - E_i)}{m} \geq 0, \quad \nu_{ij}^+ = (v^0 + \delta^2_{ij})^{1/2}.
\]

Notice that (3) includes both down and up scattering, but only one collision frequency, since the other has been eliminated, on account of microreversibility, by
\( w_{ij}(v) = v_{ij} U(v - \delta_{ij}) \nu_{ij}(v_{ij}) \) \( w_{ij}(v) = v_{ij}^+ \nu_{ij}(v_{ij}^+) \). (5)

The standard elastic collision frequency is \( \nu_i = 2\nu_{ii} \).

Peculiar feature of the Lorentz gas is that, in the \( ij \) - collision, the test particle may change its kinetic energy only by a fixed amount, \( \pm \frac{1}{2} m \delta_{ij}^2 \). We can say that two quadratic speeds \( v^2 \) and \( w^2 \) are in mutual relation when it is possible for a test particle to attain one of the speeds by collision starting from the other. It is immediately verified that this is an equivalence relation. When trying to construct the equivalence class of an arbitrary quadratic speed \( v^2 \), one easily realizes that, due to our assumptions of incommensurable energy jumps, by a basic theorem from number theory [17], the equivalence class of any \( v^2 \) is dense in \([0, +\infty)\). Notice that a completely different scenario would be in order in the purely elastic case \( L = 1 \), in which the equivalence class of \( v^2 \) would be made up by \( v^2 \) alone, as well as for the simplest inelastic case \( L = 2 \), in which \( v^2 \) is related only the other quadratic speeds which differ from it by an integer times \( \delta_{ij}^2 \). Of course, the external force always induces a coupling between different speeds in the considered problem.

The mathematical properties of the collision term have been considered in [13]. It suffices to recall here that collision invariants \( \psi(v, \Omega) \) must be angle independent, and must take the same value at all speeds which are in the same equivalence class. Since \( \psi \) is continuous, it must be a constant, and thus the space of collision invariants is one-dimensional, spanned by \( \psi = 1 \), implying that the test particle number is the only quantity conserved by collisions. A detailed balance principle [1] can also be proved, which allows to characterize completely collision equilibria as a one parameter family of Maxwellian distributions, at the same temperature and drift velocity as the host medium. In addition, by extending standard convexity arguments, several Lyapunov functionals can be constructed in order to establish an H-theorem for stability under collisions of such equilibria.

Equation (2) can be adimensionalized in terms of a typical speed \((2KT/m)^{1/2}\), and typical values \( n^* \) and \( \nu^*_{IN} \) for densities and collision frequencies. It is assumed here that elastic scattering plays the dominant role in the evolution, while all other phenomena share the same level of importance, with in particular \( \nu_{IN}^* \ll \nu^*_E \), and the Strouhal number taken to be \( O(1) \) [1]. In this frame, it is convenient to introduce \( l^* = (n^* \nu^*_IN)^{-1} (2KT/m)^{1/2} \) as a typical length, and \( F^* = (n^* \nu^*_IN)/(2KT/m)^{1/2} \) as a typical force per unit mass. All scaled (dimensionless) quantities will be denoted by a superimposed tilde, whereas the scaled energy variable \( \xi = mv^2/(2KT) \) will be used instead of speed. Correspondingly, it proves convenient resorting to the quantity

\[ \tilde{f}(\xi, \Omega) = \frac{KT}{m} f(v, \Omega) \left( \frac{2KT}{m}\xi \right)^{1/2} \] (6)

(the scalar flux of neutron transport) as new dependent variable. The Knudsen number is spontaneously defined as

\[ Kn = \frac{\nu^*_IN}{\nu^*_E} \] (7)

and it is called \( \epsilon \) since it will play the role of small parameter in the asymptotic analysis developed later. Upon dropping all tildas, the adimensionalized kinetic equation takes the singular perturbation form

\[ \frac{\partial f}{\partial t} + \xi^{1/2} \Omega \cdot \frac{\partial f}{\partial \mathbf{x}} + 2\xi^{1/2} \mathbf{F} \cdot \Omega \frac{\partial f}{\partial \xi} + \xi^{-1/2} \mathbf{F} \cdot \mathbf{e}_\theta \frac{\partial f}{\partial \theta} \\
+ \frac{\xi^{-1/2}}{\sin \theta} \mathbf{F} \cdot \mathbf{e}_\varphi \frac{\partial f}{\partial \varphi} = N_1 J_{IN}[f] = \frac{N_1}{\epsilon} J_{EL}[f], \] (8)

with

\[ J_{IN}[f] = \sum_{i=1}^{L-1} \sum_{j=i+1}^{L} J_{ij}[f] \]

\[ J_{EL}[f] = \sum_{i=1}^{L} q_i \nu^0_i(\xi) \left[ -f(\xi, \Omega) + \frac{1}{4\pi} \int f(\xi, \Omega') d_2 \Omega' \right] , \] (9)

where \( N_1 \) includes all explicit space dependence of collision integrals, and
\[ J_{ij}[\phi] = - \left[ q_i U(\xi - p_{ij}) \nu^o_{ij}(\xi) + q_j \left( \frac{\xi + p_{ij}}{\xi} \right)^{1/2} \nu^o_{ij}(\xi + p_{ij}) \right] f(\xi, \Omega) \]
\[ + q_i \nu^o_{ij}(\xi + p_{ij}) \frac{1}{4\pi} \int f(\xi + p_{ij}, \Omega') d_2\Omega' \]
\[ + q_j U(\xi - p_{ij}) \left( \frac{\xi}{\xi - p_{ij}} \right)^{1/2} \nu^o_{ij}(\xi) \frac{1}{4\pi} \int f(\xi - p_{ij}, \Omega') d_2\Omega', \]
with dimensionless (and obviously still incommensurable) jumps
\[ p_{ij} = \frac{m_0^2}{2KT} = \log \frac{q_i}{q_j}. \]

For the asymptotic analysis with respect to \( \epsilon \), the mathematical properties of the dominant operator \( J_{\text{EL}} \) are of course crucial [14]. The analysis follows the standard lines of kinetic theory (see for instance [1] and [13]) with only slight specific changes, so that technical details are omitted here. Having the elastic collision rate expression
\[ C_{\text{EL}}[\phi] = \int_0^{+\infty} d\xi \int \phi(\xi, \Omega) J_{\text{EL}}[f] d_2\Omega \]
\[ = -\frac{1}{2} \sum_{i=1}^{L} q_i \int_0^{+\infty} \nu_i(\xi) d\xi \int \int [\phi(\xi, \Omega') - \phi(\xi, \Omega)][f(\xi, \Omega') - f(\xi, \Omega)] d_2\Omega d_2\Omega' \]
in mind, elastic collision invariants are defined as continuous functions \( \psi_{\text{EL}} \) of \( \xi \) and \( \Omega \) satisfying \( \psi_{\text{EL}}(\xi, \Omega') = \psi_{\text{EL}}(\xi, \Omega) \forall \xi, \Omega, \Omega' \). They must then be isotropic, but else arbitrary functions of \( \xi \in [0, +\infty) \). The same rate expression also provides, for instance via the option \( \phi = f \), a Boltzmann inequality, implying a detailed balance principle, by which elastic collision equilibria, defined as the solutions \( f \) of
\[ J_{\text{EL}}[f] = 0 \quad \forall (\xi, \Omega) \in [0, +\infty) \times S^2, \]
are shown to coincide with elastic collision invariants. The null space of \( J_{\text{EL}} \) is thus infinite dimensional and made up by all continuous functions of \( \xi \) which are independent of \( \Omega \). This reflects clearly the physical fact that elastic collision amounts to isotropization in direction, leaving energy unchanged. Seen from a different point of view, with the partition in equivalence classes induced by elastic scattering, we may say that, for any fixed \( \xi \in [0, +\infty) \), the null space of \( J_{\text{EL}} \), as a linear integral operator acting on the variable \( \Omega \) alone, is one-dimensional. At the same time, since the trend of elastic collision invariants with respect to \( \xi \) is arbitrary, and smoothness requirements are satisfied, it is easy to show that, for any admissible distribution function \( f \), there results
\[ \int J_{\text{EL}}[f] d_2\Omega = 0 \quad \forall \xi \in [0, +\infty), \]
so that the proper hydrodynamic quantity (the one conserved under elastic collision) is \( \rho(\xi) \), the partial density of particles at energy \( \xi \), defined by
\[ \rho(\xi) = \int f(\xi, \Omega) d_2\Omega, \]
corresponding, a part from a factor \( \frac{1}{4\pi} \), to the projection, at fixed \( \xi \), of the distribution function on the null space of \( J_{\text{EL}} \). Notice that the actual test particle number density can be recovered as
\[ n = \int_0^{+\infty} \rho(\xi) d\xi. \]
From the above results there follows also existence of a one family of macroscopic equations, one for each fixed \( \xi \in [0, +\infty) \), corresponding to the conservation properties of elastic scattering. Integration of (8) over \( S^2 \) yields in fact
\[ \frac{\partial \rho}{\partial t} + \xi^{1/2} \frac{\partial}{\partial \mathbf{x}} \cdot \int \mathbf{Q} f d_2 \Omega + 2 \xi^{1/2} F \cdot \int \mathbf{Q} \frac{\partial f}{\partial \xi} d_2 \Omega \\
+ \xi^{-1/2} F \cdot \int \mathbf{e}_\theta \frac{\partial f}{\partial \theta} d_2 \Omega + \xi^{-1/2} F \cdot \int \mathbf{e}_\phi \frac{1}{\sin \theta} \frac{\partial f}{\partial \phi} d_2 \Omega = N_1 \int J_{1N} [f] d_2 \Omega, \]  

(17)

which, as usual, is exact but not closed, since it involves integrals of the unknown distribution function different from \( \rho \).

**CHAPMAN-ENSKOG EXPANSION AND ASYMPTOTIC LIMIT**

This section is devoted to the asymptotic limit of (8) when \( \epsilon \to 0 \), aiming at the derivation of a closed macroscopic balance equation with first order correction term. Only a formal standard Chapman-Enskog expansion will be applied, leaving the rigorous work and error estimate to future investigation. According to the Chapman-Enskog procedure [1], the unknown \( f \) is expanded in asymptotic series, truncated at first order terms in \( \epsilon \), but the hydrodynamic quantity, the partial density \( \rho \), is left unexpanded. The time derivative operator is expanded instead. In other words we set

\[ f = f_0 + \epsilon f_1, \]  

(18)

with

\[ \int f_0(\xi, \Omega) d_2 \Omega = \rho(\xi), \quad \int f_1(\xi, \Omega) d_2 \Omega = 0. \]  

(19)

When the ansatz (18) is inserted into (8), the first equation of the hierarchy, relevant to \( O(1) \) terms, is

\[ J_{EL} [f_0] = 0, \]  

and then, as established in the previous Section, \( f_0 \) belongs to the null space of \( J_{EL} \), uniquely determined in terms of \( \rho \), by (19), as

\[ f_0(\xi, \Omega) = \frac{1}{4\pi} \rho(\xi). \]  

(20)

\( O(\epsilon) \) terms yield the second equation of the hierarchy

\[ J_{EL} [f_1] = -J_{1N} [f_0] + \frac{1}{4\pi N_1} \left( \frac{\partial \rho}{\partial t} + \xi^{1/2} \mathbf{Q} \cdot \frac{\partial \rho}{\partial \mathbf{x}} + 2 \xi^{1/2} F \cdot \mathbf{Q} \frac{\partial \rho}{\partial \xi} \right), \]  

(21)

which can be considered, for any given \( \xi \), as a Fredholm inhomogeneous linear integral equation for \( f_1 \) with respect to the single variable \( \Omega \). Its solvability condition is then simply provided by the Fredholm alternative, and consists in the requirement that the inhomogeneous term must be orthogonal to the null space of \( J_{EL} \), which explicitly reads as

\[ \frac{\partial \rho}{\partial t} = 4\pi N_1 J_{1N} [f_0], \]  

(22)

and determines the unknown operator \( \frac{\partial}{\partial \Omega} \). Now, owing to the isotropic scattering assumption and to (19), the equation (21) for \( f_1 \) is of very easy analytical solution, and provides

\[ f_1(\xi, \Omega) = -\frac{1}{4\pi N_1 \nu_0(\xi)} \left( \xi^{1/2} \frac{\partial \rho}{\partial \mathbf{x}} + 2 \xi^{1/2} F \frac{\partial \rho}{\partial \xi} \right), \]  

(23)

with

\[ \nu_0(\xi) = \sum_{i=1}^{L} q_i \nu_i^0(\xi). \]  

(24)
Of course, a much more complicated compatibility condition would arise if inelastic scattering were dominant as well, and the solution $f_1$, though uniquely defined, could not be cast in analytical form if collision frequencies were angle-dependent, but these problems will not be considered here either.

Now the sought asymptotic limit is obtained by using the approximation (18), with $f_0$ and $f_1$ given by (20) and (23), into the macroscopic equation (17). Everything in fact can be made explicit in terms of $\rho$. In particular one ends up with

$$\int J_{1N}[f]d_2\Omega = \sum_{i=1}^{L-1} \sum_{j=i+1}^L \left\{ q_i \left[ \nu_{ij}^0(\xi + p_{ij}) \rho(\xi + p_{ij}) - U(\xi - p_{ij}) \nu_{ij}^0(\xi) \rho(\xi) \right] 
+ q_j \left[ U(\xi - p_{ij}) \left( \frac{\xi}{\xi - p_{ij}} \right)^{1/2} \nu_{ij}^0(\xi) \rho(\xi - p_{ij}) - \left( \frac{\xi + p_{ij}}{\xi} \right)^{1/2} \nu_{ij}^0(\xi + p_{ij}) \rho(\xi) \right] \right\},$$

and also integrals in the streaming terms can be performed, after some algebra, by means of the tensor identities

$$\int \Omega \otimes \Omega d_2\Omega = \frac{4\pi}{3} I, \quad \int (e_\theta \otimes e_\theta + e_\phi \otimes e_\phi) d_2\Omega = \frac{8\pi}{3} I. \quad \text{(26)}$$

The hydrodynamic approximation turns out to be a partial differential-difference equation for the quantity $\rho$ as a function of $x$, $\xi$, and $t$, with $O(\epsilon)$ correction terms. Such an equation is better rewritten in terms of the independent variables $x$, $\xi$, and $t$, where $v = \xi^{1/2}$ is the adimensionalized speed. It takes in fact the symmetric form

$$\frac{\partial \rho}{\partial t} = N_1 \int J_{1N}[f]d_2\Omega + \frac{\partial}{\partial x} \cdot \left[ D(x, v) \frac{\partial \rho}{\partial x} \right] + \frac{\partial}{\partial v} \cdot \left[ D(x, v) \frac{\partial \rho}{\partial v} \right]
+ \frac{\partial}{\partial x} \cdot \left[ (b \otimes a) \cdot \frac{\partial \rho}{\partial v} \right] + \frac{\partial}{\partial v} \cdot \left[ (a \otimes b) \cdot \frac{\partial \rho}{\partial x} \right], \quad \text{(27)}$$

where vectors $a$ and $b$ are given by

$$a(x, v) = \left[ \frac{\epsilon}{3N_1(x)\nu_0(v)} \right]^{1/2} v,$n$$
$$b(x, v) = \left[ \frac{\epsilon}{3N_1(x)\nu_0(v)} \right]^{1/2} F,$n

and provide also diffusion coefficients $D$ and $D$ as

$$D(x, v) = a \cdot a, \quad D(x, v) = b \cdot b. \quad \text{(29)}$$

There is no actual dependence in (27) on the direction of the vector $v$, since all polar coordinates but the radial one, $v = |v|$, are cancelled out by the indicated operations. The limiting equation (27) is then a generalized drift-diffusion equation with additional collision terms due to the non-dominant part of the scattering operator. More precisely, it exhibits $O(1)$ contributions from inelastic scattering, relating $\rho(\xi)$ with all other energies of the kind $\xi \pm p_{ij}$ (the same coupling due to collisions occurring at the kinetic level, which is present neither in the dominant part of scattering, nor in the asymptotic procedure, but appears again now in the final output). All contributions from streaming are instead $O(\epsilon)$, as typical in all diffusive approximations under the present scaling, with derivatives with respect to speed induced by the external force. In particular one can recover a standard diffusion term in the physical space when the external force is absent, with diffusion coefficient $D$, and an isotropic diffusion in the velocity space when spatial gradients are absent, with diffusion coefficient $D$. In the presence of both, cross interaction tensors $b \otimes a$ and $a \otimes b$ define mixed terms with spatial divergence of velocity gradients and velocity divergence of spatial gradients.

**ACKNOWLEDGMENTS**

Work performed in the frame of the activities sponsored by MURST, by the University of Parma, by the National Group for Mathematical Physics, and by the National Research Council.
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