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WAVE PROPAGATION IN DISCRETE KINETIC THEORY

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The paper is a review of shock wave propagation problems for inert and chemically reacting gases in the framework of discrete velocity models (Discrete Boltzmann Equation, DBE). The paper is divided in two parts. The former deals with the formulation of shock wave problems and with a review of results. The latter takes into account open problems and addresses the reader to future lines of research.

1. Introduction.

The analysis of the structure of shock waves and of the existence and stability of travelling shock waves is a classical topic both in continuum fluid-dynamics and in kinetic theory of gases [1].

Shock waves can be also studied in the framework of the Euler and Navier-Stokes description of fluid-dynamics. This latter mathematical model certainly provides accurate description of the flow conditions in the case of weak shock waves and small Knudsen numbers. On the other hand for strong shock waves and/or large Knudsen numbers the description provided by the Boltzmann equation appears to be more accurate if compared with experimental observations (see ref.[1] for a wide bibliography on this topic).

One can then state that the quantitative and qualitative analysis of shock waves is certainly an interesting field of application of the DBE [2]. In fact, as shown in ref.[3], this model provides an accurate description, both at a qualitative and quantitative level.

In particular, this paper tries hopefully to provide a unified review of the various mathematical and physical results available in the literature. The paper will also indicate the mathematical problems which are still open and the main difficulties to be tackled to deal with them, so that the reader can find indications for future research activities in the field.

2. Formulation of the Mathematical Problems.

The general structure of the discrete Boltzmann equation is here reported for sake of completeness and for simplicity of presentation

(1) $$\left(\frac{\partial}{\partial t} + \mathbf{v}_i \cdot \nabla_{\mathbf{x}}\right) N_i = J_i^{(2)}[\mathrm{N}] + J_i^{(3)}[\mathrm{N}] \quad , \quad i = 1, \ldots, n$$

(2) $$\mathrm{N} = \{N_i(t, \mathbf{x})\} : \ [0, T] \times \mathbb{R}^d \longmapsto \mathbb{R}_+^n \quad , \quad d = 1, 2, 3$$

where $\mathbf{v}_i$, $(i = 1, \ldots, n)$ denote the admissible velocities, N_i the number densities joined to each velocity and $J_i^{(2)}$ and $J_i^{(3)}$ are the collision operators for the binary and triple collisions respectively. The mathematical expression of such operators is related to the specific model which has been chosen, namely on the number of admissible velocities; nevertheless the operators are always of quadratic and cubic type, respectively.

If the gas includes different components which can react chemically, then to the r.h.s. of Eq.(1) *source terms* $S_i[\mathrm{N}]$ and *sink terms* $D_i[\mathrm{N}]$ should be added. For sake of simplicity in the analysis which follows we will omit these terms.

We recall briefly the principal physical mathematical properties of Eq.(1). When the number densities are equilibrium Maxwellian densities, which will be denoted by $\widehat{N}_i$, then the collision operators are equal to zero

(3) $$J_i^{(2)}[\widehat{\mathrm{N}}] = J_i^{(3)}[\widehat{\mathrm{N}}] = 0 \quad i = 1, \ldots, n.$$

Moreover a vector $\mathbf{\Phi} \in \mathbb{R}^n$ with components Φ_i, functions of the discretized velocities, is a *collisional invariant* if and only if the following scalar product satisfies the property

$$(4) \qquad < \mathbf{\Phi}, \mathbf{J}^{(s)} >= \sum_{i=1}^{n} \Phi_i J_i^{(s)} = 0 \quad , \quad s = 2, 3 \ .$$

The space of collisional invariants, which is a linear subspace of $\mathbb{R}^n$, is denoted by $\mathcal{M}$ and its dimension by δ.

Further on one can define the *hydrodynamical moments*, i.e. the macroscopic variables, by

$$(5) \qquad W_\chi(t, \mathbf{x}) =< \mathbf{\Phi}^{(\chi)}, \mathbf{N} > \quad , \quad \chi = 1, \ldots, \delta$$

where $\mathbf{\Phi}^{(\chi)}$ denotes each independent collisional invariant in the space $\mathcal{M}$. From property (4) it follows that a discrete velocity model of the Boltzmann equation admits a number δ of independent *conservation equations* which are obtained by multiplying Eq.(1) by $\Phi_i^{(\chi)}$ and summing over i. These equations can be written as

$$(6) \qquad \frac{\partial W_\chi}{\partial t} + \mathcal{F}_\chi[\mathbf{N}] = 0 \quad , \quad \chi = 1, \ldots, \delta$$

where

$$(7) \qquad \mathcal{F}_\chi[\mathbf{N}] = \sum_{i=1}^{n} \Phi_i^{(\chi)} \mathbf{v}_i \cdot \nabla_{\mathbf{x}} N_i \quad .$$

Analogously to continuum kinetic theory, these equations in general do not generate a closed system of equations in the unknown macroscopic variables W_χ.

The thermodynamical equilibrium state is determined by the well–known [2] H–theorem which assures the equivalence between the two following statements

$$(8) \qquad \log \widehat{\mathbf{N}} = \{\log \widehat{N}_1, \ldots, \log \widehat{N}_n\} \in \mathcal{M}$$

$$\mathbf{J}^{(s)}[\widehat{\mathbf{N}}] = 0 \quad , \quad s = 2, 3 \quad .$$

Then from (8), using property (4), the explicit expression of Maxwellians can be determined, i.e.

$$(9) \qquad \widehat{N}_i = \exp\left[\sum_{\chi=1}^{\delta} c_\chi \Phi_i^{(\chi)}\right] \quad , \quad i = 1, \ldots, n$$

where the coefficients $c_\chi = c_\chi(t, \mathbf{x})$ are called the *Maxwellian parameters*. Gatignol [2] has proved that the map

$$c_\chi \longmapsto \widehat{W}_\chi \tag{10}$$

is a one–to–one map, so that the Maxwellians can be expressed in terms of the hydrodynamical moments calculated in the equilibrium state.

Finally let us recall that the conservation equations (6), when are computed in the equilibrium state, become a closed system of equations which, analogously to continuum kinetic theory, are called Euler equations. These equations represent the time–space evolution of the macroscopic quantities in the equilibrium state.

In spite of the relevance of the problem, dealt with in this review, mathematical results for shock waves are available only for some special models: the Broadwell model [2] for both a simple gas (six admissible velocities) and a binary gas mixture (twelve admissible velocities), Cabannes' 14–velocity model [2] and the planar 6–velocity models [3] with triple collisions. Certainly, results for general models of the discrete Boltzmann equation would be desired, however several mathematical difficulties are still waiting to be solved.

Having in mind Eqs.(1)–(10), we have all tools to provide the mathematical descriptions of the shock wave problems which will be dealt with and reviewed in this paper:

1) Existence of shock profiles,

2) Stability of shock profiles,

3) Onset and formation of shock waves.

Since the shock wave problems studied in this paper are all in one space dimension, in what follows we will consider

$$x \in \mathbb{R} \quad \text{and} \quad N_i = N_i(t, x) \, .$$

The first problem, i.e. *existence of shock profiles*, consists in proving the existence of shock solutions

$$N_i(x - \beta t) \tag{11}$$

travelling with constant velocity β and linking, asymptotically in space, two constant Maxwellian distributions

$$(12) \qquad \widehat{N}_i^- = N_i(x \to -\infty) \quad , \quad \widehat{N}_i^+ = N_i(x \to +\infty) \; .$$

The two Maxwellians are not independent and need to be expressed one in terms of the other. This is possible using conservation equations (6) formally integrated between $x \to -\infty$ and $x \to +\infty$. Such relations, obtained at a microscopic level, can be written as

$$(13) \qquad \widehat{N}_i^+ = \widehat{N}_i^+(\widehat{N}_i^-)$$

so that one can determine the map

$$(14) \qquad \{c_\chi^+\} \longmapsto \{c_\chi^-\}$$

between the Maxwellian parameters characterizing the equilibrium states at $+\infty$ and at $-\infty$, respectively. Recalling now the map (10), relation (14) can be transferred at a macroscopic level by the new map

$$(15) \qquad \{\widehat{\rho}^+, \widehat{u}^+, \widehat{T}^+\} \longmapsto \{\widehat{\rho}^-, \widehat{u}^-, \widehat{T}^-\}$$

which links mass densities $\widehat{\rho}$, mean velocities $\widehat{u}$ and temperatures $\widehat{T}$ of the two equilibrium states. The relations (15), in analogy with those of continuum theory, are generally called Rankine-Hugoniot conditions [1].

After these preliminar calculations existence of shock profiles for the DBE can be achieved by the following investigations

— Compatibility for each β of Rankine-Hugoniot conditions (15) with the Euler equations, genuine nonlinearity and strict hyperbolicity of these equations

— Existence and uniqueness of solutions of type (11) for equation (1) with limit conditions (12).

This last step consists essentially in proving the existence of a trajectory between $x \to -\infty$ and $x \to +\infty$, linking two stable points. The existence is defined *global* if it is obtained for all values of β, namely for $|\beta|$ spanning from zero, which corresponds to

$$\{\hat{\rho}^+, \hat{u}^+, \hat{T}^+\} = \{\hat{\rho}^-, \hat{u}^-, \hat{T}^-\} ,$$

to the maximum value of $|\beta|$, which corresponds to $\hat{u}^+ = 0$. The discontinuity at $x - \beta t = 0$ is then called *shock wave*.

Various details of this problem have been studied by several authors. Following the pioneer work by Broadwell [4], Gatignol [5] and Cabannes [6] have studied several aspects related to the formulation of the Rankine-Hugoniot relations for a simple monoatomic gas. Gatignol has also provided analytical solutions generalizing the original results by Broadwell. Caflisch [7], starting from Gatignol's paper [5], has analysed the existence of shock profiles for the Broadwell model and the gap between these profiles and the ones described by the Navier-Stokes equation.

Methodological aspects are dealt with in papers [8–12] which mainly refer to mathematical aspects related to the analysis of existence of shock profiles for general models of the DBE either with binary collisions only or with both binary and triple collisions.

The problem of computation of shock profiles for a binary gas mixture has been dealt with in papers [13–16] which refer all to the 2×6–Broadwell model [2]. In particular papers [13,14] provide suitable comparisons with profiles obtained by other authors [17,18]. These comparisons show a good agreement between the results predicted by discrete kinetic theory and those obtained experimentally, or theoretically on the basis of linearized models of the full Boltzmann equation, so that one can say that shock–wave problems have been a good validation ground to test the DBE models.

Recently computation of shock profiles for binary mixtures, with both binary and triple collisions between particles, has been performed in paper [19].

Moreover exact particular shock–wave solutions have been obtained, essentially with a technique proposed by Cornille, in several papers: in [20] for the Broadwell model in one dimension, in [21] for a six planar velocity model with ternary collisions in one–space dimension, in [22] for the Broadwell model in two dimensions, in [23] for the same model in three dimensions, and finally in [24] for the cubic 14–velocity model and the hypercubic 24–velocity model in one dimension.

The analysis of the *stability of shock profiles* essentially consists in the study of the qualitative behaviour of solutions referred to the perturbation of a travelling wave

$$N_i(x - \beta t) + \varphi_i(x) \tag{16}$$

where $N_i(x - \beta t)$ is a steady shock profile and φ_i a small perturbation. The only two papers where it is possible to find original contributions to this topic are due to Kawashima and Matzumura [25] and to Caflisch and Tai Ping Liu [26]. Both papers deal with the six–velocity Broadwell model for a simple gas.

The analysis of the third topic, i.e. *onset and formation of shock waves*, consists in the analysis of the initial value problem for Eq.(1) with initial conditions

$$N_{io} = \begin{cases} \widehat{N}_i^- \quad , & \text{if } x \le 0 \\ \widehat{N}_i^+ \quad , & \text{if } x > 0 \end{cases} \tag{17}$$

where $\widehat{N}_i^-$ and $\widehat{N}_i^+$ are the Maxwellian densities defined in (12). Then one has to verify whether for $t \to \infty$ the solution tends to the steady solution (11), which is consistent with the Rankine-Hugoniot conditions.

Such a problem has been studied in paper [27] both for the Broadwell model and for binary gas mixtures with disparate masses, represented by a 2×6–Broadwell model [3]. In paper [27], at least on a numerical ground, the trend, for $t \to \infty$, to the steady shock solution has been shown. An analogous numerical experiment has been also carried on (see ref.[19]) for a binary gas mixture represented by the six planar velocity model with triple collisions [8].

Before ending this section it is worthwhile mentioning that shock–wave problems for gases admitting chemical reactions have been studied as well in discrete kinetic theory. These results deal with the onset and formation problem for a diatomic gas undergoing chemical dissociation. The effect of the reactions on the shock–wave onset has been investigated via numerical simulations in papers [28,29].

Moreover exact shock–wave solutions [30–32] for particular models admitting various reversible and irreversible reactions have been recently performed following Cornille's technique.

3. Discussion and Open Problems.

It has been shown, through the development of the content of this review, that, despite the relevance of the problem, several interesting and relevant aspects are left open. These open problems can be regarded as suitable fields for future research activity.

Keeping this in mind, let us first examine the qualitative aspects of the analysis of the problem in one space dimension. The proof of existence of shock profiles needs first the proof of existence of Euler solutions (strict hyperbolicity and genuine nonlinearity of the Euler equations and uniqueness for each β of the solution to the Rankine-Hugoniot equations), then one can deal with the direct proof of existence of shock profiles.

The proofs of the first step are necessary, but not sufficient, conditions to deal with the proof of the second step. The first step, after the paper by Kawashima and Bellomo [9] can be regarded solved at least for a discrete velocity model with only one velocity modulus. The same technique can hopefully solve the same problem for more general discrete models of the Boltzmann equation.

On the other hand, we have seen that very little is known about the second step. In fact the few results available in the literature refer to the Broadwell model. Generalizing what is known for the Broadwell model to more general discrete velocity models would certainly be of great interest.

This goal could be realized at least for *weak* shock waves. In this case one can use mathematical results which are known for the Navier-Stokes model [33,34]. Then it may be possible to show that for weak shock waves, the profiles described by the discrete Boltzmann equation remain close to the ones predicted by the Navier-Stokes equation. This may require, as already observed in [10], structural assumptions on the discrete velocity models.

Being aware of the fact that the above stated conjectures are still at the stage of speculations without useful ideas towards the solution of the problem, we need mentioning that a similar result is proved for the full Boltzmann equation by Caflisch and Nicolaenko [35].

All speculations presented in this review, refers to problems in one space dimension. Problems in two or three space dimensions, even if of great interest in fluid-dynamics, are not dealt with, at present, in the pertinent literature, apart from the aforementioned papers by Cornille. This aspect of the problem certainly deserves future research activity.

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