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Shock Waves for a Discrete Velocity Gas Mixture

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We introduce three new models for a binary mixture which have only $6+5$, $8+5$, and $12+5$ velocities and study the properties of the first two. The models are plane and have five conservation laws as expected for a binary mixture in the plane case. We look for exact solutions corresponding to traveling waves, which turn out to have the properties of a structured shock wave, and study their properties. Particular attention is paid to the overshoots in the profiles of internal energy for the mixture and the two components.

KEY WORDS: Shock wave structure; discrete velocity models; mixtures.

1. INTRODUCTION

Recently Bobylev and Cercignani[1] introduced a general approach to the problem of constructing discrete velocity models (DVM) for mixtures. They also gave two explicit examples of (plane) discrete velocity models for binary mixtures having $8+5$ and $9+16$ velocities. The first of these models, which was considered not satisfactory in ref. 1, actually turns out to have spurious conservation laws.

The aim of this paper is twofold. We first introduce a new class of models for a binary mixture which have only $6+5$, $8+5$, $12+5$ velocities and, for brevity, study the properties of only the two first ones. The models are plane and turn out to have exactly 5 conservation laws as expected for a binary mixture in the plane case.

We look at the Rankine–Hugoniot properties and later we determine exact solutions corresponding to traveling waves, following an approach introduced and used by one of us[2] in the case of DVM for a single gas.

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The properties exhibited by the solutions are studied in some detail with a particular attention to the overshoots in the profiles of internal energy for the mixture and the two components. For the possible overshoots of the mixture, taking into account only the upstream and downstream asymptotic states, we establish a criterion which generalizes a similar criterion[3] for a single gas.

2. THE NEW $11v_i$ PLANAR MODEL

We would like to retain, for the discrete models, some properties of the continuous theory, consider only binary collisions as in ref. 1 and different discrete velocities (for instance we avoid two particles at rest). For planar models we want five physical conservation laws (no more, no less): two for each component's momentum conservation, two for the mass conservation of the species and only one for the mixture energy conservation. This means that we avoid[4] either extended kinetic models without conservation laws or generalized Broadwell models with one less conservation. It can happen that models have only five conservations but some of them are "ambiguous." For instance, for one-speed species the mass and energy conservations are equivalent, then the mixture energy conservation can be considered (contrary to the continuous theory) as a sum of energy conservations for the two species. Consequently we retain different speeds for the two models. However, as discussed in ref. 1 and suggested in the book by Monaco and Preziosi,[4] this is not sufficient if the models do not allow exchange of energy between the species. So let us consider different speeds, with exchange of energy between the two species. For instance, let us consider a mixed collision with one rest particle in the loss term; then the energy of the other particle will be different from the energies of the two particles in the gain term. Is it sufficient now? Unfortunately not. We can find such models but with "spurious" conservations (more than five conservation relations), An example was the $13v_i$ model of ref. 1 but we have found many others. For some of them the "spurious" conservations disappear (for instance the $13v_i$ of ref. 1) with multiple collisions but not for all. Looking at the defects we observe that some collisions are missing. For instance for the set of light (or heavy) particles, it can happen that there exists a subset where in both loss and gain terms, one of the particles of the subset is always present. A simple but incomplete practical test, for "spurious collision invariants," is to look for solutions symmetrical with respect to one axis, even different from the coordinate axis. We can control whether the number of collision terms is not less than the number of independent densities minus the number of physical conservation relations. At the end of this section we will present a more powerful method.

For a binary mixture we denote by M the ratio between mass of the molecules of the heavy species and that of the molecules of the light ones. In Fig. 1 we present three models without "ambiguous" or "spurious" conservations, $6+5$ velocities with any integer value for M and generalizations: $8+5$ for $M=5$ and $12+5$ (not studied here) for $M=2$. For the $11v_i$ model of Fig. 1 there are 6 different momenta for the molecules of the light species: $(\pm 1, 0)$ $(\pm 1, \pm 2(M-1)^{-1/2})$ and 5 for the molecules of the heavy species: $(0, 0)$, $(\pm 2, \pm 2(M-1)^{-1/2})$. We denote by F_0 the density of the molecules of the heavy species with zero momentum, by (F_1, F_2), (F_3, F_4), the densities corresponding to the velocities $(\pm 2/M, 2(M-1)^{-1/2}/M)$, $(\mp 2/M, -2(M-1)^{-1/2}/M)$ respectively and for the densities of the light species corresponding to $(\pm 1, 0)$, $(\pm 1, 2(M-1)^{-1/2})$, $(\mp 1, -2(M-1)^{-1/2})$ by $f_1, f_2, f_3, f_4, f_5, f_6$, respectively. These $11v_i$ models are physical for any $M>1$: integer, rational or non rational, as illustration in Fig. 1 we choose the two $M=2, 5$ values. For the $M=5$, $13v_i$ model of Fig. 1, we add two

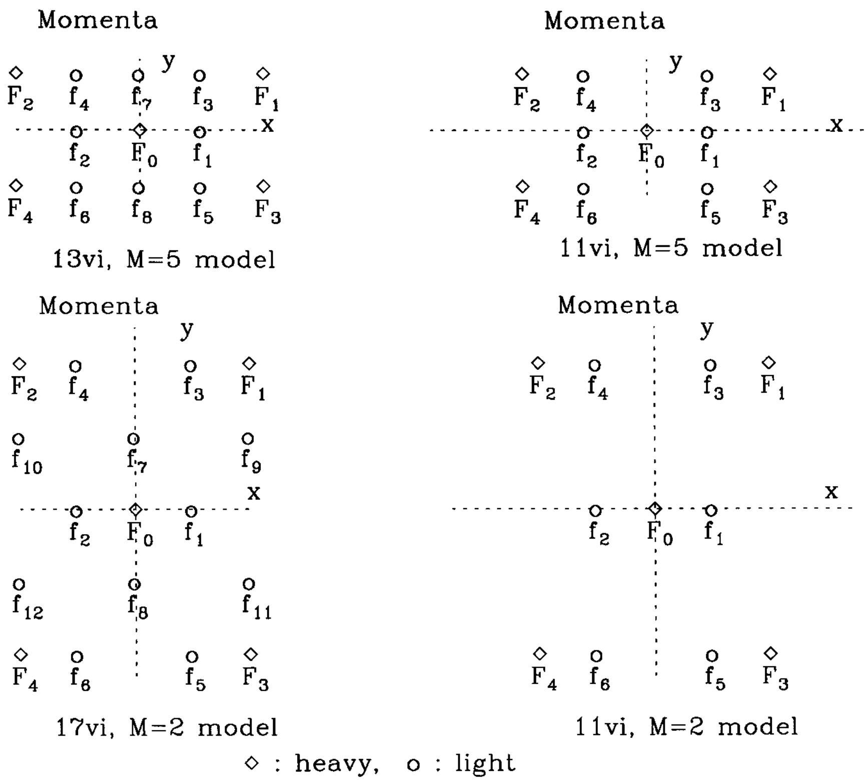

Fig. 1. Generalized $11v_i$ Models with F_0 for the particle at rest. First the $11v_i$ valid for $M>1$ and presented for $M=2$ and 5, second the $13v_i$ with $M=5$ and finally the $17v_i$ with $M=2$.

densities f_7, f_8 of the light species corresponding to $(0, \pm 1)$. For the $M=2$, $17v_i$ model, which is symmetric with respect to an exchange between the x-axis and the y-axis, to the previous f_7, f_8 we add four densities f_9, f_{10}, f_{11}, f_{12} of the light species corresponding to velocities $(\pm 2, \pm 1)$.

We have also found for $M=2$, with properties similar to the present ones, three other $11v_i$, $(5+6)$, $13v_i$, $(5+8)$, and $17v_i$, $(5+12)$ models (not studied here). For the $11v_i$, $M=2$ models the five and six velocities associated to the light f_i and heavy F_i densities are respectively $(0, 0)$, $(\pm 1, \pm 1)$ and $(\pm 1/2, 0)$, $(\pm 1, \pm 1/2)$. For the $13v_i$, $M=2$ models we add two F_i with velocities $(0, \pm 1/2)$. Finally for the symmetric $17v_i$, $M=2$ model, we add (to the $13v_i$) four heavy F_i densities with velocities $(\pm 1/2, \pm 1)$.

In the sequel of Section 1 we give properties for solutions in the plane while solutions depending on just one coordinate are treated in the other sections. The light molecules collide with each other $(1, 4) \leftrightarrow (2, 3)$, $(1, 6) \leftrightarrow (5, 2)$ and $(3, 6) \leftrightarrow (4, 5)$, with the heavy ones $((3, \mathbf{0}) \leftrightarrow (2, \mathbf{1})$, $((4, \mathbf{0}) \leftrightarrow (1, \mathbf{2})$, $(4, \mathbf{3}) \leftrightarrow (6, \mathbf{1})$, $(5, \mathbf{2}) \leftrightarrow (3, \mathbf{4})$, $(5, \mathbf{1}) \leftrightarrow (1, \mathbf{3})$ and $(6, \mathbf{2}) \leftrightarrow (4, \mathbf{4})$, while the heavy molecules collide among themselves $(\mathbf{1}, \mathbf{4}) \leftrightarrow (\mathbf{2}, \mathbf{3})$. We introduce the following notation

$$l_i = \partial_t f_i + \mathbf{v}_i \cdot \partial_{\mathbf{x}} f_i, \qquad L_{\mathbf{i}} = \partial_t F_{\mathbf{i}} + \mathbf{v}_{\mathbf{i}} \cdot \partial_{\mathbf{x}} F_{\mathbf{i}} \tag{2.1}$$

where $f_{\mathbf{i}}$ and $F_{\mathbf{i}}$ denote the densities corresponding to light and heavy particles. Let us denote by $\pm \Lambda_i$ $(i=1, 2, 3)$, $\pm \Omega$, $\pm \Gamma_i$ $(i=1, 2, 3, 4)$ the typical collision terms. We find twelve collision terms defined by:

$$\begin{aligned}
&\Lambda_1 = a(f_3 f_2 - f_4 f_1), && \Lambda_2 = a(f_5 f_2 - f_6 f_1), && \Lambda_3 = \bar{a}(f_3 f_6 - f_4 f_5)\\
&\Omega = b(F_{\mathbf{1}} F_{\mathbf{4}} - F_{\mathbf{2}} F_{\mathbf{3}}), && \Gamma_1 = c(F_{\mathbf{0}} f_3 - F_{\mathbf{1}} f_2), && \Gamma_2 = c(F_{\mathbf{0}} f_4 - F_{\mathbf{2}} f_1)\\
&\Gamma_3 = c(F_{\mathbf{0}} f_5 - F_{\mathbf{3}} f_2), && \Gamma_4 = c(F_{\mathbf{0}} f_6 - F_{\mathbf{4}} f_1), && \Gamma_5 = \bar{c}(F_{\mathbf{3}} f_4 - F_{\mathbf{1}} f_6)\\
&\Gamma_6 = \bar{c}(F_{\mathbf{4}} f_3 - F_{\mathbf{2}} f_5), && \Gamma_7 = \bar{c}(F_{\mathbf{3}} f_3 - F_{\mathbf{1}} f_5), && \Gamma_8 = \bar{c}(F_{\mathbf{4}} f_4 - F_{\mathbf{2}} f_6)
\end{aligned} \tag{2.2}$$

For hard-spheres models a and $\bar{a}$ are connected.[5] Throughout the following, for any Z_i, z_i quantities we define

$$Z^{\pm}_{i,j} = Z_i \pm Z_j, \qquad z^{\pm}_{i,j} = z_i \pm z_j$$

$$Z_{i,j\cdots p} = Z_i + Z_j + \cdots Z_p, \qquad z_{i,j\cdots p} = z_i + z_j + \cdots z_p$$

and the evolution equations read as follows:

$$
\begin{gathered}
L_{\mathbf{0}} = -\Gamma_{1,2,3,4}, \qquad L_{\mathbf{1}} = -\Omega + \Gamma_{1,5,7}, \qquad L_{\mathbf{2}} = \Omega + \Gamma_{2,6,8} \\
L_{\mathbf{3}} = \Omega + \Gamma_3 - \Gamma^+_{5,7}, \qquad L_{\mathbf{4}} = -\Omega + \Gamma_{\mathbf{4}} - \Gamma^+_{6,8} \\
l_1 = \Lambda^+_{1,2} + \Gamma^+_{2,4}, \qquad l_2 = -\Lambda^+_{1,2} + \Gamma^+_{1,3}, \qquad l_3 = -\Lambda^+_{1,3} - \Gamma_{1,6,7} \\
l_4 = \Lambda^+_{1,3} - \Gamma_{2,5,8}, \qquad l_5 = -\Lambda^-_{2,3} - \Gamma_3 + \Gamma^+_{6,7}, \qquad l_6 = \Lambda^-_{2,3} - \Gamma_4 + \Gamma^+_{5,8}
\end{gathered}
\tag{2.3}
$$

There are several conservation relations; 5 of them are independent as appropriate for a plane model for a binary mixture. We start (proof given in Appendix 0, Theorem 1) with three sets: either only for the light species $[l_i]$ or for the heavy $[L_i]$ and finally for the $[l_i, L_i]$ except L_o. In each case, with linear combinations of the l_i, L_i and l_i, L_i, we eliminate successively the associated collision terms. In the two first cases we find only one linear combination vanishing and interpreted as the only conservation laws of mass (or number of particles) for the two species: light and heavy.

$$
\mathscr{M}_l = \sum_1^6 l_i = 0, \qquad \mathscr{M}_h = \sum_0^4 L_{\mathbf{i}} = 0 \tag{2.4}
$$

In the last case (see Theorem 1), we find three vanishing linear combinations of the l_i, L_i which can be combined (with $\mathscr{M}_l = 0$) to give the two components of the momentum conservation and the energy conservation equations:

$$
\begin{gathered}
\mathscr{J}_x = 2(L^+_{\mathbf{1},\mathbf{3}} - L^+_{\mathbf{2},\mathbf{4}}) + l_{1,3,5} - l_{2,4,6} = 0, \qquad \mathscr{J}_y \simeq L^+_{\mathbf{1},\mathbf{2}} - L^+_{\mathbf{3},\mathbf{4}} + l^+_{3,4} - l^+_{5,6} = 0 \\
2\mathscr{E} = (4/(M-1)) \left(\sum_1^4 L_{\mathbf{i}} + \sum_3^6 l_i \right) + \sum_1^6 l_i = 0
\end{gathered}
\tag{2.5}
$$

This method is powerful, for instance it can be applied to prove that the $13v_i$, $17v_i$ models of Fig. 1 are without spurious invariants. A simplification can occur using a "minimal number of collisions." For the proof of Theorem 1, instead of the 12 collisions, we can retain only Γ_i, $i = 1,..., 4$, Γ_6, Λ_i, $i = 1, 2$. When, with only binary collisions, spurious invariants exist, we can see the missing collisions and the geometrical defect of,the model. For instance this has been done (not presented here), with a "minimal number of collisions" for the $13v_i$ and the $25v_i$, $M = 2, 5$ models of ref. 1, proving that only the $25v_i$ $M = 2$ model is without spurious invariants.

A defect of the model, that we call semi-symmetric, is that it is not symmetric with respect to an exchange between the x- and the y-axis. The equilibrium solutions will be studied in the next sections for solutions along the x or y axis, here we write only the relations when the right hand sides of the evolution equation vanish:

$$\Gamma^{+}_{1,3} = \Gamma^{+}_{2,4} = \Lambda^{+}_{1,2} = \Gamma_{1,2,5,6,7,8} = 0, \qquad \Lambda^{+}_{1,3} = \Gamma_{2,5,8}, \qquad \Omega = \Gamma_{1,5,7} \tag{2.6}$$

3. EQUILIBRIUM STATES FOR SOLUTIONS ALONG ONE COORDINATE AXIS

We restrict our study (at equilibrium all $\Gamma_i = \Lambda_j = \Omega$ vanish) to the two simple cases of shock waves along one coordinate-axis. First for solutions along the x-axis, the usual assumption for the $F_{\mathbf{i}}$, f_i (independent of the y coordinate) which are symmetric with respect to the x-axis, is that they are equal, leading to new relations between the collision terms:

$$F_{\mathbf{3}} = F_{\mathbf{1}}, \qquad F_{\mathbf{4}} = F_{\mathbf{2}}, \qquad f_5 = f_3, \qquad f_6 = f_4 \tag{3.1}$$

$$\Gamma_3 = \Gamma_1, \Gamma_4 = \Gamma_2, \Lambda_2 = \Lambda_1, \qquad 0 = \Lambda_3 = \Omega = \Gamma_5 = \Gamma_6 = \Gamma_7 = \Gamma_8 \tag{3.2}$$

Substituting (3.2) into (2.6) we get $\Lambda_1 = \Gamma_1 = \Gamma_2 = 0$ and all collision terms vanish at equilibrium. Second, for solutions along the y-axis, we assume that the $F_{\mathbf{i}}$, f_i (independent of the x coordinate) which are symmetric with respect to the y-axis, are equal, leading to new relations:

$$\begin{gathered} F_{\mathbf{2}} = F_{\mathbf{1}}, F_{\mathbf{4}} = F_{\mathbf{3}}, f_2 = f_1, f_4 = f_3, f_6 = f_5 \\ \Gamma_2 = \Gamma_1, \Gamma_4 = \Gamma_3, \Gamma_5 = \Gamma_6 = \Gamma_7 = \Gamma_8, \qquad 0 = \Lambda_2 = \Lambda_1 = \Lambda_3 = \Omega \end{gathered} \tag{3.3}$$

We substitute (3.3) into (2.6) and get for the nonzero equilibrium terms

$$\Gamma^{+}_{1,3} = 0, \qquad \Gamma_1 + 2\Gamma_5 = 0 \tag{3.4}$$

but this simple argument, which does not exploit the structure of the collision terms, is not enough to conclude that the terms Γ_j are zero. We can reach the conclusion that all the $\Gamma_j = 0$ by exploiting the circumstance that the terms $\Gamma^{+}_{1,3} = \Gamma_1 + 2\Gamma_5 = 0$ that we rewrite, defining $\tilde{c} = \bar{c}/c > 0$:

$$\begin{gathered} F_{\mathbf{0}} = -2\tilde{c}F_{\mathbf{3}} + F_{\mathbf{1}}(f_1 + 2\tilde{c}f_5)/f_3 = f_1 F^{+}_{\mathbf{1},\mathbf{3}}/f^{+}_{3,5} \\ [2\tilde{c}f^{+}_{3,5} + f_1][F_{\mathbf{3}}f_3 - F_{\mathbf{1}}f_5] = 0 \end{gathered} \tag{3.5}$$

If the first factor vanishes then, due to positivity, $f_1 = f_3 = f_5 = 0$ leading to $\Gamma_1 = \Gamma_5 = 0$. If the second factor vanishes then $\Gamma_5 = 0$, leading to $\Gamma_1 = 0$. In both cases all collision terms vanish at equilibrium.

4. ONE-DIMENSIONAL SOLUTIONS ALONG THE *x*-AXIS

For solutions depending on just time t and the space coordinate x we have the obvious symmetry with respect to the x-axis, just 7 unknown densities with the (3.1)-(3.2) conditions and the following equations hold:

$$l_1 = 2\Lambda_1 + 2\Gamma_2, \qquad l_2 = -2\Lambda_1 + 2\Gamma_1, \qquad l_3 = -\Lambda_1 - \Gamma_1, \qquad l_4 = \Lambda_1 - \Gamma_2$$

$$L_{\mathbf{0}} = -2\Gamma_1 - 2\Gamma_2, \qquad L_{\mathbf{1}} = \Gamma_1, \qquad L_{\mathbf{2}} = \Gamma_2 \tag{4.1}$$

As a consequence, we have just 7 equations to solve. There are now 4 conservation equations because the momentum conservation equation along the y-axis is trivially satisfied. They are:

$$\begin{aligned} l^+_{1,2} + 2l^+_{3,4} = 0, \qquad L_{\mathbf{0}} + 2L^+_{\mathbf{1},\mathbf{2}} = 0 \\ L^+_{\mathbf{1},\mathbf{2}} + l^+_{3,4} = 0, \qquad 2L^-_{\mathbf{1},\mathbf{2}} + l_1 + 2l_3 = 0 \end{aligned} \tag{4.2}$$

or suitable linear combinations of them.

For a parametric representation of equilibria we introduce as a first parameter λ the ratio between f_2 and f_1 and as a second σ the ratio between f_3 and f_1. From the vanishing of the collision terms $\Lambda_1, \Gamma_1, \Gamma_2$ we can assign arbitrarily f_1 and F_0, as well as the two parameters λ and σ, to obtain:

$$f_2 = \lambda f_1, \qquad f_3 = \sigma f_1, \qquad f_4 = \lambda\sigma f_1, \qquad F_{\mathbf{1}} = (\sigma/\lambda)\, F_{\mathbf{0}}, \qquad F_{\mathbf{2}} = \lambda\sigma F_{\mathbf{0}} \tag{4.3}$$

5. THE RANKINE–HUGONIOT CONDITIONS

For a shock-like solution to exist, the upstream and downstream values must satisfy the conditions which arise from the conservation equations, which are known as the Rankine–Hugoniot conditions in both the theory of continuous media and the theory of shock wave structure in the kinetic theory of gases with a continuous set of velocities. Here something similar must occur, with an important difference. Usually one chooses a reference system in which the shock is steady. This is not possible, in general, for a discrete velocity gas, because Galilei invariance does not hold and the kinetic equations hold in a preferred reference frame.

Thus we look for solutions which depend on $z = x - \xi t$, where ξ is a parameter having the physical meaning of the speed of propagation of the shock. We denote by q_i ($q_{\mathbf{i}}$, respectively) the relative velocity $v_i - \xi$ ($v_{\mathbf{i}} - \xi$, respectively), where v_i ($v_{\mathbf{i}}$, respectively) is now the component of the ith (**i**th, respectively) molecular velocity along the x-axis. The conservation equations then give, if we denote the upstream and downstream values of f_i and $F_{\mathbf{i}}$ by a_i, $A_{\mathbf{i}}$ and c_i, $C_{\mathbf{i}}$, respectively:

$$\begin{aligned} q_1 a_1 + q_2 a_2 + 2q_3 a_3 + 2q_4 a_4 = q_1 c_1 + q_2 c_2 + 2q_3 c_3 + 2q_4 c_4 = K_1 \\ q_{\mathbf{0}} A_{\mathbf{0}} + 2q_{\mathbf{1}} A_{\mathbf{1}} + 2q_{\mathbf{2}} A_{\mathbf{2}} = q_{\mathbf{0}} C_{\mathbf{0}} + 2q_{\mathbf{1}} C_{\mathbf{1}} + 2q_{\mathbf{2}} C_{\mathbf{2}} = K_2 \\ q_{\mathbf{1}} A_{\mathbf{1}} + q_{\mathbf{2}} A_{\mathbf{2}} + q_3 a_3 + q_4 a_4 = q_{\mathbf{1}} C_{\mathbf{1}} + q_{\mathbf{2}} C_{\mathbf{2}} + q_3 c_3 + q_4 c_4 = K_3 \\ 2q_{\mathbf{1}} A_{\mathbf{1}} - 2q_{\mathbf{2}} A_{\mathbf{2}} + q_1 a_1 + 2q_3 a_3 = 2q_{\mathbf{1}} C_{\mathbf{1}} - 2q_{\mathbf{2}} C_{\mathbf{2}} + q_1 c_1 + 2q_3 c_3 = K_4 \end{aligned} \tag{5.1}$$

where K_k $(k = 1, 2, 3, 4)$ are four constants. We have found four relations which permit to relate the, upstream values of seven quantities to the downstream values of the same quantities. Since the upstream and the downstream values are equilibrium states, we can express both sets of values in terms of four parameters each, according to the relations found at the end of the previous section. Thus we can express, in principle, these parameters on one side in terms of the parameters on the other side, or, equivalently, in terms of the constants K_k. There is still a hidden parameter, ξ.

We introduce the differences $b_i = c_i - a_i$, $B_{\mathbf{i}} = C_{\mathbf{i}} - A_{\mathbf{i}}$, define $\xi_{\pm M} = \xi \pm 2/M$ and, with the explicit values of the discrete velocities, obtain:

$$\begin{aligned} \xi B_{\mathbf{0}} + 2(B_{\mathbf{1}} \xi_{+M} + B_{\mathbf{2}} \xi_{-M}) = (\xi - 1)(b_1 + 2b_3) + 2(B_{\mathbf{1}} \xi_{+M} - B_{\mathbf{2}} \xi_{-M}) = 0 \\ (\xi - 1)\, b_1 + (\xi + 1)\, b_2 + \xi B_{\mathbf{0}} = (\xi - 1)\, b_3 + (\xi + 1)\, b_4 - \xi B_{\mathbf{0}}/2 = 0 \end{aligned} \tag{5.2}$$

In Appendix 1 we first rewrite (5.2) in terms, of (A_j, a_i), (C_j, c_i), calling $\langle A \rangle$ and $\langle C \rangle$ the associate states. In Appendix 11, in agreement with the representation given at the end of Section 4 we rewrite the four relations in terms of ξ and $\langle A \rangle$: $\lambda_a, \sigma_a, a_1, A_0$, $\langle C \rangle$: $\lambda_c, \sigma_c, c_1, C_0$. We find two expressions for the ratio C_0/c_1 from which ξ is root of a polynomial with the asymptotic states parameters $\lambda_a, \sigma_a, \lambda_c, \sigma_c$. It is useful to check whether well known properties of the Rankine–Hugoniot polynomial for single gas can be extended to mixtures. A very important property is that $|\xi|$ is bounded, from positivity constraints, by the smallest modulus of the discrete v_i velocity along the x-axis. Here this means $|\xi| < 1$ and any exact or numerical solutions must satisfy this constraint.

In Appendix 12, for brevity, we restrict our study to a "homogeneous $\langle A \rangle$ state" with all a_i, A_j equal respectively to a_1, A_0 or equivalently $\lambda_a = \sigma_a = 1$. We first write explicitly the cubic ξ polynomial with M and $\lambda := \lambda_c$, $\sigma := \sigma_c$ as parameters. Second (proof given in Appendix 13, Theorem 2), we prove analytically the existence of this upper bound $|\xi| < 1$.

In Appendix 14, Theorem 3, always for a "homogeneous $\langle A \rangle$ state," we prove other constraints for ξ depending on the $\lambda > 1$, < 1, $\sigma > 1$, < 1 subdomains, for instance where ξ is necessarily positive or negative. Numerically, always with a "homogeneous" $\langle A \rangle$ state, we have also found, like for single gas models, intervals around 0 where ξ cannot be present. For $M = 2$ we find $19/23 \leqslant |\xi| < 1$ and we explain the origin of this lower bound.

6. THE STRUCTURE OF THE SHOCK WAVE

As is well known, the Rankine–Hugoniot conditions are not enough to solve the problem of shock structure and we must study the equations for the non-conserved quantities. Here we make an *ansatz* that turns out to be exact for the model under study, i.e., that the profile is given by a hyperbolic tangent, or, following the previous approach of one of the authors,[2, 3] that the shock structure is described by a function $F = F(z)$ such that:

$$dF/dz = \gamma F(F-1), \qquad F(z) = [1 + e^{\gamma z}]^{-1} \tag{6.1}$$

We assume F_i, f_i linear in F, substitute into three nonlinear equations:

$$\begin{gathered} f_i = a_i + b_i F(z), \qquad F_i = A_i + B_i F(z), \qquad L_j = \Gamma_j \\ j = 1, 2, \qquad l_1 + 2l_4 = 4\Lambda_1 \end{gathered} \tag{6.2}$$

use the equation satisfied by f_i, F_i and equate terms of zeroth, first and second degree in F. We obtain, after some simplification, three equations

$$\frac{\mathbf{B_0} b_3 - \mathbf{B_1} b_2}{-\xi_{-M} B_1} = \frac{\mathbf{B_0} b_4 - \mathbf{B_2} b_1}{-\xi_{+M} B_2} = \frac{\gamma}{c} = (4a/c)\,\frac{b_3 b_2 - b_4 b_1}{(-\xi + 1)\, b_1 - 2(\xi + 1)\, b_4} \tag{6.3}$$

containing the parameter γ (essentially the inverse of the shock thickness), with $\xi_{\pm M} = \xi \pm 2/M$ and 6 equations involving just the asymptotic states:

$$\begin{aligned} &\mathbf{A_0} a_3 - \mathbf{A_1} a_2 = 0, \qquad \mathbf{B_0} b_3 - \mathbf{B_1} b_2 + \mathbf{A_0} b_3 + \mathbf{B_0} a_3 - \mathbf{A_1} b_2 - \mathbf{B_1} a_2 = 0 \\ &\mathbf{A_0} a_4 - \mathbf{A_2} a_1 = 0, \qquad \mathbf{B_0} b_4 - \mathbf{B_2} b_1 + \mathbf{A_0} b_4 + \mathbf{B_0} a_4 - \mathbf{A_2} b_1 - \mathbf{B_2} a_1 = 0 \\ &a_3 a_2 - a_4 a_1 = 0, \qquad b_3 b_2 - b_4 b_1 + a_3 b_2 + a_2 b_3 - a_4 b_1 - a_1 a_4 = 0 \end{aligned} \tag{6.4}$$

The equations Eqs. (5.2), Eqs. (6.3) do not contain the unknowns $\mathbf{A_i}$, a_i.

This permits to find the values of the unknowns $B_{\mathbf{i}}$ and b_i ignoring Eqs. (6.4). If we let $B_{\mathbf{i}}=\psi_i B_{\mathbf{0}}$, $b_i=\eta_i B_{\mathbf{0}}$ and $\gamma=\bar{\lambda} c B_{\mathbf{0}}$, $B_{\mathbf{0}}$ factors throughout and remains as a free parameter. We rewrite the (5.2) relations:

$$\begin{aligned} \xi_{+M}\psi_2 &= \xi_{-M}\psi_1+\xi/2, \qquad (\xi+1)\,\eta_2=(1-\xi)\,\eta_1-\xi \\ (\xi+1)\,\eta_4 &= (1-\xi)\,\eta_3+\xi/2, \qquad \eta_1+2\eta_3=[4\psi_1\xi_{-M}+\xi]/(1-\xi) \end{aligned} \tag{6.5}$$

giving a first relation between η_1 and η_3 while another (see Eq. (A2.1) in Appendix 2) is obtained from the two first Eq. (6.3). From these 5 relations we obtain all η_i and ψ_2 as functions of ξ and ψ_1. From one of the remaining two relations Eq. (6.3) we determine γ itself, or $\bar{\lambda}=\gamma(cB_0)^{-1}$ while the last one becomes a compatibility between a, c, ξ, ψ_1. Physically, it is reasonable to assign a, c and one of the ξ, ψ_1; however, numerical evaluations are easier if we assign ξ, ψ_1 and one of a, c and deduce the other.

There remain three nonlinear algebraic equations containing $A_{\mathbf{i}}$, a_i and three relations involving in addition $B_{\mathbf{i}}$, b_i, which are known. If we let $A_{\mathbf{i}}=\overline{a_i}A_{\mathbf{0}}$, the $A_{\mathbf{i}}$ and a_i equations can be used to express $\overline{a_4}$ and the $A_{\mathbf{i}}$ in terms of $A_{\mathbf{0}}$ and of the remaining $\overline{a_i}$. The equations containing both types of constants can then be used to produce three different expressions of $B_{\mathbf{0}}/A_{\mathbf{0}}$.

A particular class of solutions is obtained by letting $\overline{a_1}=\eta_1$. Then $B_{\mathbf{0}}=-A_{\mathbf{0}}$ and $b_1=-a_1$. If we assume $\overline{a_2}\neq\eta_2$, then $b_3=-a_3$, $B_{\mathbf{1}}=-A_{\mathbf{1}}$ and $B_{\mathbf{2}}\neq -A_{\mathbf{2}}$, $b_2\neq -a_2$, $b_4\neq -a_4$. Otherwise $\overline{a_2}=\eta_2$, and $b_3\neq -a_3$, $B_{\mathbf{1}}\neq -A_{\mathbf{1}}$, $B_{\mathbf{2}}\neq -A_{\mathbf{2}}$, $b_2=-a_2$, $b_4\neq -a_4$.

If, on the other hand, we assume $\overline{a_1}\neq\eta_1$, then we are led to solving a cubic equation in $\overline{a_3}$, with coefficients depending on $\overline{a_1}$, η_1, η_2, η_3, η_4, ψ_1, ψ_2.

For any given set of values for the free parameters, we can solve for $\overline{a_3}$ and then compute $\overline{a_2}$ and the other quantities (see Appendix 2 and Appendix 3 for the characteristics). We retain only the solutions with non-negative asymptotic states: a_i, a_i+b_i and A_i, A_i+B_i. The monotonic densities $f_i(z)=a_i+b_iF(z)\in(a_i, a_i+b_i)$, $F_i=\cdots$ are positive for $z=x-\xi t\in(-\infty, +\infty)$ only if these constraints are satisfied. If only one is positive then f_i (or F_i) is positive, negative for some z intervals but this does not mean that for t fixed, for instance $t=0$, we have $f_i>0$ (or $F_i>0$) $\forall x$.

7. POSSIBLE OVERSHOOTS IN THE THERMAL ENERGIES

It is well-known that for a continuous velocity model, the thermal energy per unit mass E has a not so marked overshoot[6] but in a mixture the thermal energy E of the heavy gas can have a rather pronounced maximum.[7] Here we avoid using the term temperature, which cannot be given a clear and simple meaning outside an equilibrium state for a discrete velocity gas.[8]

In the case of a single gas, E is essentially the ratio between the pressure p and the mass density ρ. If W is the energy per unit volume and D the number of dimensions (2 in our case), we have:

$$2E = pD/\rho = 2W/\rho - (J/\rho)^2 \tag{7.1}$$

With the densities $f_i(z) = a_i + b_i F(z)$, written in (6.2), the mass $\rho(z)$, mass flow $J(z)$ and energy $W(z)$ are linear in the function F which satisfies the Riccati equation and is monotonic with z. We write ρ, J, W and the "a" and "c" asymptotic states: $\rho_a, \rho_c = \rho_a + \rho_b$, $J_a, J_c = J_a + J_b$. W_a, $W_c = W_a + W_b$:

$$\rho = \sum f_i = \sum a_i + F \sum b_i = \rho_a + F\rho_b$$

$$J = \sum \alpha_i f_i = \sum a_i \alpha_i + F \sum b_i \alpha_i = J_a + FJ_b$$

$$W = \sum e_i f_i = \sum a_i e_i + F \sum b_i e_i = W_a + FW_b$$

with α_i for the projection of the velocity along the x-axis and e_i for the energy. More generally let us assume "shock profiles" solutions with F monotonic and $F \in [0, 1]$. We denote by a prime all derivatives with respect to z: $E' = dE/dz$, ρ'. W', J', F', we shall have extrema (overshoots or undershoots) if and only if E' vanishes. We have:

$$\rho^3 E' = \rho(W'\rho - \rho' W - JJ') + J^2 \rho' = F'[\rho(\rho W_b - \rho_b W) + J(J\rho_b - \rho J_b)]$$

$$= F'[\rho(\rho_a W_b - \rho_b W_a) + J(J_a \rho_b - J_b \rho_a)]$$

$$\rho^3 E'/F' = Q_1 = \Lambda_a + F\Lambda_b, \qquad \Lambda_a = \rho_a(\rho_a W_c - \rho_c W_a) + J_a(\rho_c J_a - \rho_a J_c)$$

$$\Lambda_c = \Lambda_a + \Lambda_b = \rho_c(\rho_a W_c - \rho_c W_a) + J_c(\rho_c J_a - \rho_a J_c) \tag{7.2}$$

Theorem 4. E' can vanish (or not), E is monotonic (or not), depending on whether the asymptotic state values satisfy $\Lambda_a \Lambda_c \geqslant 0$ (or <0).

For the proof we notice that in (7.2), Q_1 is linear in F and F monotonic with $F \in (0.1)$. Λ_a, Λ_c depending only on the asymptotic states $\langle A \rangle$ and $\langle C \rangle$, we have a criterion[3] based only on the knowledge of the asymptotic states. For a monotonic behavior it is sufficient that one of the two Λ_a, Λ_c be zero. This was important to distinguish the models with a "homogeneous (densities associated to the same speed are equal) asymptotic state" or not. For instance for a "homogeneous" $\langle C \rangle$ state then $J_c = 0$ and $\Lambda_c/\rho_c = \rho_a W_c - \rho_c W_a$. For one speed models, like the Broadwell models, it is clear that the right hand side is zero, $\Lambda_c = 0$ and E is monotonic. The same property can occur for other models, like the $9v_i$, $15v_i \cdots$ models, and other more general models with assumptions[3] on the $\langle A \rangle$ state.

In the case of a mixture, things become a bit more complicated because it is the energy per particle, proportional to p/n (where n is the number density for the mixture) that one must consider in order to have a proper equivalent of what is called temperature in the continuous case. Then we consider:

$$2E = \frac{pD}{n} = 2\frac{W}{n} - \frac{J^2}{\rho n} \tag{7.3}$$

$$2\rho^2 n^2 E' = 2\rho^2 (W'n - Wn') + J(J\rho n' + J\rho' n - 2J'\rho n) \tag{7.4}$$

$$\begin{aligned} 2\rho^2 n^2 E'/F' &= 2\rho^2 (W_b n_a - W_a n_b) + (J_a + J_b F)[(J_a + J_b F)(\rho_a + \rho_b F)\, n_b \\ &\quad + (J_a + J_b F)\, \rho_b (n_a + n_b F) - 2J_b(\rho_a + \rho_b F)(n_a + n_b F)] \\ &= Q_2 = \tilde{A} F^2 + \tilde{B} F + \tilde{C} \end{aligned}$$

where $\tilde{A}$, $\tilde{B}$, $\tilde{C}$ still depend only on the asymptotic values:

$$\begin{aligned} \tilde{A} &= 2\rho_b^2 (W_b n_a - W_a n_b) - J_b^2 (\rho_b n_a + \rho_a n_b) + 2\rho_b n_b J_a J_b \\ \tilde{B} &= 4\rho_a \rho_b (W_b n_a - W_a n_b) - 2J_b^2 \rho_a n_a + 2J_a^2 \rho_b n_b \\ \tilde{C} &= 2\rho_a^2 (W_b na_{\_} W_a n_b) + J_a^2 (\rho_b n_a + \rho_a n_b) - 2\rho_a n_a J_a J_b \end{aligned} \tag{7.5}$$

In the case of a single gas we can identify n with ρ (apart from an inessential, constant factor) and the second degree polynomial factorizes into the product of ρ ($\neq 0$) and the previous first degree polynomial: $Q_2 = 2\rho Q_1$.

There are real roots for $Q_2(F)$ if, and only if, $\tilde{B}^2 \geqslant 4\tilde{A}\tilde{C}$.

Theorem 5. A sufficient condition for E' nonmonotonic or for a root between 0 and 1 is $\tilde{C}(\tilde{A} + \tilde{B} + \tilde{C}) < 0$. (Proof: still $F \in (0, 1)$ in Q_2, (7.5)) We can find more complete conditions. If $\tilde{C}(\tilde{A} + \tilde{B} + \tilde{C}) > 0$, there might be two real roots between 0 and 1; a necessary condition for this is $-2\tilde{A}^2 < \tilde{A}\tilde{B} < 0$, to which $\tilde{A}\tilde{C} > 0$ must be added to make it sufficient.

8. A 13v_i MODEL WHICH GENERALIZES THE 11v_i ONE FOR $M=5$

To the $11v_i$ model for $M=5$ we add (see Fig. 1) two light species f_7, f_8 with momenta 0, ± 1 and three collisions to the twelve (2.2):

$$\Lambda_4 = a(f_3 f_8 - f_5 f_7), \qquad \Lambda_5 = a(f_4 f_8 - f_6 f_7), \qquad \Lambda_6 = \tilde{a}(f_1 f_2 - f_7 f_8)$$

We still find only five linear relations which are physical conservation laws. We restrict our study to one-dimensional solutions with space coordinate x. With a new independent density $f_8 = f_7$, one $\Lambda_4 = \Lambda_5 = 0$, $\Lambda_6 \neq 0$, we write the changes in the linear and nonlinear equations:

$$l_7 = \Lambda_6 = \tilde{a}(f_1 f_2 - f_7^2), \qquad l_1 + 2l_4 + l_7 = 4\Lambda_1 \qquad l_1 = \cdots - \Lambda_6$$

$$l_2 = \cdots - \Lambda_6, \qquad l_1 + l_2 + 2(l_3 + l_4 + l_7) = 0$$

$$2(L_1 - L_2) + l_1 + 2l_3 + l_7 = 0$$

We still assume F_i, f_i linear in F and compatible different scalar Riccati equations (the same γ in (6.1)). In (6.3) the two first relations for γ/c are the same, the third is modified, we add a fourth one and two new ones in (6.4):

$$\frac{\gamma}{4a} = \frac{b_3 b_2 - b_4 b_1}{(-\xi + 1)\, b_1 - 2(\xi + 1)\, b_4 - \xi b_7}, \qquad \frac{\gamma}{\tilde{a}} = \frac{b_1 b_2 - b_7^2}{-\xi b_7}$$

$$a_1 a_2 - a_7^2 = 0, \qquad b_1 b_2 - b_7^2 - 2a_7 b_7 + a_1 b_2 + a_2 b_1 = 0$$

To the same $\gamma = \bar{\lambda} c B_0$, $B_i = \psi_i B_0$, $b_i = \eta_i B_0$ we add a new $b_7 = \eta_7 B_0$ and write down the two changes in (6.5):

$$(\xi + 1)\, \eta_2 + \xi(\eta_7 + 1) = (1 - \xi)\, \eta_1, \qquad \eta_1 + 2\eta_3 = \frac{4\psi_1(\xi - 0.4) + \xi(1 + \eta_7)}{1 - \xi} \tag{6'.5'}$$

In Appendix 4 we consider, for a, $\tilde{a}$, models where they are independent or other, like hard-spheres, where they are linked by $\tilde{a}\sqrt{5} = 2a$.

9. NUMERICAL CALCULATIONS

We exhibit now and discuss some plots of the thermal energies for the two species and for the mixture. We present shock waves in Figs. 2 for the $11v_i$ model with always the Lax criterion and the shock inequalities satisfied. As was said in Section 2 these $11v_i$ are physical for $M > 1$: integer, rational or non rational. Here in Figs. 2 we present shock waves for $M = 2$, 3, 5 and 10, but results have been obtained for other integer values (not reported because we have not found new features). Let us call $\xi_{\pm\infty}$ the characteristics associated to the asymptotic states at $\pm\infty$. For the Lax criterion we must satisfy $\xi_{+\infty} < \xi < \xi_{-\infty}$ ($\xi_{\pm\infty}$ with the same index among the characteristics associated to $\pm\infty$). If we define

$$v_{\pm\infty} = J_{\pm\infty}/\rho_{\pm\infty} - \xi, \qquad w_{\pm\infty} = J_{\pm\infty}/\rho_{\pm\infty} - \xi_{\pm\infty}$$

for the mixtures, we must verify $|v| > |w|$ (or $|v| < |w|$) at the upstream (downstream) state. We always find compressive shocks for the mixture (mass and pressure increasing from the upstream to the downstream states). For the three curves: mixture, heavy and light particles, we present examples with three, two, one or zero overshoots and the $F_i(z = 0)$, $f_i(z = 0)$ values. Is it true that, for the mixture, the internal energy E still always increases from the upstream to the downstream state?

We begin with the general solutions for the $11v_i$ model. In Fig. 2a for $M = 5$, the three curves E_l, E_h, E for the light, heavy species and the mixture have overshoots and they increase from the upstream to the downstream state. In Fig. 2b for $M = 5$, only the mixture and heavy species have overshoots but, contrary to the heavy species, the mixture (also the light species) decreases from the upstream to the downstream state. In Fig. 2c for $M = 3$, like in Fig. 2b we have overshoots for the mixture and heavy species, but here the three curves are dominant at the upstream state which means that E for the mixture decreases from the upstream to the downstream state. In Fig. 2d for $M = 10$, we find the most important overshoot for the heavy species and the three curves increase from they upstream to the downstream state. For the general solutions, we can, roughly speeking, say that the highest overshoot is always for the heavy species and that it increases with M.

We go on with the particular solutions $C_0 = C_1 = c_1 = c_3 = 0$ which in fact depend on only two parameters ξ, ψ_1 so that we can explore numerically all possibilities. We always find that the mixture increases from the upstream to the downstream state; nevertheless we find two different cases $M \neq 2$ and $M = 2$. For $M > 2$ we do not find overshoots for the mixture but the three curves are always dominant at the downstream state. In Fig. 2e $M = 5$ we present the three monotonic curves for one particular solution. For $M = 2$, in general we find the same features but there exist cases where we find overshoots for the mixture and the heavy species curve, contrary to the other two, is dominant upstream. In Fig. 2f we present such an example with very small overshoots for the mixture and light species curves.

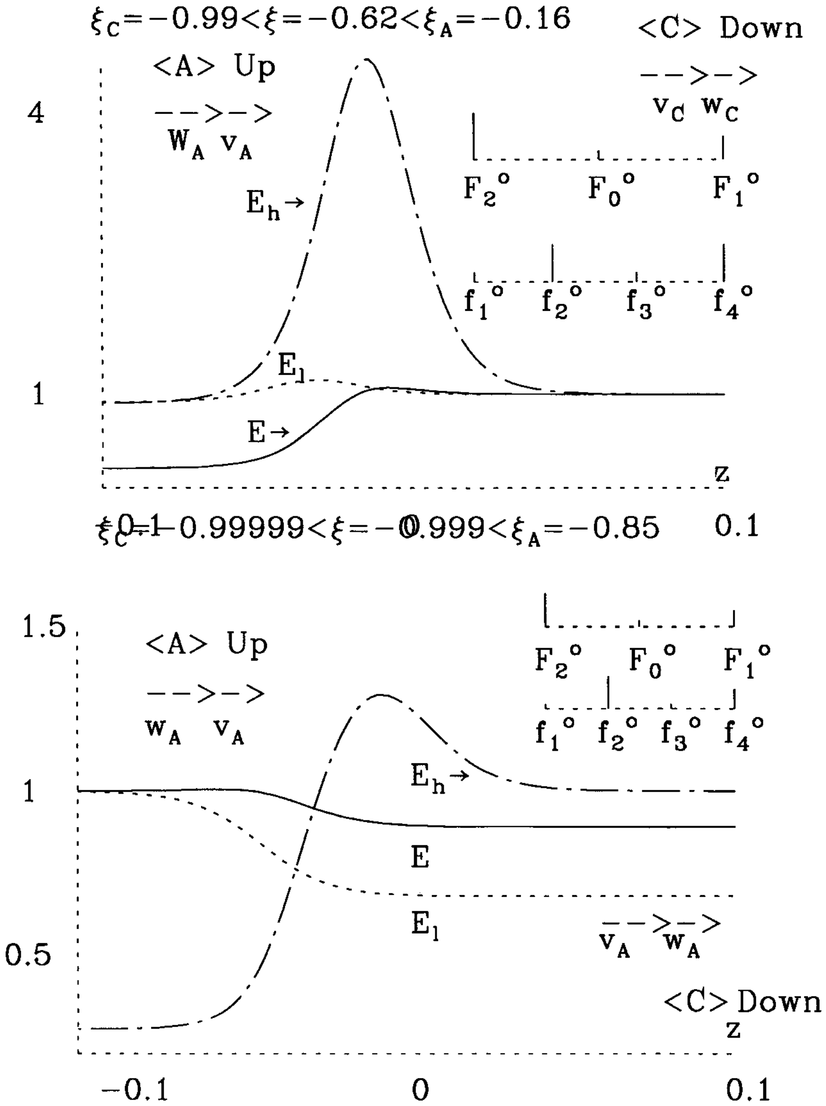

Fig. 2. (a) First 11vx, $M=5$ General Solution, the three curves E, E_l, E_h have overshoots. (b) Second 11vx, $M=5$ General Solution. Overshoots only for E, E_h and only E_h dominant at the downstream state. (c) Third 11vx, $M=3$ General Solution. Overshoots only for E, E_h with the three curves dominant at the upstream. (d) Fourth 11vx, $M=10$ General Solution. Very important overshoot for E and the three curves are dominant at the downstream. (e) 11vx, $M=5$ Particular Solution: $C_0=C_1=c_1=c_3=0$. The three curves are monotonic. (f) 11vx, $M=2$ Particular Solution $C_0=C_1=c_1=c_3=0$. Overshoot only for E. E_l, E are (contrary to to E_h) dominant at the downstream.

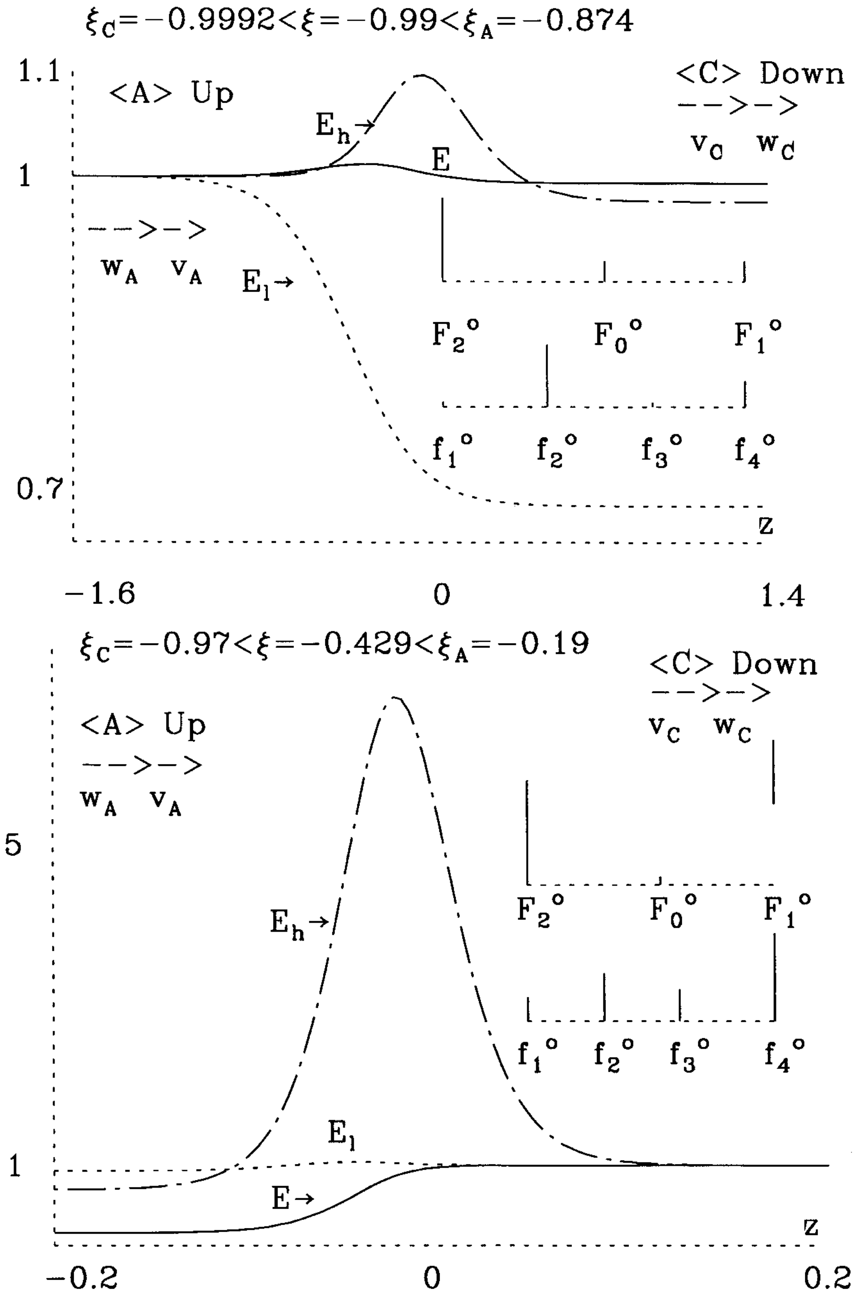

Fig. 2. (*Continued*)

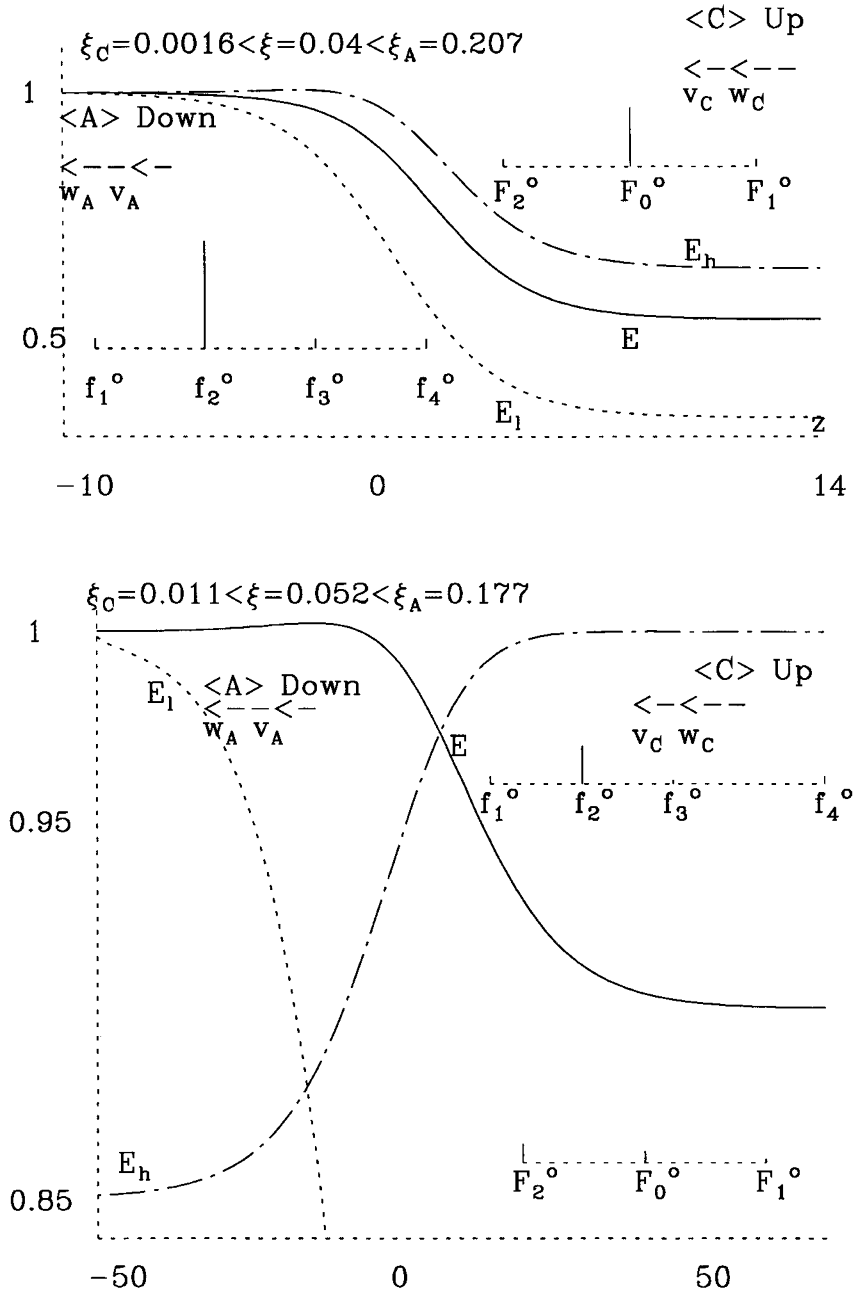

Fig. 2. (*Continued*)

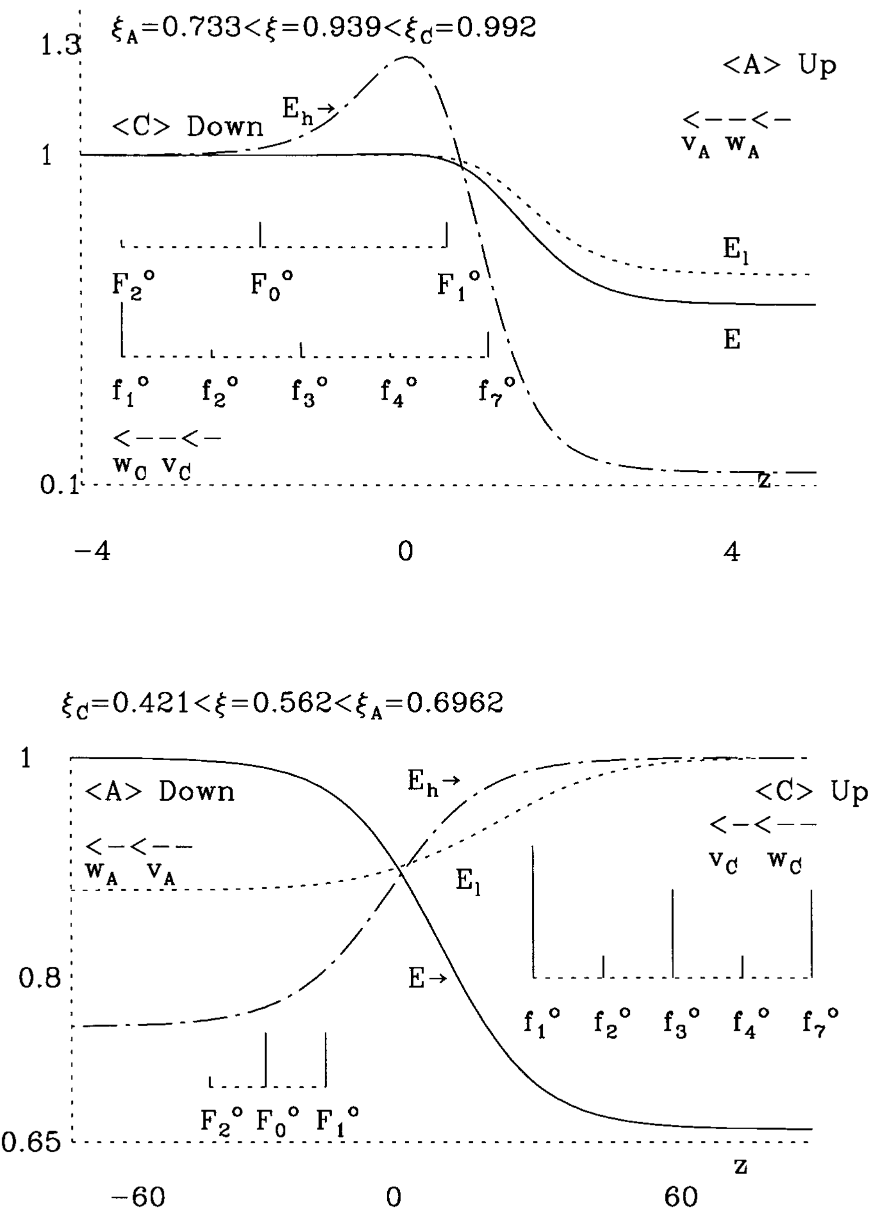

Fig. 3. (a) Fist 13vx, $M = 5$ General Solution with overshoots (small for E, E_l). (b) Second 13vx, $M = 5$ General Solution with hard-spheres. The three curves are monotonic with E_h, E_l (contrary to E) dominant at the upstream. (c) 13vx, $M = 5$ Particular Solution: $c_1 = c_3 = c_7 = C_0 = C_1 = 0$. The three curves are monotonic and dominant at the downstream.

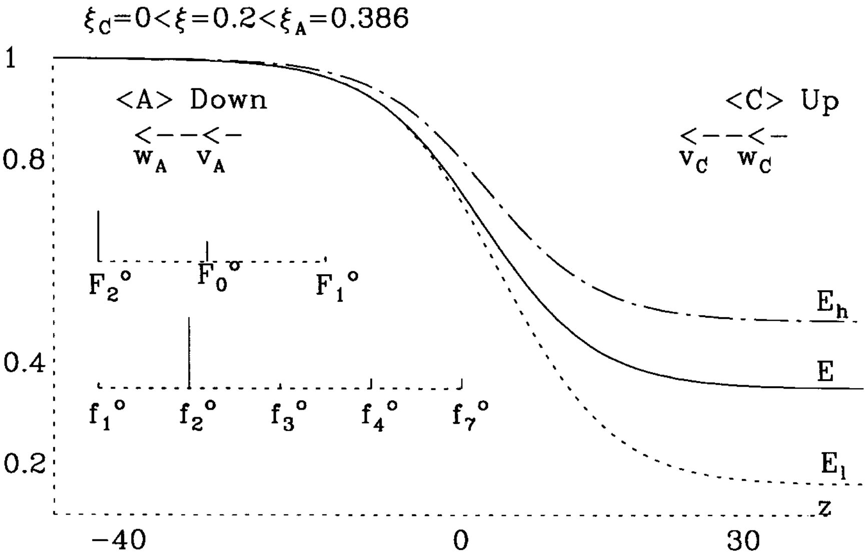

Fig. 3. (*Continued*)

Now we present for the $13v_i$, $M=5$ model three figures with the curves dominant downstream (except in Fig. 3b with light and heavy curves dominant upstream). In Fig. 3a the three curves have overshoots (very small for the light species and mixture), in Fig. 3b (hard-spheres) and Fig. 3c (a particular solution), they are monotonic.

Finally, for the solutions with a "homogeneous" $\langle A \rangle$ state ($A_i = A_0$, $a_i = a_1$), we present results for the $11v_i$ model with $M=5$ and $M=10$. For the thermal energy, we always find monotonic curves for the mixture, small overshoots for either the light species or both species.

APPENDIX 0. ONLY FIVE PHYSICAL CONSERVATION RELATIONS

Theorem 1. There are only 5 physical conservation laws for the $11v_i$ model. We define $\bar{\in} := (\in \text{ only in})$. In the following proofs for the 12 collision terms in l_i, L_i (2.2)–(2.3) we can retain only Γ_i, $i=1, 2, 3, 4, 6$, Λ_j, $j=1, 2$.

(1) $[l_i]$ set: First, $\Gamma_2 \bar{\in} l_1, l_4$ and is eliminated in $l_{1,4}$; $\Gamma_4 \bar{\in} l_{1,4}, l_6$ and disappears in $l_{1,4,6} = 2\Lambda^+_{1,2}$. Second, Γ_1 is eliminated in $l_{2,3}$ and Γ_3 in

$l_{2,3,5} = -2\Lambda^{+}_{1,2} = -l_{1,4,6}$ leading finally to the only light mass relation $\sum_1^6 l_i = \mathscr{M}_l = 0$.

(2) $[L_i]$ set: $\Gamma_1 \bar{\in} L_0$, L_1 is eliminated in $L_{0,1}$, Γ_2 in $L_{0,1,2}$ and Γ_3 in $L_{0,1,2,3} = -L_4$ leading to the only heavy mass relation $\sum_0^4 L_i = \mathscr{M}_h = 0$.

(3) set $[l_i, L_i]$ except L_0. First $\Gamma_1 \bar{\in} L_1, l_2, l_3$ and is eliminated in $X_1 = L_1 + l_3 + al_{2,3}$ with a arbitrary. Second $\Gamma_3 \bar{\in} X_1$, L_3, l_5 and is eliminated in $X_2 = L_1 + l_3 + a(l_{2,3} - L_3) + b(l_5 + L_3)$ with b arbitrary. Third, $\Gamma_6 \bar{\in} X_2$, L_2, L_4 and is eliminated in $X_3 = X_2 - (a+1-c-b) L_4 + cL_2$ with c arbitrary. Fourth, $\Gamma_2 \bar{\in} X_3$, l_3, l_4 and is eliminated in $X_4 = X_3 + cl_4 + dl_{3,4}$ with d arbitrary. Finally $\Gamma_4 \bar{\in} X_4$, l_6 and disappears in $X_5 = X_4 + l_6(c+b-1-a)$:

$$X_5 = L^{-}_{1,4} + l^{-}_{3,6} + a(l^{+}_{2,3} - l_6 - L^{+}_{3,4}) + c(L^{+}_{2,4} + l^{+}_{4,6}) + dl_{1,4,6} + b\mathscr{X}$$

$$\mathscr{X} = L^{+}_{3,4} + l^{+}_{5,6} = 0 \rightarrow X_5 = \Lambda^{+}_{1,2}(-1 - 2a + c + 2d)$$

With $c = 1 + 2a - 2d$ we rewrite $X_5 = \mathscr{Y} + a\mathscr{Z} - d(\mathscr{X} + \mathscr{Z} - \mathscr{M}_l) = 0$,

$$\mathscr{Y} = L^{+}_{1,2} + l^{+}_{3,4} = 0, \qquad \mathscr{Z} = L^{-}_{4,3} + 2L_2 + l_{2,3,4} + l^{+}_{4,6} = 0$$

$$\mathscr{Y} - \mathscr{Z} = (\mathscr{J}_x - \mathscr{M}_l)/2, \qquad \mathscr{Y} - \mathscr{X} = \mathscr{J}_y, \qquad \mathscr{Y} + \mathscr{X} = (2\mathscr{E} - \mathscr{M}_l)(M-1)/4$$

and see that $\mathscr{X}$, $\mathscr{Y}$, $\mathscr{Z}$ are linear combinations of $\mathscr{E}$, $\mathscr{M}_l$, $\mathscr{J}_x$, $\mathscr{J}_y$.

APPENDIX 1. A DISCUSSION OF THE RANKINE–HUGONIOT CONDITIONS

A11. We define $\xi_{\pm M} = \xi \pm 2/M$ and the conservation equations can be written in terms of $\langle A \rangle$: $(\lambda_a, \sigma_a, a_1, A_{\mathbf{0}})$, $\langle C \rangle$: $(\lambda_c, \sigma_c, c_1, C_{\mathbf{0}})$:

$$\begin{aligned}
&A_{\mathbf{0}}[\xi + 2\xi_{-M}\sigma_a\lambda_a^{-1} + 2\xi_{+M}\lambda_a\sigma_a] \\
&\quad = C_{\mathbf{0}}[\xi + 2\xi_{-M}\sigma_c\lambda_c^{-1} + 2\xi_{+M}\lambda_c\sigma_c] \\
&\xi A_{\mathbf{0}} + (\xi - 1)\, a_1 + (\xi + 1)\, \lambda_a a_1 \\
&\quad = \xi C_{\mathbf{0}} + (\xi - 1)\, c_1 + (\xi + 1)\, \lambda_c c_1 \\
&(\xi - 1)\, \sigma_a a_1 + (\xi + 1)\, \lambda_a \sigma_a a_1 - \xi A_{\mathbf{0}}/2 \\
&\quad = (\xi - 1)\, \sigma_c c_1 + (\xi + 1)\, \lambda_c \sigma_c c_1 - \xi C_{\mathbf{0}}/2 \\
&2\xi_{-M}\sigma_a\lambda_a^{-1} A_{\mathbf{0}} - 2\xi_{-M}\lambda_a\sigma A_{\mathbf{0}} + (\xi - 1)\, a_1(2\sigma_a + 1) \\
&\quad = 2\xi_{-M}\sigma_c\lambda_c^{-1} C_{\mathbf{0}} - 2\xi_{+M}\lambda_c\sigma_c C_{\mathbf{0}} + (\xi - 1)\, c_1(2\sigma_c + 1)
\end{aligned} \tag{A1.1}$$

The first equation and a suitable combination of the next two give

$$R := \frac{A_0}{C_0} = \frac{\xi + 2\xi_{-M}\sigma_c\lambda_c^{-1} + 2\xi_{+M}\lambda_c\sigma_c}{\xi + 2\xi_{-M}\sigma_a\lambda_a^{-1} + 2\xi_{+M}\lambda_a\sigma_a} \tag{A1.2}$$

$$r := \frac{a_1}{c_1} = \frac{(2\sigma_c + 1)[(\xi - 1) + (\xi + 1)\,\lambda_c]}{(2\sigma_a + 1)[(\xi - 1) + (\xi + 1)\,\lambda_a]} \tag{A1.3}$$

With R, r defined in (A1.3) we get from the first and fourth (A1.2):

$$\frac{C_0}{c_1} = \frac{(\xi - 1)(1 - r) + (\xi + 1)(\lambda_c - \lambda_a r)}{\xi(R - 1)}$$
$$\frac{C_0}{c_1} = \frac{(\xi - 1)[2(\sigma_c - \sigma_a r) + (1 - r)]}{(R\sigma_a\lambda_a^{-1} - \sigma_c\lambda_c^{-1})\,2\xi_{-M} - 2\xi_{+M}(R\lambda_a\sigma_a - \lambda_c\sigma_c)} \tag{A1.4}$$

A12. We assume $\langle A \rangle$ homogeneous: $\lambda_a = \sigma_a = 1$, define $\lambda = \lambda_c > 0$, $\sigma = \sigma_c > 0$ and rewrite both $R > 0$, $r > 0$ and the two $C_0/c_1 > 0$:

$$R = \frac{\xi[1 + 2\sigma(\lambda + 1/\lambda)] + (4/M)\,\sigma(\lambda - 1/\lambda)}{5\xi}, \qquad r = (2\sigma + 1)\,\frac{\xi(\lambda + 1) + \lambda - 1}{6\xi}$$

$$\alpha_{\pm} = (1 - \sigma)(\lambda \pm 1)/3, \qquad \alpha = (2/M)\,\sigma(\lambda - 1/\lambda), \qquad \beta = -2 + \sigma(\lambda + 1/\lambda)$$

$$\delta_2 = 5M\alpha/2, \qquad \delta_1 = 2\beta/M, \qquad \delta_0 = -(8/M)\,\alpha, \qquad \gamma = (2\sigma + 1)(1 - \lambda)/2$$

$$Y(\xi) = \delta_2\xi^2 + \delta_1\xi + \delta_0 = (2/M)\,X(\xi) + \alpha 5M\xi_{-M}\xi_{+M}/2 \tag{A1.5}$$

$$X(\xi) = \xi\beta + \alpha, \qquad C_0/c_1 = 5\,\frac{(\xi\alpha_+ + \alpha_-)}{X(\xi)}, \qquad C_0/c_1 = 5\,\frac{(\xi^2 - 1)\,\gamma}{2\,Y(\xi)} \tag{A1.6}$$

We deduce a cubic polynomial $\sum_{i=0}^{3} X_i\xi^i = 0$ with $X_3 = 2\delta_2\alpha_+ - \beta\gamma$ and $X_0 = 2\delta_0\alpha_- + \alpha\gamma$, $X_1 = 2\delta_1\alpha_+ + 2\delta_0\alpha_+ + \gamma\beta$, $X_2 = 2\delta_2\alpha_- + 2\delta_1\alpha_+ - \gamma\alpha$. We define $\mathscr{C}$, $\mathscr{CC}$ as the signs of the first and second C_0/c_1 (A1.6) expressions which must be positive and for any Z quantity we write "Z" for the sign. For instance "$\lambda - 1$" = "α," "$\xi(\lambda + 1) + \lambda - 1$" = "$\xi$" from $r > 0$,

$$\mathscr{C} = \text{“}\xi(1 - \sigma)\,X(\xi)\text{,”} \qquad \mathscr{CC} = \text{“}(\xi^2 - 1)(1 - \lambda)\;Y(\xi)\text{”} \tag{A1.7}$$

A.13. Theorem 2. For $M \geqslant 2$ and a "homogeneous" state $\lambda_a = \sigma_a = 1$, then $|\xi| > 1$ violates positivity. For the proofs we have eight different cases:

First: (1), (2) $\lambda \lessgtr 1$, $\sigma \gtrless 1$, $\xi > 1 \rightarrow \alpha \lessgtr 0$, $\mathscr{C} = -\mp$"$X(\xi)$" $\rightarrow X(\xi) \lessgtr 0$, (A1.5) gives $Y(\xi) \lessgtr 0 \rightarrow \mathscr{CC} = \pm$"$Y$" < 0. (3), (4) $\lambda \gtrless 1$, $\sigma \gtrless 1$, $\xi < -1 \rightarrow \alpha \gtrless 0$, $\mathscr{C} = \pm$"$X(\xi)$" $\rightarrow X \gtrless 0$, (A.15) gives $Y(\xi) \gtrless 0 \rightarrow \mathscr{CC} = \mp$"$Y$" < 0.

Second with Lemma 1: If $\sigma > 1$ then $\beta > 0$. Proof: $\lambda > 0 \to \lambda + 1/\lambda > 2 \to \beta = -2 + \sigma(\lambda + 1/\lambda) > 2(\sigma - 1) > 0$. (5), (6): $\lambda \gtrless 1$, $\sigma > 1$, $\xi > 1$, < -1, $\to \alpha \gtrless 0$, $\beta > 0 \to X(\xi) \gtrless 0$. But $\mathscr{C} = \mp$"$X(\xi)$"< 0.

Third: (7), (8) $\lambda \gtrless 1$, $\sigma < 1$, $\xi = \mp(1+\eta)$, $\eta \geqslant 0 \to \alpha \gtrless 0$ and $\mathscr{C}\mathscr{C} = \mp$"$Y(\xi)$"$\to Y(\xi) \lessgtr 0$. This contradicts the following Lemmas 2–3:

Lemma 2: With (7), then $Y(-1) > 0$ and $Y(-1-\eta) > 0$.

Proof: $MY(-1)/2 = 2(1-\sigma/\lambda) + \sigma(\lambda - 1/\lambda)(M-2)(5/2 + 4/M) > 0$, $Y(\xi) = Y(-1) + (2\eta/M)[2(1-\sigma/\lambda) + \sigma(\lambda - 1/\lambda)(-1 + 5M(1+\eta/2)] > 0$.

Lemma 3: With (8), then $Y(1) < 0$, $Y(1+\eta) < 0$:

Proof: $MY(1)/2 = 2(\sigma - 1) + \sigma(1/\lambda - \lambda)(2-M)(5/2 + 4/M) < 0$, $Y(\xi) = Y(1) + (2\eta/M)[2(\sigma\lambda - 1) + \sigma(\lambda - 1/\lambda)(5M-1)] + 5\alpha M\eta^2/2 < 0$.

A.14. Theorem 3. For $M = 2$, $\langle A \rangle$ "homogeneous," $|\xi| < 1$ and (1), (2): $\lambda \lessgtr 1$, $\sigma \gtrless 1$, $\xi < 0$, (3), (4): $\lambda \gtrless 1$, $\sigma \gtrless 1$, $\xi > 0$, then positivity is violated.

Proofs: (1), (2): $\mathscr{C}\mathscr{C} = \mp$"$Y$", $Y \lessgtr 0$, $\mathscr{C} = \pm X$, $X \gtrless 0$, $\alpha \lessgtr 0$ and (A.1.5) $\to Y \gtrless 0$. (3), (4): $\mathscr{C}\mathscr{C} = \pm$"$Y$", $Y \gtrless 0$, $\mathscr{C} = \mp X$, $X \lessgtr 0$, $\alpha \lessgtr 0$ and (A.1.5) $\to Y \lessgtr 0$.

Numerically, from the cubic ξ polynomial and $M = 2$, we have found $19/23 \leqslant |\xi| < 1$ and we give the origin of the lower bound:

$$\lim_{\lambda \to \infty,\, 0 < \sigma < 1} \frac{C_{\mathbf{0}}}{c_1} = \frac{5(1-\sigma)}{3\sigma} = \frac{5(2\sigma+1)(1-\xi)}{4\sigma(5\xi - 4)} \to \xi = \frac{19 - 10\sigma}{23 - 14\sigma} \geqslant 19/23$$

$$\lim_{\lambda \to 0,\, 0 < \sigma < 1} \frac{C_{\mathbf{0}}}{c_1} = \frac{5(1-\sigma)}{3\sigma} = \frac{5(2\sigma+1)(1+\xi)}{4\sigma(5\xi + 4)} \to \xi = \frac{10\sigma - 19}{23 - 14\sigma} \leqslant -19/23$$

APPENDIX 2. EXACT SOLUTIONS FOR THE 11v_i MODEL

We complete the discussion of the shock structure with $\xi_{\pm M} = \xi \pm 2/M$, $B_{\mathbf{i}} = \psi_i B_{\mathbf{0}}$, $b_i = \eta_i B_{\mathbf{0}}$, $\gamma = \lambda c B_{\mathbf{0}}$, where $B_{\mathbf{0}}$, ψ_1 and ξ are parameters. Equation (6.5) gives both ψ_2, η_2 and η_4 in terms of η_1, η_3, ψ_1 ξ and a first η_1, η_3 linear relation while the first two Eq. (6.3) equations gives a second:

$$\eta_1 \left[\frac{1}{\xi_{+M}} - \frac{1-\xi}{\xi_{-M}(1+\xi)} \right] + \eta_3 \left[\frac{1}{\psi_1 \xi_{-M}} - \frac{1-\xi}{\xi_{+M}(1+\xi)} \right]$$
$$= \frac{\xi}{1+\xi} \left[\frac{1}{\xi + 2\psi_1 \xi_{-M}} - \frac{1}{\xi_{-M}} \right] \tag{A2.1}$$

Thus η_1 and η_3, and, as a consequence, η_2 and η_4 and ψ_2 are determined. One of the two (6.3) relations containing γ can be used to determine γ or $\bar{\lambda}$:

$$\bar{\lambda} = \gamma(cB_0)^{-1} = (\psi_1\eta_2 - \eta_3)/\psi_1\xi_{-M} = (\psi_2\eta_1 - \eta_4)/\psi_2\xi_{+M} \quad \text{(A2.2)}$$

There is still a compatibility relation between a, c, ξ, ψ_1:

$$4a/\bar{\lambda}c = [(1-\xi)\,\eta_1 - 2(1+\xi)\,\eta_4]/(\eta_3\eta_2 - \eta_1\eta_4) \quad \text{(A2.3)}$$

We define $a_{\mathbf{i}} = \overline{a_i}A_{\mathbf{0}}$, then the $A_{\mathbf{i}}$, a_i equations give $\overline{a_4}$ and the $A_{\mathbf{i}}$ in terms of $A_{\mathbf{0}}$, $\bar{a}_{i\neq 4}$ while the $A_{\mathbf{i}}$, a_i, $B_{\mathbf{i}}$, b_i equations give three $B_{\mathbf{0}}/A_{\mathbf{0}}$ expressions.

$$\frac{\bar{a}_3\eta_2/\bar{a}_2 + \psi_1\bar{a}_2 - \eta_3 - \bar{a}_3}{\eta_3 - \psi_1\eta_2} = \frac{\bar{a}_2\bar{a}_3(\eta_1 - a_1)/\bar{a}_1^2 + \psi_2\bar{a}_1 - \eta_4}{\eta_4 - \psi_2\eta_1}$$
$$= \frac{\bar{a}_2\bar{a}_3\eta_1/\bar{a}_1 + \bar{a}_1\eta_4 - \bar{a}_3\eta_2 - \bar{a}_2\eta_3}{\eta_3\eta_2 - \eta_1\eta_4} = B_0/A_0 \quad \text{(A2.4)}$$

We assume $\overline{a_1} \neq \eta_1$ ($\overline{a_1} = \eta_1$ discussed in the main text) leading to a cubic equation $\sum_{i=0}^{3} \overline{A_i}\,\overline{a_3}^{\,i} = 0$. From $\bar{a}_1$, $\bar{a}_3$, A_0 known we get all A_i, a_i, B_i, b_i. We write (A2.4) for a "homogeneous" $\langle A \rangle$ state $A_i = A_0$, $a_i = a_1$,

$$\frac{\eta_2 - \eta_3 + (a_1/A_0)(\psi_1 - 1)}{\eta_3 - \psi_1\eta_2}$$
$$= \frac{(\eta_1 - \eta_4) + (a_1/A_0)(\psi_2 - 1)}{\eta_4 - \psi_2\eta_1}$$
$$= (a_1/A_0)(\eta_1 + \eta_4 - \eta_2 - \eta_3)/(\eta_3\eta_2 - \eta_1\eta_4) = B_0/A_0 \quad \text{(A2.5)}$$

deduce a_1/A_0, B_0/A_0 and a compatibility condition between ξ and ψ_1. Assuming A_0 as given, we deduce a_1, B_0 and all parameters are known.

APPENDIX 3. THE IDEAL FLUID LIMIT

An interesting problem is the investigation of the ideal fluid limit for our model. This is given by the conservation equation in which the densities are local equilibrium states. We introduce $f_1 = \mu$ and $F_0 = v$ and deduce:

$$f_2 = \lambda\mu, \qquad f_3 = \sigma\mu, \qquad f_4 = \lambda\sigma\mu, \qquad F_{\mathbf{1}} = \sigma\lambda^{-1}v, \qquad F_{\mathbf{2}} = \lambda\sigma v \quad \text{(A3.1)}$$

with λ, μ, v, σ functions of x, t. We write the conservation equations:

$$\partial_t(v+2\sigma\lambda^{-1}v+2\lambda\sigma v)+\frac{4}{M}\partial_x(\sigma\lambda^{-1}v-\lambda\sigma v)=0$$

$$\partial_t(v+\mu+\lambda\mu)+\partial_x(\mu-\lambda\mu)=0, \qquad \partial_t\left(\sigma\mu+\partial\sigma\mu-\frac{v}{2}\right)+\partial_x(\sigma\mu-\lambda\sigma\mu)=0$$

$$\partial_t[2(\sigma\lambda^{-1}v-\lambda\sigma v+\sigma\mu)+\mu]+\partial_x\left[\frac{4}{M}(\sigma\lambda^{-1}v+\lambda\sigma v)+2\sigma\mu+\mu\right]=0 \tag{A3.2}$$

For these equations the shock wave solutions are generalized (or weak) solutions with discontinuities. Other disturbances travel along the characteristic lines and involve at most discontinuities in the first order derivatives.

For the characteristic velocities, we first differentiate the various terms in the above equations, define $\lambda_\pm:=\lambda^{-1}\pm\lambda$ and obtain:

$$\begin{gathered}
(1+2\lambda^{-1}\sigma+2\lambda\sigma)\,\partial_t v+2\lambda_+ v\partial_t\sigma-2v\sigma(\lambda^{-2}-1)\,\partial_t\lambda \\
+\frac{4}{M}\lambda_-(\sigma\partial_x v+v\partial_x\sigma]-\frac{4}{M}v\sigma(\lambda^{-2}+1)\,\partial_x\lambda=0 \\
\partial_t v+(1+\lambda)\,\partial_t\mu+\mu\partial_t\lambda+(1-\lambda)\,\partial_x\mu-\mu\partial_x\lambda=0 \\
(1+\lambda)[\mu\partial_t\sigma+\sigma\partial_t\mu]+\sigma\mu\partial_t\lambda-\frac{1}{2}\partial_t v+(1-\lambda)[\sigma\partial_x\mu+\mu\partial_x\sigma]-\mu\sigma\partial_x\lambda=0 \\
2\sigma\lambda_-\partial_t v+[2\lambda_- v+\mu]\,\partial_t\sigma-2v\sigma(\lambda^{-2}+1)\,\partial_t\lambda+(1+2\sigma)\,\partial_t\mu+(4/M) \\
\times[(\lambda_+ v+2\mu)\,\partial_x\sigma+\lambda_+\sigma\partial_x v-v\sigma(\lambda^{-2}-1)\,\partial_x\lambda]+(1+2\sigma)\,\partial_x\mu=0
\end{gathered} \tag{A3.3}$$

For a travelling wave with $z=x-\xi t$, we obtain a homogeneous system for the derivatives $\partial_z v$, $\partial_z\mu$, $\partial_z\lambda$, $\partial_z\sigma$ with vanishing determinant.

Another method is to linearize about the $\langle A\rangle$ state, $F_i\simeq A_i+X_i$, $f_i\simeq a_i+x_i$, leading to a quartic polynomial for the characteristics

$$0=\begin{vmatrix}
-\xi/2 & -\xi_{-M} & -\xi_{+M} & 0 & 0 & 0 & 0 \\
-\xi & 0 & 0 & -\xi+1 & -\xi-1 & 0 & 0 \\
\xi/2 & 0 & 0 & 0 & 0 & -\xi+1 & -\xi-1 \\
0 & -2\xi_{-M} & 2\xi_{+M} & -\xi+1 & 0 & -2\xi+2 & 0 \\
-a_3 & a_2 & 0 & 0 & A_1 & -A_0 & 0 \\
-a_4 & 0 & a_1 & A_2 & 0 & 0 & -A_0 \\
0 & 0 & 0 & a_4 & -a_3 & -a_2 & a_1
\end{vmatrix}$$

The characteristics for the class with only $c_2 \neq 0$, $c_4 \neq 0$, $C_2 \neq 0$ at the $\langle C \rangle$ state are: $\xi = \xi_{\langle C \rangle} = -1, -1, -2/M, \xi_+ = [c_2 c_4 + c_4^2]/[C_2 c_2 + c_2 c_4 + 2c_4^2]$.

APPENDIX 4. EXACT SOLUTIONS FOR THE $13v_i$ MODEL

Firstly, from the first and last (6.5), the two (6′.5′) and (A2.2) relations we have a linear system for η_i, $i = 1, 2, 3, 4$ with ψ_1, η_7, ξ as parameters. From, (A2.4), the three A_0/B_0 with $\bar{a}_1$ arbitrary, give a cubic $\bar{a}_3$ polynomial, then $\bar{a}_2$ and B_0 from A_0 given. It remains $\bar{a}_7$ deduced from another B_0/A_0; η_7 from a compatibility condition $\bar{a}_7^2 = \bar{a}_1 \bar{a}_2$ and a, $\tilde{a}$:

$$B_0/A_0 = [2\bar{a}_7\eta_7 - \bar{a}_1\eta_2 - \bar{a}_2\eta_1]/[\eta_1\eta_2 - \eta_7^2] \qquad \text{(A4.1)}$$

$$\frac{4a}{\bar{\lambda}c} = \frac{(1-\xi)\,\eta_1 - 2(1+\xi)\,\eta_4 - \xi\eta_7}{\eta_3\eta_2 - \eta_1\eta_4}, \qquad \frac{\tilde{a}}{\bar{\lambda}c} = \frac{\xi\eta_7}{\eta_7^2 - \eta_1\eta_2} \qquad \text{(A4.2)}$$

Secondly for hard-spheres $2a = \tilde{a}\sqrt{5}$, (A4.1) gives a new η_i relation:

$$(\eta_7^2 - \eta_1\eta_2)[\eta_1(1-\xi) - 2\eta_4(1+\xi) - \eta_7\xi] = 2\sqrt{5}\,\eta_7\xi[\eta_3\eta_2 - \eta_1\eta_4] \qquad \text{(A4.3)}$$

leading (with the four above linear η_i relations) to a cubic η_7 polynomial, still one compatibility condition $\bar{a}_7^2 = \bar{a}_1\bar{a}_2$ and (A4.3) giving either a or $\tilde{a}$.

Thirdly for the particular solutions with $\bar{a}_1 = \eta_1$, $A_0/B_0 = -1$ we get two classes: (i): $\bar{a}_2 = \eta_2$, $\bar{a}_7 = \eta_7$, $c_1 = c_2 = c_7 = C_0 = 0$; (ii): $\bar{a}_3 = \eta_3$, $\bar{a}_7 = \eta_7$, $\psi_1 = \bar{a}_3/\bar{a}_2 = A_1/A_0$, $c_1 = c_3 = c_7 = C_0 = C_1 = 0$ with characteristic values at the $\langle C \rangle$ state: $\xi_{\langle C \rangle}$: $-1, -1, -2/5, 0$.

Finally we write the general quartic polynomial for the characteristics.

$$0 = \begin{vmatrix}
-\xi/2 & -\xi+0.4 & -\xi-0.4 & 0 & 0 & 0 & 0 & 0 \\
-\xi & 0 & 0 & -\xi+1 & -\xi-1 & 0 & 0 & -2\xi \\
\xi/2 & 0 & 0 & 0 & 0 & -\xi+1 & -\xi-1 & \\
0 & -2\xi+0.8 & 2\xi+0.8 & -\xi+1 & 0 & -2\xi+2 & 0 & -\xi \\
-a_3 & a_2 & 0 & 0 & A_1 & -A_0 & 0 & 0 \\
-a_4 & 0 & a_1 & A_2 & 0 & 0 & -A_0 & 0 \\
0 & 0 & 0 & a_4 & -a_3 & -a_2 & a_1 & 0 \\
0 & 0 & 0 & a_2 & -a_1 & 0 & 0 & 2a_7
\end{vmatrix}$$

REFERENCES

1. A. V. Bobylev and C. Cercignani, Discrete velocity models for mixtures, *J. Stat. Phys.* **91**:327–342 (1998); *21st International Symposium on Rarefied Gas Dynamics*, *RGD* **I**:71–78 (1999).
2. H. Cornille, *JMP* **28**:1567–79 (1987); *JPA*: *Math. Gen.* **31**:671–86 (1998).
3. H. Cornille, *Trans. Theo. Stat. Phys.* **24**:709–29 (1995) and **26**:359–71 (1997); *WASCOM95*, S. Rionero and T. Ruggeri, eds. (World Scientific, 82–91, 1995); *J. Stat. Phys.* **81**:335–46 (1995); H. Cornille and A. d'Almeida, *J. Math. Phys.* **37**:5476–95 (1998).
4. G. L. Caraffini and G. Spiga, *Trans. Theo. Stat. Phys.* **23**:9–25, (1994); R. Monaco and L. Preziosi, *Fluid Dynamic Applications of the Discrete Boltzmann Equation* (World Scientific, Singapore, 1991).
5. H. Cabannes, The discrete Boltzmann equation, Lecture notes (University of California, Berkeley, 1980).
6. G. A. Bird, Shock wave structure in gas mixture, in *RGD*, H. Ogushi, ed., pp. 175–182 (University of Tokyo Press, 1984); The search for solutions in RGD, in *RGD*, J. Harvey and G. Lord, eds, Vol. 2, 753–762 (Oxford University Press, Oxford, 1995).
7. Ching Shen, Shock wave in gas mixtures with internal energy relaxation (1986).
8. C. Cercignani, On the thermodynamics of a discrete velocity gas, *Transp. Th. Stat. Phys.* **23**:1–8 (1994); Temperature, entropy and kinetic theory, *J. Stat. Phys.* **87**:1097–1109 (1997).