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Hexagonal Discrete Boltzmann Models With and Without Rest Particles

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We consider seven different hexagonal discrete Boltzmann models corresponding to one, two, three, and five hexagons with or without rest particles. In the microscopic collisions the number of particles associated with a given speed is not necessarily conserved, except for two models without rest particles. We compare different behaviors for the macroscopic quantities between models with and without rest particles and when the number of velocities (or hexagons) increases. We study similarity waves with two asymptotic states and consider two classes of solutions at one asymptotic state: either isotropic (densities associated with the same speed are equal) or anisotropic. Two macroscopic quantities seem useful for such studies: internal energy and mass ratio across the asymptotic states, which satisfy a relation deduced from continuous theory. Here we report results for the isotropic solutions, which only exist, for both models, in the subdomains where the propagation speed is larger than some well-defined value. Outside these subdomains, modifications occur when the rest particle density becomes large. For both models we find a monotonic internal energy and subdomains with a mass ratio equal to the one in continuous theory.

KEY WORDS: Nonlinear discrete Boltzmann models; Rankine–Hugoniot relations.

1. INTRODUCTION

In this paper (see Fig. 1) we discuss the one- ($6v_i$), two- ($12v_i$, $14v_i$) FHP,[1] three- ($18v_i$, $19v_i$) GBL,[2] and five- ($30v_i$, $31v_i$) hexagon models.

1. Only one speed exists for the $6v_i$ model,[1] so that the mass and energy are not independent.

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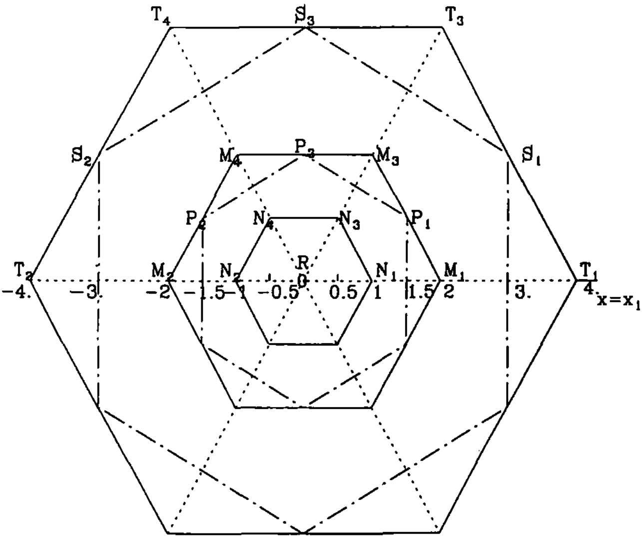


Fig. 1. The one-, two-, three-, four-, and five-hexagon models.

2. Two speeds exist for the $12v_i$ model; the mass and energy are different; however, the slow and fast particles give separately mass and energy conservation laws. If we consider such models as binary mixtures,[3] these conserved quantities have a physical meaning. If we consider them for a simple gas, it could be interesting to check whether, at the macroscopic level, differences occur from other models without such conserved quantities.

3. Three speeds exist for the $14v_i$ model with two rest particles. Collisions of the type $[1]+[1]+[1] \rightarrow [\sqrt{3}]+[0]+[0]$ exist. The *numbers of slow and fast particles are not separately conserved.*

4. We obtain the same result for the three-speed $18v_i$ model (similarly for the $30v_i$ model) with collisions of the type $[\sqrt{3}]+[\sqrt{3}]+[\sqrt{3}] \rightarrow [1]+[2]+[2]$. The total number of particles is conserved, but not the numbers of slow, intermediate, or fast particles separately. However, a conserved relation exists including both slow and fast particles.

5. At least four speeds, including 0, exist in the $19v_i$, $31v_i$ models with only energy conservation between the slow, intermediate, and fast particles.

For one-dimensional similarity solutions along the x axis (cf. Fig. 1) with propagation speed ζ we take into account the three Rankine–Hugoniot relations and the vanishing of the collision terms (binary and ternary collisions excluding spurious conservation laws). We determine an arbitrary space, including ζ, from which we construct the two asymptotic states and the associated macroscopic quantities. We want to find the differences between the isotropic solutions at one state (mass larger than at the other) and the anisotropic ones. We seek the subdomains where the internal energy E_I is monotonic or not.[4] We also study the mass ratio ρ across the asymptotic states and compare with the corresponding ρ_C of the continuous theory.[4] An intermediate step consists in replacing E_I by the temperature: Cercignani[5] has given arguments showing that *this is valid only for discrete models with an infinite number of velocities.*

For the different hexagonal models of Fig. 1 we consider one-dimensional solutions along the x axis. The x coordinates for the independent densities are for R: 0 and N_i: ± 1, $\pm 1/2$ ($6v_i$), P_i: $\pm 3/2$, 0 ($12v_i$), M_i: ± 2, ± 1 ($18v_i$), T_i: ± 4, ± 2, S_i, ± 3, 0 ($30v_i$). To each "hexagon" we associate a mass and a momentum. For the total mass M, momentum J, energy E, and $E_I = E/M - (J/M)^2/2$ we have two types of components:

$$M = M_N + M_P + M_M + M_S + M_T + \lambda R$$

($\lambda = 2$, $14v_i$ and $\lambda = 1$, $19v_i$, $31v_i$)

$$J = J_N + J_M + J_P + J_S + J_T$$

$$E = M_N/2 + 3M_P/2 + 2M_M + 6M_S + 8M_T$$

with $M_X = X_1 + X_2 + 2(X_3 + X_4)$, $J_X = a(X_1 - X_2 + X_3 - X_4)$ for $(X_i, a) = (N_i, 1)$, $(M_i, 2)$, $(T_i, 4)$ and $M_Y = 2(Y_1 + Y_2 + Y_3)$, $J_Y = b(Y_1 - Y_2)$, $(Y_i, b) = (P_i, 2)$, $(S_i, 6)$.

We define $d_Z = \partial_t M_Z + \partial_x J_Z$ and write the mass and energy conservation laws:

$$-\lambda \partial_t R = (2d_N - d_M - 13d_T - 9d_S)/3 = (3d_N + d_P - 12d_T - 8d_S)/4 \quad (1.1)$$

Theorem 1. For multispeed models without a rest particle, conservation relations exist between the slow, intermediate, and fast particles or equivalently between the "hexagons".

For the $12v_i$ model we get $d_N = d_M = 0$, leading for slow and fast particles to mass and energy conservations. For the $18v_i$ model the relations $2d_N = d_M$, $3d_N = -d_P$ between the "hexagons" cannot lead to both energy and mass conservation for each "hexagon" because, with the ternary collisions, $d_N \neq 0$, $d_P \neq 0$. For the "hexagons" of the $14v_i$, $19v_i$, $31v_i$ models there exists only energy conservation in collisions among slow, intermediate, and fast particles, but no conservation laws involving only slow and fast particles.

We consider similarity solutions with variable $\eta = x - \zeta t$. With the densities N_i, P_j, M_i, S_j, T_i, R we associate two asymptotic states:

$$\begin{aligned} &\text{(i)} \quad n_{01} = 1, n_{0i}, p_{0j}, m_{0i}, s_{0j}, t_{0i}, r_0 \\ &\text{(ii)} \quad n_{si} = n_{0i} + n_i, \quad p_{sj} = p_{0j} + p_j, \quad m_{si} = m_{0i} + m_i \\ &\qquad s_{sj} = s_{0j} + s_j, \quad t_{si} = t_{0i} + t_i \\ &\qquad r_s = r_0 + r, \qquad i = 1, 2, 3, 4, \quad j = 1, 2, 3 \end{aligned} \tag{1.2}$$

We associate $\mathscr{R} = -\zeta r$ to R and to the N_i, P_i, M_i, S_i, T_i of the different "hexagons":

$$\begin{aligned} \mathscr{X}_i &= [(3-2i)\,a - \zeta]\,x_i \\ \mathscr{X}_{i+2} &= [(3-2i)a/2 - \zeta]\,x_{i+2} \\ \mathscr{Y}_i &= [(3-2i)\,b - \zeta]\,y_i, \qquad i = 1, 2 \\ \mathscr{Y}_3 &= -\zeta y_3 \end{aligned} \tag{1.3}$$

with a, $x_i = 1$, $n_i = 2$, $m_i = 4$, t_i and b, $y_i = 3/2$, $p_i = 3$, s_i; $\mathscr{X}^{\pm} = \mathscr{X}_1 + \mathscr{X}_2 + (3 \pm 1)(\mathscr{X}_3 + \mathscr{X}_4)/2$ with $\mathscr{X} = \mathscr{N}$, $\mathscr{M}$, $\mathscr{T}$ and $\mathscr{Y}^{\pm} = \mathscr{Y}_1 + \mathscr{Y}_2 + (1 \pm 1)\,\mathscr{Y}_3/2$ with $\mathscr{Y} = \mathscr{P}$, $\mathscr{S}$.

We write the three conservation laws associated with the Rankine–Hugoniot relations:

$$\begin{aligned} [M] &= \mathscr{M}^+ + \mathscr{N}^+ + 2\mathscr{P}^+ + \mathscr{T}^+ + 2\mathscr{S}^+ + \lambda\mathscr{R} = 0 \\ [E] &= 2\mathscr{M}^+ + \mathscr{N}^+/2 + 8\mathscr{T}^+ + 12\mathscr{S}^+ + 3\mathscr{P}^+ = 0 \\ [J] &= \mathscr{N}^- + 2\mathscr{M}^- + 3\mathscr{P}^- + 4\mathscr{T}^- + 6\mathscr{S}^- = 0 \\ -\lambda\mathscr{R} &= [3\mathscr{N}^+ + 2\mathscr{P}^+ - 12\mathscr{T}^+ - 16\mathscr{S}^+]/4 \\ &= [2\mathscr{N}^+ - \mathscr{M}^+ - 13\mathscr{T}^+ - 18\mathscr{S}^+]/3 \\ &= -[4\mathscr{P}^+ + 3\mathscr{M}^+ + 15\mathscr{T}^+ + 22\mathscr{S}^+] \end{aligned} \tag{1.4}$$

with $\mathscr{R} \neq 0$ or $=0$ depending on whether the rest particle is present or not. Consequently at the (i) isotropic state due to $r_0 = m_{01}^{-1/3} = p_{01}^{-1/2}$ or $=0$ we see that in subdomains the rest particle, if it is present, can be the dominant term and similarly for the anisotropic state.

Corollary 1. For the models without rest particles [$\mathscr{R}=0$ in (1.4)], there always exist jump relations between the slow, intermediate, and fast particles or between the "hexagons".

From (1.4) we deduce $\mathscr{N}^+=0$ ($6v_i$), $\mathscr{N}^+=\mathscr{P}^+=0$ ($12v_i$, mass and energy conservation for slow and fast particles). For the $18v_i$ model we have, for instance, the relation $\mathscr{M}^+=2\mathscr{N}^+$ between fast and slow particles, but with $\mathscr{N}^+\neq 0$, $\mathscr{M}^+\neq 0$, $\mathscr{P}^+\neq 0$, and similar relations for the $30v_i$ model. On the contrary, for the $14v_i$, $19v_i$, $31v_i$ models with $\mathscr{R}\neq 0$, only the energy relation exists between the masses of the different "hexagons".

We report (without proof) results obtained from the weak shock theory. *For isotropic solutions the characteristic velocities* $\zeta_i^{(j)}=\zeta_{i\pm}$, 0 *are*

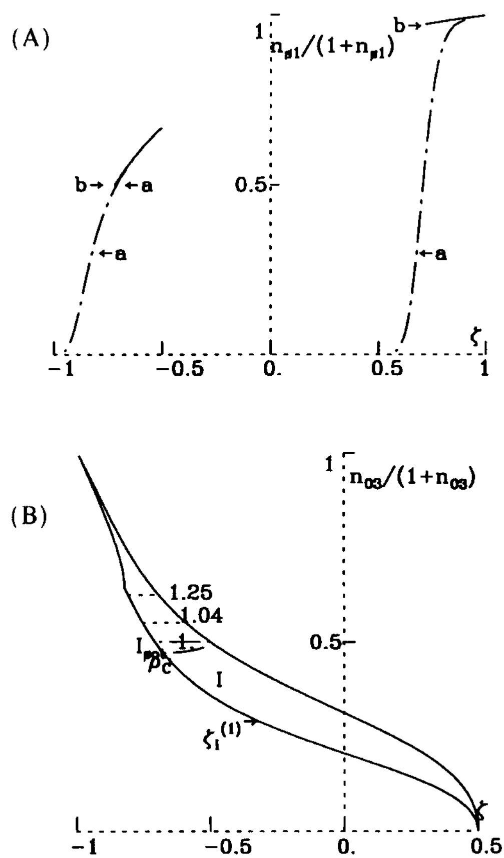


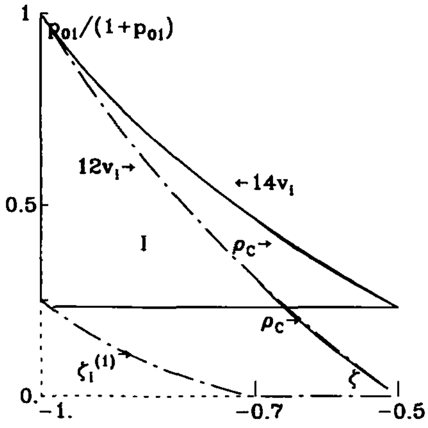
Fig. 2. (A) $6v$ isotropic, $n_{0i}=1$, $n_{si}\neq 0$. (B) $6v$ anisotropic, (ii) $n_{s3}\neq 0$, $n_{s1}\neq 0$.

the same for the $12v_i$, $14v_i$, *the* $18v_i$, $19v_i$, *as well as for the* $30v_i$, $31v_i$ *models* and the shock inequalities have been verified. Here

$$\zeta_{i\pm} = \pm[(1+9p_{01}+16m_{01}+144s_{01}+256t_{01})/2(1+3p_{01}+4m_{01}+12s_{01}+16t_{01})]^{1/2} \quad (1.5)$$

2. ISOTROPIC AND ANISOTROPIC (i) STATE SOLUTIONS

1. *For isotropic solutions we have verified* (Appendix) *the constraint* $|\zeta| \geqslant 1/2$, *observed monotonic internal energy* (I in the figures) E_I, $\rho = \rho_C$



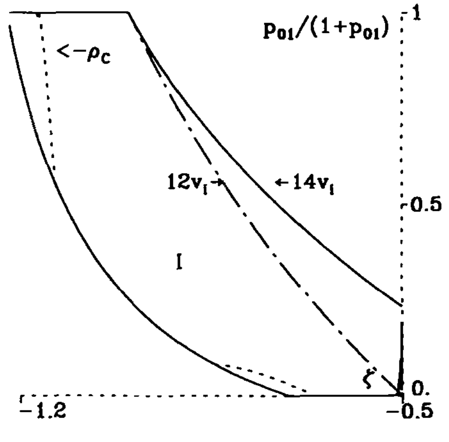


Fig. 3. (A) Top: $12v$, $14v$ isotropic, (ii) $n_{s1} \neq 0$, $n_{s3} \neq 0$, $p_{s1} \neq 0$; (B) bottom: $12v$, $14v$ isotropic, (ii) densities $\neq 0$. (C) $12v$, $14v$ anisotropic, (ii) state only $n_{s1} \neq 0$, $p_{s1} \neq 0$.

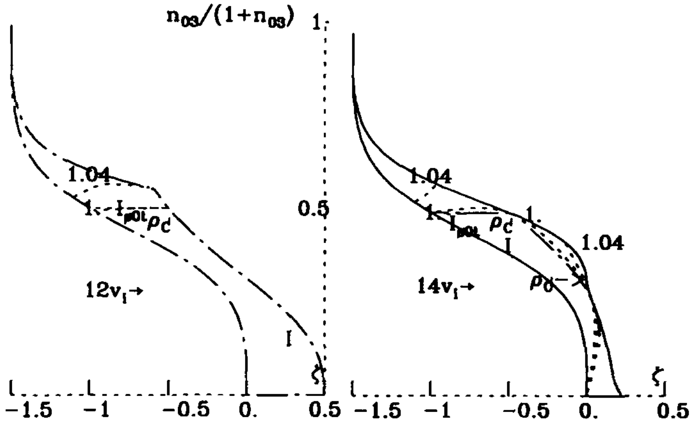


Fig. 3. *(Continued)*

curves, and found larger domains for the models with rest particles: $14v_i$, $19v_i$, $31v_i$. In Fig. 2A we find $\rho=\rho_C$ for $\zeta=-1/2$, $n_{s1}=2$, solutions with all (ii) state densities nonzero (curves a) and only two of them (b). In Fig. 3A (left) with three nonzero (ii) state densities the domain is limited by $p_{01}\geqslant 0$ ($12v_i$), $p_{01}=r_0^{-2}\geqslant(1/6)^{2/3}$ ($14v_i$) and by a characteristic $\zeta_i^{(1)}$. In Fig. 3A (right) all (ii) state densities are different from zero. For the $19v_i$, $31v_i$ models, when $m_{01}\to 0$, $r_0=m_{01}^{-1/3}\to\infty$. In Figs. 4A (left) and 5A [three (ii) state densities nonzero] and Fig. 4A (right) (all nonzero) we see modifications of the domains when the rest particle is large (m_{01} small).

2. *For anisotropic solutions with* $|\zeta|\geqslant 1/2$ *we observe, for both models, the* $\rho=\rho_C$ *curve and nonmonotonic* E_I (some values for the strength of the effect are given) *and only for models with rest particles for* $|\zeta|<1/2$. In Fig. 2B the domain is limited from positivity and from a characteristic velocity $\zeta_i^{(1)}$. In Fig. 3B we see the difference when $|\zeta|<1/2$ and R is present. For the $18v_i$, $30v_i$ models $r_0=0$, while $r_0\simeq m_{02}^{-1/3}$ for the $19v_i$, $31v_i$ models. We find differences for m_{02} small [Figs. 4B (top) and 5B] except if it is forbidden by positivity [Fig. 4B (bottom)].

3. DISCUSSION

1. Let us consider two models differing by the presence of rest particles ($12v_i$, $14v_i$, $18v_i$, $19v_i$, $30v_i$, $31v_i$). They have *common properties for the isotropic solutions which introduce new symmetries:* They have the *same characteristic velocities,* using the energy and momentum conserva-

tion laws, which do not involve rest particles densities, they only *exist in some intervals of the propagation speed* ($|\zeta| \geqslant 1/2$) with *monotonic internal energy. However, for these isotropic solutions, we observe great modifications of the positivity domain when the rest particle density is large.* For the connection with the continuous theory ($p = p_C$ curves) we do not see great differences even when the number of "hexagons" increases.

2. *For anisotropic solutions* we have observed that an additional subdomain can exist for $|\zeta| < 1/2$ with $p = p_C$ curves and nonmonotonic E_I

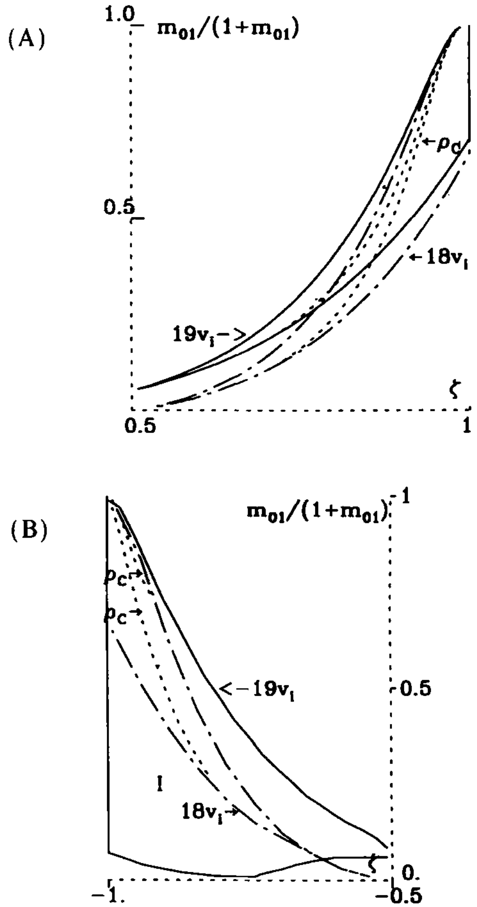
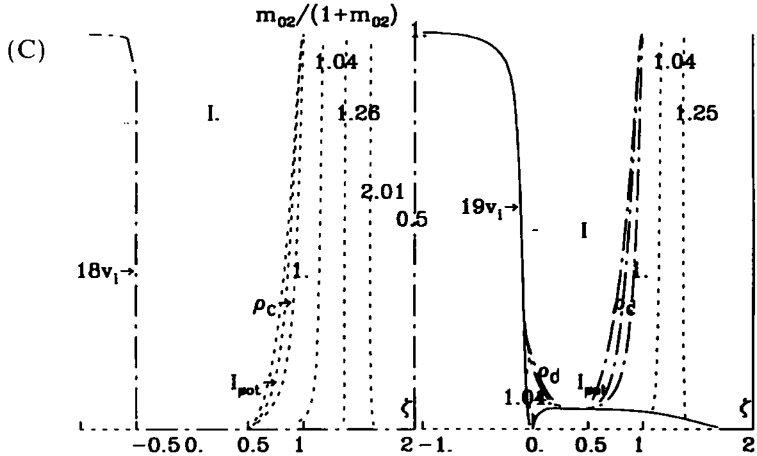


Fig. 4. (A) Top: $18v$, $19v$ isotropic, (ii) $m_{s2} \neq 0$, $p_{s2} \neq 0$, $n_{s2} \neq 0$; (B) bottom: $18v$, $19v$ isotropic, (ii) densities $\neq 0$. (C) Top: $18v$, $19v$ anisotropic, (ii) state only $n_{s2} \neq 0$, $m_{s2} \neq 0$; (D) bottom: $18v$, $19v$ anisotropic, (ii) $m_{s2} \neq 0$, $p_{s2} \neq 0$.



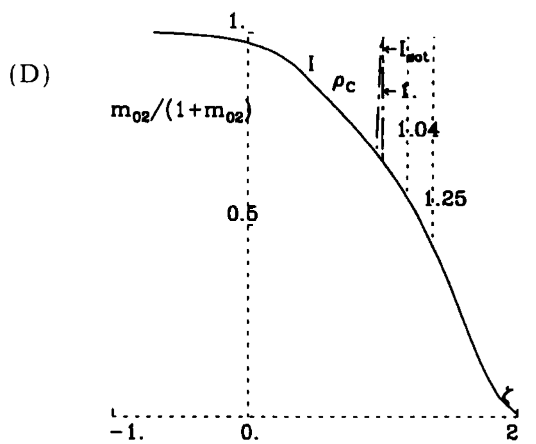


Fig. 4. *(Continued)*

only in the models with rest particle. This happens when the rest particle density is large, $|\zeta|$ small, and these subdomains are not forbidden by positivity. Outside this $|\zeta|$ interval we have found for both models *some nonmonotonic internal energy. On comparison with the above isotropic solutions, this seems to be an anisotropic effect.*

3. These results have been obtained in a general framework which represents the minimal constraints. We could be more specific and retain

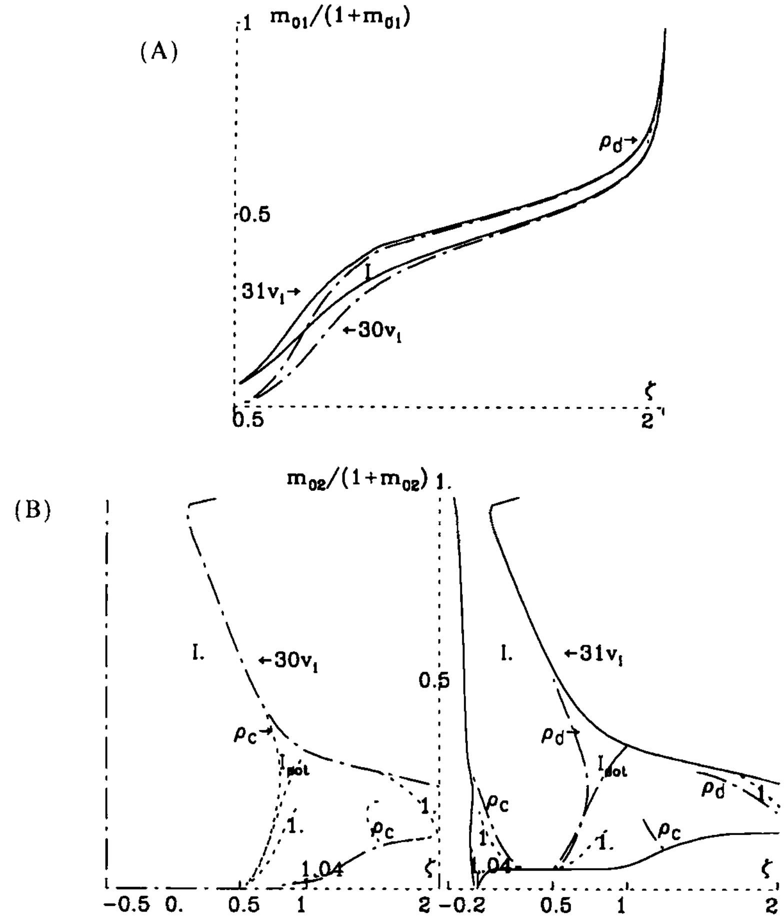


Fig. 5. (A) $30v$, $31v$ isotropic, (ii) $n_{s2}\neq 0$, $m_{s2}\neq 0$, $t_{s2}\neq 0$. (B) $30v$, $31v$ anisotropic, (ii) state only $n_{s2}\neq 0$, $p_{s2}\neq 0$.

only $\rho=\rho_C$ domains (only one point in Fig. 2a and curves in other figures), only isotropic solutions (results for $|\zeta|<1/2$ disappear). For the nonlinear equations we could try to solve the equations (not only the vanishing of the collision terms), which means *for the* $31v_i$ *model the resolution of a 19×19 system* (Riccati type for quadratic collisions) and it seems difficult to handle the problem with more and more velocities. Finally *no boundary conditions, which could affect the present results*, were considered.

APPENDIX. ISOTROPIC (i) STATE WITH NONZERO (ii) STATE DENSITIES

We define $\bar{n}_{s2}=n_{s2}/n_{s1}$. For the (ii) state we choose as arbitrary parameters n_{s1}, n_{s2}, p_{s1}, or m_{s1} and for the isotropic (i) state $n_{0i}=1$, $p_{01}=m_{01}^{2/3}=s_{01}^{2/11}=t_{01}^{2/15}=r_0^{-2}$ or $r_0=0$:

$$\begin{array}{lll} n_{s3}=n_{s1}\bar{n}_{s2}^{1/4}, & n_{s4}=n_{s1}\bar{n}_{s2}^{3/4} & \\ p_{s2}=p_{s1}(\bar{n}_{s2})^{3/2}, & p_{s3}=p_{s1}(\bar{n}_{s2})^{3/4} & \\ r_s^2 p_{s1}=n_{s3}^3, & p_{s1}^3=m_{s1}^2 n_{s3} & \\ m_{s2}=m_{s1}\bar{n}_{s2}^{-2}, & m_{s3}=m_{s1}\bar{n}_{s2}^{1/2}, & m_{s4}=m_{s1}\bar{n}_{s2}^{-3/2} \\ s_{s2}=s_{s1}\bar{n}_{s2}^{3}, & s_{s3}=s_{s1}\bar{n}_{s2}^{-3/2}, & s_{s1}n_{s1}^{8/3}=m_{s1}^{11/3}\bar{n}_{s2}^{-5/2} \\ t_{s2}=t_{s1}\bar{n}_{s2}^{3}, & t_{s3}=t_{s1}\bar{n}_{s2} & \\ t_{s4}=t_{s1}\bar{n}_{s2}^{3}, & t_{s1}n_{s1}^4=m_{s1}^5\bar{n}_{s2} & \end{array} \tag{A.1}$$

Theorem 2. $|\zeta|\geqslant 1/2$ for isotropic (i) state and nonzero (ii) state densities. We have

$$\begin{aligned} & x_i := n_i, m_i, t_i, \qquad x^{\pm}=x_1 \pm x_2+(3\pm 1)(x_3\pm x_4)/2 \\ & x^{++}=2(x_1+x_2)+x_3+x_4 \\ & y_j := p_j, s_j, \qquad y^{\pm}=y_1\pm y_2+(1\pm 1)\,y_3/2, \qquad y^{++}=y_1+y_2 \\ & A := 0.5n^- +4m^- +32t^- +36s^- +4.5p^- \\ & B := 0.5n^+ +2m^+ +8t^+ +3p^+ +12s^+ \\ & C := 2m^{++}+8t^{++}+0.5n^{++}+18s^{++}+4.5p^{++} \\ & D := n^- +2m^- +4t^- +3p^- +6s^- \\ & [E]=0\rightarrow\zeta=A/B, \qquad [J]=0\rightarrow\zeta=C/D \end{aligned} \tag{A.2}$$

From (A.1) if $\bar{n}_{s2}<1$ we find positive x^-, y^-, A, deduce the inequalities $x_{s1}>x_{s3}>x_{s4}>x_{s2}$, $y_{s1}>y_{s3}>y_{s2}$ (with $x_i\rightarrow x_{si}$,... when $n_i\rightarrow n_{si}$,...). If $A>0$, $0<\zeta<1/2$, it follows that $X:=2A-B+C-D/2<0$ with

$$\begin{aligned} X= & (n_1-n_4)+.9(m_1-m_4)+5(m_3-m_2) \\ & +54(t_1-t_4)+70(t_2-t_3)+(75s_1-63s_2-12s_3)+(9p_1-6p_2-3p_3) \end{aligned}$$

In each bracket we replace x_i by x_{si} and due to the inequalities, $X>0$. Similarly, $A<0$ leads to incompatibilities.

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