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A BKW mode for the extended Boltzmann equation

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Abstract. We consider a gaseous mixture where the constituting particles interact through binary elastic collisions and removal processes. This system is described by an extended Boltzmann equation for which we derive exact solutions of similarity type, and determine existence conditions. Finally we write explicit solutions for some particular choices of the collision and removal frequencies.

1. Introduction

The nonlinear Boltzmann equation (NLBE) describes the evolution of the distribution function $f(r, v, t)$ for a dilute gas, whose particles undergo binary elastic collisions. Several years ago, Krook and Wu [1], and, independently Bobylev [2], found an exact analytic solution known as the BKW mode, for this equation. This particular solution is valid for spatially homogeneous systems and Maxwell molecules [3]. In this model, collision cross-sections have the form

$$\sigma(b, \chi) = K\varphi(\chi)/g \tag{1}$$

where b is the impact parameter, χ is the deflection angle, and g stands for the relative velocity between the interacting particles before the collision. In the case of a multi-component system, a BKW mode can be found, and the particular solution corresponding to species a, reads [4]

$$f_a(v, t) = (2\pi\alpha_a)^{-3/2} \exp(-v^2/2\alpha_a)(P_a(t) + v^2 Q_a(t)) \tag{2}$$

where α_a, P_a and Q_a are functions of time. This solution exists if all the components have the same mean kinetic energy,

$$m_a \alpha_a(t) = \xi(t) \qquad \forall a \tag{3}$$

and certain parameters defining the system satisfy specifed relations [4]. Let n_a be the number density of particles belonging to species a, m_a their mass and K^s_{ba} the elastic

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collision frequency between two particles, one belonging to species a, and the other to species b. If we consider a two-species system and define the following parameters:

$$
\begin{aligned}
S_1 &= K^s_{22} - K^s_{21}\mu_{21}(3-2\mu_{21}) \\
S_2 &= K^s_{11} - K^s_{12}\mu_{12}(3-2\mu_{21})
\end{aligned} \tag{4}
$$

$$\mu_{ab} = 4m_a m_b/(m_a+m_b)^2 \tag{5}$$

the condition to be satisfied at all times turns out to be

$$(n_2 S_1 - n_1 S_2)\left(2\mu^2_{12}\left(\frac{K^s_{21}}{S_1}+\frac{K^s_{12}}{S_2}\right)-1\right)=0. \tag{6}$$

Recently, the Boltzmann equation has been extended (ENLBE) in order to consider not only elastic collisions but also removal and creation events [5]. This enables the ENLBE to be applied in different areas such as chemical kinetics, nuclear reactor physics, etc, where, as a general rule, the particle number does not remain constant. Several schemes have been proposed in order to find solutions for the ENLBE, specially for Maxwell models [6, 7]. In particular, the BKW mode has been generalized to the ENLBE for a single–species gas [8].

In the next section, we shall derive the conditions for the existence of a BKW mode for the ENLBE in the case of a binary gas mixture. Section 3 is devoted to setting up the general form of this particular exact solution, and in section 4 we present some particular cases in which a closed form for this solution can be written.

2. Existence conditions

Let us consider a two-component gaseous mixture of Maxwell molecules, in which isotropic elastic collisions as well as removal processes take place. In this case, the ENLBE for the velocity distribution function of species a is written

$$\frac{\partial}{\partial t}f_a(v,t)=\sum_b\int \mathrm{d}w\int \mathrm{d}\boldsymbol{n}\, K^s_{ba}(f_a(v')f_b(w')-f_a(v)f_b(w))-\sum_b\int \mathrm{d}w\int \mathrm{d}\boldsymbol{n}\, K^r_{ba}f_a(v)f_b(w) \tag{7}$$

where K^r_{ba} is the removal frequency corresponding to removal of a particle a in one b–a collision.

We write

$$f_a(v,t)=n_a(t)g_a(v,t) \tag{8}$$

such that

$$\int g_a(v,t)\,\mathrm{d}v=1. \tag{9}$$

If we substitute equations (9) in equation (8) and then integrate with respect to v, we obtain an autonomous evolution equation for the number densities:

$$\frac{\mathrm{d}}{\mathrm{d}t}n_a=-4\pi\sum_b K^r_{ba}n_a n_b. \tag{10}$$

This system can be solved without solving the entire BE. In addition, we get the equation that determines the evolution of $g_a(v,t)$

$$\frac{\partial}{\partial t}g_a(v,t)=\sum_b n_b(t)\int \mathrm{d}w\int \mathrm{d}n\, K^s_{ba}(g_a(v')g_b(w')-g_a(v)g_b(w)). \tag{11}$$

The structure of this equation is identical to that for the case without removal, i.e. equation (7) without the last term. Accordingly, we propose for $g_a(v,t)$ the structure of the BKW mode, equivalent to that of $f_a(v,t)$, in the case without removal (equation (2)):

$$g_a(v,t)=(2\pi\alpha_a)^{-3/2}\exp(-v^2/2\alpha_a)(P_a(t)+v^2Q_a(t)). \tag{12}$$

Again, we shall assume that both species have equal mean kinetic energy

$$m_a\alpha_a(t)=m_b\alpha_b(t)=\xi(t). \tag{13}$$

Let us define

$$R_a(t)=Q_a(t)\xi(t)/m_a. \tag{14}$$

Conservation of particle number and of energy implies that

$$P_a+3R_a=1 \qquad (a=1,2) \tag{15}$$

$$\xi(t)\sum_a n_a(t)(P_a+5R_a)=(n_1+n_2)K_\mathrm{B}T \tag{16}$$

where K_B is the Boltzmann constant and T is the system temperature.

When equation (12) is substituted into equation (11), integrations in the right-hand side can be explicitly performed. We obtain one equation for each gas species consisting of an equality of expressions quadratic in v^2. Equating coefficients results in a system of six nonlinear differential equations for the five functions $\xi(t)$, $P_a(t)$ and $Q_a(t)$:

$$-\frac{P_a}{\xi}\frac{\mathrm{d}\xi}{\mathrm{d}t}-2\frac{\partial R_a}{\partial t}=\sum_b 4\pi n_b(t)K^s_{ba}(\mu_{ab}(R_a-R_b)+\frac{5}{3}\mu_{ab}(3-2\mu_{ab})R_aR_b) \tag{17}$$

$$(-R_a+1)\frac{1}{2\xi}\frac{\mathrm{d}\xi}{\mathrm{d}t}+\frac{\partial R_a}{\partial t}=\sum_b 4\pi n_b(t)K^s_{ba}\left(\frac{\mu_{ab}}{2}(R_b-R_a)-\frac{5}{3}\mu_{ab}(3-2\mu_{ab})R_aR_b\right) \tag{18}$$

$$\frac{1}{\xi}\frac{\mathrm{d}\xi}{\mathrm{d}t}=\sum_{b}\frac{4\pi}{3}n_b(t)K^s_{ba}R_b\mu_{ab}(3-2\mu_{ab}). \tag{19}$$

Equation (19) must hold for $a=1,2$. This yields a simple relation between R_1 and R_2:

$$R_2(t)=\frac{n_1(t)S_2}{n_2(t)S_1}R_1(t). \tag{20}$$

Substituting equation (20) in equation (18), and after some algebra, two different equations are obtained for one of the functions R_i. Solution to this system exists if one condition is satisfied at all times. The new 'compatibility' condition for the case with both removal processes and elastic collisions turns out to be

$$n_1(t)\left(-\frac{K^s_{11}}{6}-K^r_{11}+K^r_{12}+\frac{K^s_{21}\mu^2_{12}S_2}{3S_1}+\frac{K^s_{12}\mu_{12}}{2}\right)$$
$$=n_2(t)\left(-\frac{K^s_{22}}{6}-K^r_{22}+K^r_{21}+\frac{K^s_{12}\mu^2_{12}S_1}{3S_2}+\frac{K^s_{21}\mu_{12}}{2}\right). \tag{21}$$

As the evolution of $n_1(t)$ and $n_2(t)$ is determined independently, equation (21) should hold for any $n_1(t)$, $n_2(t)$. If $n_1(t)$ is not proportional to $n_2(t)$, this implies

$$-\frac{K^s_{11}}{6}-K^r_{11}+K^r_{12}+\frac{K^s_{21}\mu^2_{12}S_2}{3S_1}+\frac{K^s_{12}\mu_{12}}{2}=0 \tag{22}$$

$$-\frac{K^s_{22}}{6}-K^r_{22}+K^r_{21}+\frac{K^s_{12}\mu^2_{12}S_1}{3S_2}+\frac{K^s_{21}\mu_{12}}{2}=0. \tag{23}$$

As stated earlier, the relations above do not involve the species densities, whose evolution is ruled independently by equation (10); instead they are relations between collisions and removal frequencies and masses.

When we set all the removal frequencies equal to zero in (21), both densities remain constant, so we recover the original Krook and Wu compatibility relation, equation (6).

In [6], the 2D BKW mode for the ENLBE was deduced as a particular case of a more general solution consisting in a modified Laguerre series. Such a solution involves conditions similar to (22) and (23) between collison frequencies and masses. It is worth mentioning that this 2D bkw mode is also valid for Maxwell models with non-isotropic collision cross-sections. The condition that allows truncation of the Laguerre expansion in [6] (equation (57)) seems to be inherent to the BKW mode, since it is the 2D equivalent of (19), which is deduced here starting from different grounds.

3. General-case solution

Having established the conditions that the system given by (9) should satisfy in order to have a BKW solution, we are in position to derive it. Thus, from the differential equation system, (17)–(19), we find

$$R_1(t)=\left(-\exp\left(-\int_0^t (Bn_1+Cn_2)\,\mathrm{d}t\right)\left(\int_0^t An_1\exp\left(\int_0^t (Bn_1+Cn_2)\mathrm{d}t+Z\right)\right)\right)^{-1} \tag{24}$$

where

$$A=-\frac{2}{3}\pi\left(K_{11}^s+\mu(3-2\mu)\frac{S_2}{S_1}K_{21}^s\right) \tag{25}$$

$$B=\frac{2}{3}\pi\left(-K_{11}^s+\mu^2\frac{S_2}{S_1}K_{21}^s\right) \tag{26}$$

$$C=-2\pi\mu K_{21}^s \tag{27}$$

and Z is an initial condition.

Let us define:

$$I_1(t)=\exp\left(-\int_0^t (Bn_1+Cn_2)\,\mathrm{d}t'\right) \tag{28}$$

and

$$J_1(t)=\int_0^t \frac{An_1(t')}{I_1(t')}\,\mathrm{d}t'. \tag{29}$$

Then $R_1(t)$ is written

$$R_1(t)=\left[-I_1(t)\left(J_1(t)-\frac{1}{R_1(0)}\right)\right]^{-1}. \tag{30}$$

Once $R_1(t)$ is known, equation (20) may be used to calculate $R_2(t)$.

When the collision frequencies satisfy (22) and (23), equation (24) gives an explicit form for $f_a(v,t)$, provided the equations for the number densities, (10), can be solved in a closed form.

4. Particular cases

Equation (10) has been studied in the framework of extended kinetic theory, and some analytical solutions for particular choices of the parameters, namely, the removal frequencies, are known [9].

In this section we will derive the BKW mode for particular cases considered in [9]

Case 1. When

$$K'_{12}=\frac{2K'_{22}-K'_{21}}{K'_{22}}K'_{11} \tag{31}$$

the solution of (10) yields [8]

$$\begin{aligned} n_1(t)&=\frac{N_1 D}{a_1(1+Dt)+a_2(1+Dt)^{\alpha}} \\ n_2(t)&=\frac{N_2 D}{a_1(1+Dt)^{2-\alpha}+a_2(1+Dt)} \end{aligned} \tag{32}$$

where

$$a_i=K'_{ii}N_i \qquad N_i=n_i(0) \qquad \alpha=\frac{K'_{21}}{K'_{22}} \qquad D=a_1+a_2. \tag{33}$$

From (28) and (32) we get

$$I_1(t)=\left(\frac{(1+Dt)^{\alpha-1}D}{a_1+a_2(1+Dt)^{\alpha-1}}\right)^{-BN_1/(\alpha-1)a_1}\left(\frac{(1+Dt)^{1-\alpha}D}{a_2+a_1(1+Dt)^{1-\alpha}}\right)^{-CN_2/(1-\alpha)a_2}. \tag{34}$$

Equation (29) can be explicitly written in the following form:

$$J_1(t)=\frac{AN_1D^{(\nu-1)}}{(\alpha-1)}\int_1^{X(t)}\frac{X^{\mu-1}}{(a_1+a_2X)^{\nu}}\,\mathrm{d}X \tag{35}$$

where

$$\begin{aligned} \mu&=\frac{BN_1}{(\alpha-1)a_1} \\ \nu&=\frac{BN_1}{(\alpha-1)a_1}+\frac{CN_2}{a_2(1-\alpha)}+1 \\ X&=(1+Dt)^{\alpha-1}. \end{aligned} \tag{36}$$

It is always possible, making an adequate change of variables, to express (35) in terms of a hypergeometric function. For instance, if $\alpha<1$, and $a_1\geqslant a_2$, we have

$$J_1(t)=\frac{AN_1D^{\nu-1}}{(\alpha-1)a_1^{\nu}}\left(\frac{X^{\mu}}{\mu}\,{}_2F_1\!\left(\nu,\mu;1+\mu;\,-\frac{a_2}{a_1}X\right)-\frac{1}{\mu}\,{}_2F_1\!\left(\nu,\mu;1+\mu;\,-\frac{a_2}{a_1}\right)\right). \tag{37}$$

From the analytic continuation properties of the hypergeometric function, it is possible to find $J_1(t)$ for any choice of the parameters α, a_1 and a_2.

For the particular case $\alpha=1$, we have $K'_{21}=K'_{22}$. From the condition imposed by (31), we have

$$K'_{21}=K'_{22} \qquad K'_{12}=K'_{11} \tag{38}$$

and we get

$$n_1(t)=\frac{N_1}{1+Dt} \qquad n_2(t)=\frac{N_2}{1+Dt} \tag{39}$$

i.e. the number densities of both species evolve proportionally as time elapses. From (30) we obtain

$$R_1(t)=\left(-[1+Dt]^{-\varepsilon}\left(\frac{AN_1}{BN_1+CN_2}[1+Dt]^{\varepsilon}-\left(\frac{1}{R_1(0)}+\frac{AN_1}{BN_1+CN_2}\right)\right)\right)^{-1} \tag{40}$$

where

$$\varepsilon=\frac{BN_1+CN_2}{D} \tag{41}$$

Case 2. $k_{ii}^r=0$. In this case we have

$$I_1(t)=\left(\frac{\gamma\tau-\delta}{(\gamma-\delta)\tau}\right)^{\rho-1}\left(\frac{\gamma\tau-\delta}{\gamma-\delta)}\right)^{1-\eta} \tag{42}$$

where

$$\gamma=K_{21}^r N_2 \qquad \delta=K_{12}^r N_1 \qquad \eta=-\frac{CN_2}{\gamma}+1 \qquad \rho=\frac{BN_1}{\delta}+1 \tag{43}$$

and

$$\tau=\exp\left[(\gamma-\delta)t\right]. \tag{44}$$

We can choose $\delta>\gamma$ (the case $\delta=\gamma$ will be treated later on) and obtain for $B>0$ ($\rho>1$)

$$J_1(t)=\frac{AN_1}{(\gamma-\delta)^{\rho-\eta}(-\delta)^{(\eta-\rho+1)}}(-1)\left(\frac{-\gamma}{\delta}\right)^{(2\rho-\eta-1)}\frac{1}{(\rho-\eta)}$$
$$\times\left({}_2F_1\left(\rho,\rho-\eta;\rho-\eta+1;\frac{\gamma}{\delta}\right)-\left(\frac{1}{\tau}\right)^{\eta-\rho}{}_2F_1\left(\rho,\rho-\eta;\rho-\eta+1;\frac{\gamma\tau}{\delta}\right)\right) \tag{45}$$

and

$$J_2(t)=\frac{AN_1}{(\gamma-\delta)^{\rho-\eta}(-\delta)^{(\eta-\rho+1)}}\left(\frac{\delta}{\gamma}\right)^{(-\rho+1)}$$
$$\times\left(\frac{(-1)^{\rho}}{(\rho-\eta)}\left(\left(\frac{\delta}{\delta-\gamma}\right)^{\eta-\rho}{}_2F_1(\rho,\rho-\eta;\rho-\eta+1;\frac{\delta-\gamma}{\delta}\right)\right.$$
$$\left.\left.-\left(\frac{\delta}{\delta-\gamma\tau}\right)^{\eta-\rho}{}_2F_1\left(\rho,\rho-\eta+1;\frac{\delta-\gamma\tau}{\delta}\right)\right)\right). \tag{46}$$

These results simplify when $\delta=\gamma$. In this case the solution to (10) yields

$$n_1(t)=\frac{N_1}{1+K_{12}^r N_1 t} \qquad n_2(t)=\frac{N_2}{1+K_{21}^r N_2 t}. \tag{47}$$

Again, in this particular case, both densities evolve proportionally to each other, and $R_1(t)$ can be easily calculated:

$$R_1(t)=\left(-\frac{AN_1}{BN_1+CN_2}+\left(\frac{1}{R_1(0)}+\frac{AN_1}{BN_1+CN_2}\right)(1+K'_{12}N_1t)^{\eta-\rho}\right)^{-1}. \tag{48}$$

Case 3. $K'_{12}=0$; $K'_{21}=K'_{22}$. In this case we have

$$I_1(t)=\exp\left(-\int_0^t (Bn_1+Cn_2)\,\mathrm{d}t\right)=(1+\vartheta\ln\tau)^{\varphi}\tau^{\xi} \tag{49}$$

with

$$\tau=1+K'_{22}N_2t \tag{50}$$

$$\vartheta=\frac{K'_{11}N_1}{K'_{22}N_2} \qquad \varphi=\frac{B}{K'_{11}} \qquad \xi=-\frac{C}{K'_{22}} \tag{51}$$

and finally we get

$$\begin{aligned}J_1(t)=&-\frac{AN_1\exp[\xi/\vartheta]}{C}\left(\frac{1}{\xi}\right)^{\varphi-1}\\&\times\{\xi^{(\varphi-1)/2}\exp[\xi/2\vartheta]W_{(\varphi-1)/2;\,\varphi/2}(\xi)-\xi(1+\vartheta\ln\tau)^{(\varphi-1)/2}\\&\times\exp[\xi(1+\vartheta\ln\tau)/2\vartheta]W_{(\varphi-1)/2;\,\varphi/2}(\xi(1+\vartheta\ln\tau))\}\end{aligned} \tag{52}$$

where $W_{a,b}(z)$ stands for Whittaker's function [9]. As remarked before, these are just a few particular examples of the BKW mode for a binary mixture with removal processes and, of course, they are not the only ones.

Finally we can show that our solution reduces to that derived by Spiga when there is only one species [8]. Starting from (32) and setting $N_2=0$ we have

$$\begin{aligned}n_1(t)&=\frac{N_1}{1+a_1t}\\n_2(t)&=0.\end{aligned} \tag{53}$$

Equation (34) reduces to

$$I(t)=(1+a_1t)^{-(BN_1/a_1)} \tag{54}$$

and (35) yields

$$J(t)=I(t)-1 \tag{55}$$

finally giving

$$\frac{1}{R(t)=I(t)}\left(-1+I(t)-\frac{1}{R(0)}\right) \tag{56}$$

which is essentially the behaviour described in detail in [8].

Up to now, we have set up exact similarity solutions of the ENLBE for different systems, regardless of their physical meaning. So we have to analyse the conditions for these solutions to be acceptable from a physical point of view.

First we observe that the velocity distribution function of both species should be positive since they represent probability densities. From (12) and (16) we see that $f(\mathbf{v}, t)$ will be positive if

$$0 \leqslant R_a(t) \leqslant \tfrac{1}{3} \qquad a = 1, 2. \tag{57}$$

Also, equation (20) links $R_1(t)$ and $R_2(t)$ yielding

$$\frac{n_a(t) S_b R_a(t)}{n_b(t) S_a} \leqslant \frac{1}{3} \qquad a = 1, 2 \qquad b \neq a. \tag{58}$$

These relations are valid at all times, in particular they hold for the initial time, so we are not free to choose $R_1(0)$ and $R_2(0)$ independently. Furthermore, the velocity distribution functions of both species must obey the H-theorem, that is, they must approach Maxwellian distributions as $t \to \infty$. We can see from (12) and (16) that this is the case if $R_a(t \to \infty) \to 0$ $(a = 1, 2)$.

From (24) we see that $R_a(t)$ remain positive if the initial conditions are positive, and tend monotonicallly to zero when $t \to \infty$ if $B \leqslant 0$. Fortunately, this is physically possible and does not contradict general compatibility conditions defined by (22) and (23). So we conclude that if $R_1(0)$ and $R_2(0)$ are chosen according to (57) and (58), then (24) ensures that $R_a(t)$ will obey (57) at all times, and compatibility conditions guarantee that the relation given by (58) will also hold at all times, regardless of the temporal evolution of both species number densities.

5. Conclusion

We have studied a gaseous mixture of Maxwell molecules, taking into account binary elastic collisions as well as removal processes between them.

We have found the conditions that this system must fulfil in order to evolve towards equilibrium according to a BKW mode. Furthermore, we have derived the mathematical structure of this solution for a general case, and it has been set up explicitly for several particular cases in which the particle densities evolution was known as an explict function of time. Rather complicated expressions involving hypergeometric functions have been obtained, except for cases in which the particle densities of both species remain proportional as the system evolves.

Our results are shown to reduce to those previously known for both cases of a single-species gas with self-removal, and of a mixture with elastic collision processes only.

Finally, we have analysed some conditions that the solutions obtained must obey in order to be acceptable from a physical point of view, and the restrictions these conditions put on the system parameters.

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