A note on a Discrete Boltzmann Equation with multiple collisions

Filipe Oliveira*and Ana Jacinta Soares†

* Centro de Matemática e Aplicações, FCT – Universidade Nova de Lisboa, Portugal
† Centro de Matemática, Universidade do Minho, Braga, Portugal

Abstract

We compute a non-trivial explicit solution for the one-dimensional plane 6-velocity discrete Boltzmann model with multiple collisions introduced in [4] which asymptotically connects two particular Maxwellian states. We prove that such a solution exists provided that a suitable condition on the differential elastic cross sections holds.

AMS Classification Numbers: 76P05, 74J40, 35L50
Keywords: Discrete Boltzmann Equation, Shock wave solutions, Hyperbolic PDEs

1 Introduction

The Discrete Boltmann Equation (DBE) constitutes a mathematical model in kinetic theory of gases which describes the time-space evolution of a gas whose particles are only allowed to move with a finite number of selected velocities. It is well known that this model provides an alternative tool to the full Boltzmann equation in terms of an hyperbolic set of partial differential equations for the number densities joined to the selected velocities. There exists a rather vast bibliography on this topic. In the context of the DBE for gases with binary collisions only, we can mention, among others, the pioneering paper by Broadwell [1], where a 6-velocity model for one component gas is proposed, the lecture notes by Gatignol [2], with an exhaustive treatment of generalized DBE and the paper [3], which provides a systematic theory of gas mixtures. On the other hand, in the context of the DBE for gases with multiple encounters, we cite the paper [4], where a plane 6-velocity model with triple and binary collisions is proposed, and the paper [5] which refers to the general model with multiple collisions.

Although the inclusion of multiple collisions implies rather complex collision terms involving higher degree polynomials, it represents an advantage from both physical and mathematical point of view. In fact, it allows to simulate moderately dense gas effects and, at the same time, it reduces the collision invariants of the model to the ones with physical meaning only, resulting better stability properties, as shown in paper [6].

Besides a rather simple mathematical structure, the DBE presents the capability of deriving interesting hydrodynamic equations. For this reason, it provides an adequate description of

*fso@fct.unl.pt
†ajsoares@math.uminho.pt

several relevant fluid dynamical problems as, for example, the shock wave propagation in rarefied or moderately dense gases. Several authors have studied this problem within different particular models [1, 7, 8, 9, 10, 11] and the conclusions have shown a satisfactory qualitative agreement with experimental and theoretical results. In particular, in paper [11], the present authors have obtained a non-trivial explicit solution for the 14-velocity Cabannes model introduced in [7], where only binary collisions are taken into acount.

In the present paper, for the one space dimensional version of the plane 6-velocity model with binary and triple collisions introduced in [4], we obtain an explicit shock profile solution of the kinetic equations, under a suitable condition on the differential elastic cross sections and a pertinent choice of the Maxwellian parameters of the state behind the shock. Such a solution represents a plane shock wave which travels with constant velocity and asymptotically connects two particular equilibrium Maxwellian states.

From the solution profiles obtained both in paper [11] and in the present work, we strongly believe that the inclusion of triple encounters in the collision mechanism contributes to improve the model properties.

The knowledge of an explicit shock solution is of theoretical and practical importance, for both modelling problems and numerical simulations. The explicit solutions give some understanding of the physical process, allow to extract comparisons with approximate solutions and provide the validation of experimental predictions. To our knowledge, explicit traveling wave solutions of the above mentioned model does not exist so far in the literature.

The paper is organized in three sections. After this introduction, in Section 2, we summarize the relevant equations of the considered model in the one space dimension. In Section 3, we integrate the model conservation equations between limiting states, deriving the corresponding Rankine-Hugoniot conditions, and finally we obtain the explicit shock wave solution.

2 The model equations

We consider the 6-velocity DBE with multiple collisions introduced in [4]:

$$\left\{\begin{array}{rcl} \partial_t F_1 + \partial_x F_1 & = & \sigma_1 q_1(F) + \sigma_2 q_2(F) \\ 2\left(\partial_t F_2 + \frac{1}{2}\partial_x F_2\right) & = & -\sigma_1 q_1(F) - 2\sigma_2 q_2(F) \\ 2\left(\partial_t F_3 - \frac{1}{2}\partial_x F_3\right) & = & -\sigma_1 q_1(F) + 2\sigma_2 q_2(F) \\ \partial_t F_4 - \partial_x F_4 & = & \sigma_1 q_1(F) - \sigma_2 q_2(F), \end{array}\right. \tag{1}$$

where $(x,t) \in \mathbb{R} \times \mathbb{R}^+$, σ_1 and σ_2 are positive constants depending on differential cross sections, collision frequencies and relative velocity of the colliding particles, and the nonlinear collision terms on the *r.h.s.* of Eqs. (1) are given by

$$q_1(F) := F_2F_3 - F_1F_4 \ \text{ and } \ q_2(F) := F_2^2F_4 - F_1F_3^2. \tag{2}$$

Here, F_i denotes the number density of particles with velocity v_i along the (Ox) direction, for

$$(v_1, v_2, v_3, v_4) = (1, \frac{1}{2}, -\frac{1}{2}, -1).$$

Let us introduce the new variables ρ, m, z and $\tilde{z}$ defined by

$$\begin{array}{ll} \rho = F_1 + 2F_2 + 2F_3 + F_4, & m = F_1 + F_2 - F_3 - F_4, \\ z = 2F_1 + F_2 + F_3 + 2F_4, & \tilde{z} = 3(F_2 - F_3). \end{array} \tag{3}$$

where ρ is the total mass density of the gas, m the total x-momentum component, $\tilde{z}/3$ the x-flux of particles with velocity at angle with the x-axis and $z/2$ the x-flux of total x-momentum component. The old variables can be expressed in terms of the new ones in the following way:

$$
\begin{aligned}
F_1 &= \frac{1}{2}m - \frac{1}{6}\rho + \frac{1}{3}z - \frac{1}{6}\tilde{z}, \qquad & F_2 &= \frac{1}{6}\tilde{z} - \frac{1}{6}z + \frac{1}{3}\rho, \\
F_3 &= \frac{1}{3}\rho - \frac{1}{6}z - \frac{1}{6}\tilde{z}, \qquad & F_4 &= -\frac{1}{6}\rho + \frac{1}{3}z + \frac{1}{6}\tilde{z} - \frac{1}{2}m,
\end{aligned} \tag{4}
$$

and the system (1) can be re-written as

$$\partial_t \rho + \partial_x m = 0, \tag{5a}$$

$$\partial_t m + \frac{1}{2}\partial_x z = 0, \tag{5b}$$

$$\partial_t z + \partial_x (2m - \frac{1}{2}\tilde{z}) = \frac{\sigma_1}{4} Q_1, \tag{5c}$$

$$\partial_t \tilde{z} + \partial_x (\rho - \frac{1}{2} z) = \frac{\sigma_2}{6} Q_2, \tag{5d}$$

where

$$Q_1(\rho, m, z, \tilde{z}) = \rho^2 - z^2 + 3m^2 - 2m\tilde{z} \tag{6a}$$

and

$$Q_2(\rho, m, z, \tilde{z}) = -\frac{1}{3}\tilde{z}^3 + \tilde{z}(z^2 + \tilde{z}m) - 2z(\rho\tilde{z} + 2m\rho - \frac{1}{2}zm) + 4\rho^2 m\,. \tag{6b}$$

Equations ($5a$) and ($5b$) express conservation of total mass density and total x-momentum component, respectively.

A local Maxwellian state associated to Eqs. ($5a$-d) is characterized by equilibrium parameters (a, b, c, d) such that $Q_i(a, b, c, d) = 0$, for i=1,2. Therefore, it results

$$a^2 - c^2 + 3b^2 - 2bd = 0, \qquad -\frac{1}{3}d^3 + d(c^2 + bd) - 2c(ad + 2ba - \frac{1}{2}cb) + 4a^2 b = 0. \tag{7}$$

3 Shock profile solutions

We are interested in steady shock profile solutions to Eqs. ($5a$–d) of the form

$$(\rho(x,t), m(x,t), z(x,t), \tilde{z}(x,t)) = (A(\xi), B(\xi), C(\xi), D(\xi))\,, \tag{8}$$

where

$$\xi = x + t, \tag{9}$$

traveling from right to left with unit velocity and connecting, asymptoticaly in space, two Maxwellian states (a, b, c, d) and $(\alpha, \beta, \gamma, \delta)$, that is

$$
\begin{aligned}
&\lim_{\xi\to+\infty} (A(\xi), B(\xi), C(\xi), D(\xi)) = (a, b, c, d), \\
&\lim_{\xi\to-\infty} (A(\xi), B(\xi), C(\xi), D(\xi)) = (\alpha, \beta, \gamma, \delta).
\end{aligned} \tag{10}
$$

Solutions of type (8-9) with limiting conditions (10) correspond to state variables which are close to their local equilibrium, far from the shock at $x = -t$.

Now we write system ($5a$-d) in terms of the new variable ξ. We obtain the following system of ordinary differential equations

$$
\begin{aligned}
A' + B' &= 0, & (11a)\\
B' + \frac{1}{2}C' &= 0, & (11b)\\
C' + 2B' - \frac{1}{2}D' &= \frac{\sigma_1}{4}Q_1(A,B,C,D), & (11c)\\
D' + A' - \frac{1}{2}C' &= \frac{\sigma_2}{6}Q_2(A,B,C,D), & (11d)
\end{aligned}
$$

where the primes indicate total derivative with respect to ξ.

The two Maxwellian states introduced in (10) are not independent and need to be expressed one in terms of the other through the so called Rankine-Hugoniot conditions. Integration of the conservation equations ($11a$-b) between $-\infty$ and $+\infty$ with limiting conditions (10) yields

$$
\begin{aligned}
a + b &= \alpha + \beta, & (12a)\\
b + \frac{1}{2}c &= \beta + \frac{1}{2}\gamma, & (12b)
\end{aligned}
$$

which constitute the jump Rankine-Hugoniot conditions and express a relation between the properties of the gas in the limiting Maxwellian states.

If we assume a Maxwellian state behind the shock of type $(a,b,c,d) = (6u,0,6u,0)$, where $u > 0$, corresponding to a state for which $F_1 = F_2 = F_3 = F_4 = u$, we get the solution

$$\alpha = 4u, \quad \beta = 2u, \quad \gamma = 2u, \quad \delta = 6u, \qquad (13)$$

defining a Maxwellian state ahead the shock for which $F_1 = F_3 = F_4 = 0$, $F_2 = 2u$.

Again, integration of the conservation laws ($11a$-b), now from x to $+\infty$, leads to

$$
\begin{aligned}
B(\xi) &= b - (A(\xi) - a), & (14a)\\
C(\xi) &= c + 2(A(\xi) - a). & (14b)
\end{aligned}
$$

Inserting conditions ($14a$-b) into Eqs. ($11c$-d), we obtain the system

$$-\frac{1}{2}D'(\xi) = \frac{\sigma_1}{4}Q_1(A(\xi),B(\xi),C(\xi),D(\xi)), \qquad (15a)$$

$$\sigma_1 Q_1(A(\xi),B(\xi),C(\xi),D(\xi)) = -\frac{\sigma_2}{3}Q_2(A(\xi),B(\xi),C(\xi),D(\xi)). \qquad (15b)$$

Putting $\tilde{A}(\xi) = A(\xi) - a$, from Eqs. ($14a$-$b$) we get

$$Q_1 = 2\tilde{A}(\xi)D - 12u\tilde{A}(\xi)$$

and

$$Q_2 = -\frac{1}{3}D(\xi)^3 - 36u^2(\tilde{A}(\xi) + D(\xi)) - 12u\tilde{A}(\xi)D(\xi) - \tilde{A}(\xi)D(\xi)^2.$$

¿From ($15b$) we get

$$\tilde{A}(\xi) = -\frac{D(\xi)(D(\xi)^2 + 108u^2)}{3(-2SD(\xi) + 12Su + 36u^2 + 12uD(\xi) + D(\xi)^2)}, \qquad (16)$$

where we have put $S = 3\dfrac{\sigma_1}{\sigma_2}$. Finally, using this last identity, Eq. (15a) transforms to

$$D'(\xi) = \frac{\sigma_1}{3} \frac{(D(\xi)^2 - 6uD(\xi))(D(\xi)^2 + 108u^2)}{-2SD(\xi) + 12uS + 36u^2 + 12uD(\xi) + D(\xi)^2}. \tag{17}$$

Equation (17) cannot be explicitly integrated. However, putting $S = 6u$, which means that $\dfrac{\sigma_1}{\sigma_2} = \dfrac{1}{2}u$, Eq. (17) reduces to the separable equation

$$D'(\xi) = \sigma_1(\frac{1}{3}D^2(\xi) - 2uD(\xi)). \tag{18}$$

Solutions to Eq. (18) are obtained in the form

$$D(\xi) = \frac{6u}{Ce^{2u\sigma_1\xi} + 1},$$

for some constant C that we choose positive in order to guarantee that D is defined for all ξ. Finally, from Eqs. (8), (14a-b) and (16), we get the exact solutions

$$\begin{aligned}
\rho(x,t) &= A(x+t) = \frac{-2u}{Ce^{2u\sigma_1(x+t)} + 1} + 6u, \\
m(x,t) &= B(x+t) = \frac{2u}{Ce^{2u\sigma_1(x+t)} + 1}, \\
z(x,t) &= C(x+t) = \frac{-4u}{3(Ce^{2u\sigma_1(x+t)} + 1)} + 6u, \\
\tilde{z} &= D(x+t) = \frac{6u}{Ce^{2u\sigma_1(x+t)} + 1}.
\end{aligned} \tag{19}$$

Note that, as expected,

$$\lim_{\xi \to -\infty} (A(\xi), B(\xi), C(\xi), D(\xi)) = (4u, 2u, 2u, 6u). \tag{20}$$

In Figure 1 we have drawn the shock profile for the gas density ρ versus ξ , with $C = 1$, $u = 1$ and $\sigma_1 = 1$. This profile corresponds to a continuous shock solution to the model Boltzmann equation traveling from right to left and interpolating the corresponding limit Maxellian states. The solution shows a finite and nonzero wave thickness.

Acknowledgements

The paper is partially supported by Minho University Mathematics Centre and Portuguese Foundation for Science and Technology (CMAT-FCT,CMA-FCT) through programme POCTI.

References

[1] J. E. Broadwell, "Shock structure in a simple discrete velocity gas", *Phys. Fluids*, **7**, pp. 1243-1247, 1964.

[2] R. Gatignol, *Théorie cinétique des gaz à répartition discrète des vitesses*, Lect. Notes in Phys., **36**, Berlin (Springer–Verlag), 1975.

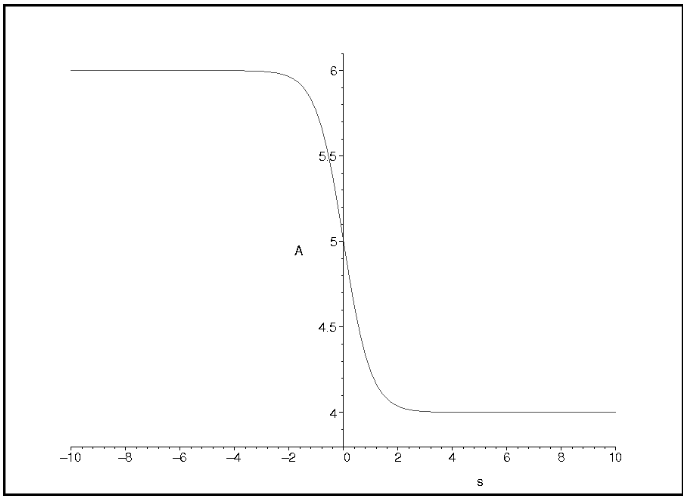

Figure 1: Exact shock profile solutions for the gas density.

[3] E. Longo and R. Monaco, *On the thermodynamics of the discrete models of the Boltzmann equation for gas mixtures*, Trans. Theory Statist. Phys., **17**, pp. 423-442, 1988.

[4] E. Longo and R. Monaco, *On the discrete kinetic theory with multiple collisions: plane six-velocity and unsteady Couette flow*, in the proceedings of *Rarefied Gas Dynamics*, Eds. Muntz *et al*, AIAA Publ., **118**, pp. 118-130, 1989.

[5] R. Gatignol and F. Coulouvrat, *OConstitutive Laws for discrete velocity models*, in *Discrete Kinetic Theory, Lattice Gas Dynamics and Foundations of Fluid Dynamics*, Ed. R. Monaco, World Scientific, Singapore, pp. 121-145, 1989.

[6] S. Kawashima and N. Bellomo, "The discrete Boltzmann equation with multiple collisions: Global existence and stability for the initial value problem", J. Math. Phys. , **31**, pp. 245-253, 1990.

[7] H. Cabannes, "Etude de la Propagation des Ondes dans un Gaz à Quatorze Vitesses", *J. Mécanique*, **4**, pp. 705-744, 1975.

[8] R. Gatignol, "Kinetic theory for a discrete velocity gas and application to the shock structure", *Phys. Fluids*, **18**, pp. 153-161, 1975.

[9] R. Caflish, "Navier-Stokes and Boltzmann shock profiles for a model of gas dynamics", *Commun. Pure Appl. Math.*, **32**, pp. 521-554, 1979.

[10] S. Kawashima, S. Nishibata, "Stationary waves for the discrete Boltzmann equation in the half space with reflective boundaries", *Commun. Math. Phys.*, **211**, pp. 183-206, 2000.

[11] Filipe Oliveira and A. J. Soares "A non-trivial explicit solution for the 14-velocity Cabannes kinetic model", *Nonlinear Analysis TMA*, to appear.