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POLYSOLITON SOLUTIONS FOR PLANE DISCRETE VELOCITY MODELS OF A GAS WITH CHEMICAL REACTIONS

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Exact polysoliton solutions are given for plane discrete velocity models of a gas with chemical reactions. A technique due to Osland and Wu is sistematically applied [3].

1. Introduction.

The discrete velocity models in kinetic theory are models of the Boltzmann equation where the gas particles can attain only to a finite set of allowed velocities.

In this paper we shall deal with exact particular solutions for certain discrete velocity models of reacting gases.

Let us first sketch briefly the background of this kind of research.

Exact solutions for the DBE (discrete Boltzmann equation) have been given in the past mainly by Cornille (a number of soliton and polysoliton solutions [1]) and by Wu (initial value problems for particular scattering models [2,3]).

Boffi and Spiga have studied problems which include absorption and creation of particles (extended kinetic theory [4]).

A DBE for gases with chemical reactions has been introduced recently by Monaco et al. [5]. Exact solutions for these equations have been given for the 1D case by Monaco and Platkowski [6].

The aim of this paper is to study exact solutions for plane discrete velocity models of a gas with chemical reactions by applying a technique suggested by Osland and Wu [3].

In spite of the different physical situation they considered, this method turns out to be useful in our case too.

We study the following reaction schemes:

$$\mathcal{A} \; + \; \mathcal{A} \longrightarrow \mathcal{B}$$

$$\mathcal{A} \; + \; \mathcal{A} \longrightarrow \mathcal{B} \; + \; \mathcal{C}.$$

Under the hypothesis that the cross sections of reaction are much greater than the cross section of scattering, our model contains only the collisional terms due to reactions. The equations for particles $\mathcal{A}$ are then decoupled from the ones for the products.

We shall confine our analysis to the number densities for particles $\mathcal{A}$, whose form allows the application of the Osland–Wu technique. Particular exact solutions are found for both the reaction schemes.

2. The two velocity problem.

The results we shall obtain here will be recalled in the study of the full plane discrete velocity models and they have to be considered only preliminaries.

Consider particles $\mathcal{A}$ endowed with only two velocities,$\mathbf{v}_i$ and $\mathbf{v}_j$, in the plane.

They can interact between themseves only according the following scheme:

$$\mathcal{A}_i \; + \; \mathcal{A}_j \longrightarrow \textit{products}.$$

The equations for the number densities f_i *and* f_j are given by

$$\left(\frac{\partial}{\partial t} \; + \; \mathbf{v}_i \cdot \nabla\right) f_i \;=\; -a_{ij} f_i f_j$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_j \cdot \nabla\right) f_j = -a_{ij} f_i f_j$$

where

$$\nabla = \mathbf{i}\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y}$$

and a_{ij} is the collision frequency of the reaction.

Following Osland and Wu we set

$$f_l(\mathbf{x}, t) = g_l(\mathbf{x}, t) / D(\mathbf{x}, t)$$

l=i,j, so that

$$D\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) g_l - g_l\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) D = -a_{ij} g_i g_j .$$

We may satisfy this equation by imposing simultaneously

(1) $$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) g_l = \alpha_l g_l$$

(2) $$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) D = a_{nl} g_n + \alpha_l D$$

$l = i, j \quad n \neq l$ where α_l is an arbitrary constant.

Now look for solutions of the following kind

$$g_l(\mathbf{x}, t) = C_l A_l E_l(\mathbf{x}, t)$$

$$D(\mathbf{x}, t) = C_i E_i(\mathbf{x}, t) + C_j E_j(\mathbf{x}, t)$$

where $E_l = exp(p_l t + \mathbf{q}_l \cdot \mathbf{x})$, $C_l > 0$, $A_l > 0$, $l = i, j$.

Once we have inserted this ansatz into (1) and (2) we get the following conditions:

(3) $$p_l + \mathbf{q}_l \cdot \mathbf{v}_l = \alpha_l$$

(4) $$p_l + \mathbf{q}_l \cdot \mathbf{v}_n = a_{nl} A_l + \alpha_n$$

$l = i, j \quad n \neq l.$

By eliminating α_i and α_j we are reduced to

$$p_i - p_j + \mathbf{v}_j \cdot (\mathbf{q}_i - \mathbf{q}_j) = a_{ij} A_i \tag{5a}$$

$$p_j - p_i + \mathbf{v}_i \cdot (\mathbf{q}_j - \mathbf{q}_i) = a_{ij} A_j \tag{5b}$$

which can be regarded as two equations for the three unknowns $p_i - p_j$ and $\mathbf{q}_i - \mathbf{q}_j$.

Setting $\gamma_{ij} = p_i - p_j$ $\mathbf{B}_{ij} = \beta \mathbf{u} = (\mathbf{q}_i - \mathbf{q}_j)/(p_i - p_j)$ $(\beta > 0,\ |\mathbf{u}| = 1)$ equations (5) give

$$\beta = -(A_i + A_j)/(A_i w_i + A_j w_j)$$

$$\gamma_{ij} = a_{ij}(A_i w_i + A_j w_j)/(w_i - w_j)$$

where $w_l = \mathbf{v}_l \cdot \mathbf{u}$.

In correspondence to given values of A_i,A_j and $\mathbf{u}$ such that $(A_j \mathbf{v}_j + A_i \mathbf{v}_i) \cdot \mathbf{u} < 0$, the number densities are given by

$$f_l(\mathbf{x}, t) = C_l A_l / \{C_l + C_n exp[\gamma_{nl}(t + \mathbf{B}_{nl} \cdot \mathbf{x})]\}$$

$n \neq l$ which is a well known soliton solution [1].

3. Reaction $\mathcal{A} + \mathcal{A} \to \mathcal{B}$.

Particles $\mathcal{M}$ $(\mathcal{M} = \mathcal{A}, \mathcal{B})$ are endowed with the following 6 velocities in the plane: $\mathbf{v}_{lM} = \mathbf{e}_l v_M$ l=1,2,...,6 M=A,B where

$$\mathbf{e}_1 = -\mathbf{e}_4 = \mathbf{j}$$

$$\mathbf{e}_2 = -\mathbf{e}_5 = -\frac{1}{2}(\mathbf{j} + \sqrt{3}\mathbf{i})$$

$$\mathbf{e}_3 = -\mathbf{e}_6 = -\frac{1}{2}(\mathbf{j} - \sqrt{3}\mathbf{i}).$$

The only possible events are

$$\mathcal{A}_1 + \mathcal{A}_2 \to \mathcal{B}_6, \quad \mathcal{A}_4 + \mathcal{A}_5 \to \mathcal{B}_3$$

$$\mathcal{A}_2 + \mathcal{A}_3 \to \mathcal{B}_4, \quad \mathcal{A}_5 + \mathcal{A}_6 \to \mathcal{B}_1$$

$$\mathcal{A}_3 + \mathcal{A}_1 \rightarrow \mathcal{B}_5, \quad \mathcal{A}_6 + \mathcal{A}_4 \rightarrow \mathcal{B}_2.$$

Momentum conservation imposes $m_A v_A = m_B v_B = \mathcal{P}$. Energy and mass conservation are expressed as follows

$$\frac{1}{2}\mathcal{P}^2(2/m_A - 1/m_B) = \epsilon > 0 \tag{6}$$

$$m_B = 2m_A$$

where ϵ is the chemical link energy of the reaction.

Equation (6) fixes $\mathcal{P}$:

$$\mathcal{P} = 2\sqrt{m_A \epsilon/3}.$$

Observe that particles $\mathcal{A}_1$, $\mathcal{A}_2$ and $\mathcal{A}_3$ interact only among themselves. The same holds for particles $\mathcal{A}_4$, $\mathcal{A}_5$ and $\mathcal{A}_6$. The equations for particles $\mathcal{A}_1$, $\mathcal{A}_2$ and $\mathcal{A}_3$ are decoupled from the ones for $\mathcal{A}_3$, $\mathcal{A}_4$ and $\mathcal{A}_5$ and are written as follows:

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) f_l = -k f_l (f_{l+1} + f_{l+2}) \tag{7}$$

$l = 1, 2, 3 \quad (l + 3 \rightarrow l)$ where $\mathbf{v}_l = \mathbf{v}_{lA}$ and k is the collision frequency of the reaction. Now, following the Osland–Wu approach we are led to

$$D\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) g_l - g_l \left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) D = -k g_l (g_{l+1} + g_{l+2})$$

and

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) g_l = \alpha_l g_l \tag{8}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) D = k(g_{l+1} + g_{l+2}) + \alpha_l D \tag{9}$$

l=1,2,3, which are 6 equations in 4 unknowns.

We look for solutions of this kind:

$$g_l(\mathbf{x}, t) = C_l A_l E_l(\mathbf{x}, t)$$

$$D(\mathbf{x}, t) = \sum_{l=1}^{3} C_l E_l(\mathbf{x}, t).$$

Conditions (3) and (4) hold again (with $a_{nl} = k$) but now they represent 9 equations for the 9 unknowns

$$p_l, \quad \mathbf{q}_l$$

$l = 1, 2, 3$.

It is convenient to set

$$p_l = P + P_l, \quad \mathbf{q}_l = \mathbf{Q} + \mathbf{Q}_l$$

where P and $\mathbf{Q}$ solve the following system:

$$P + \mathbf{v}_l \cdot \mathbf{Q} = \alpha_l \quad l = 1, 2, 3.$$

The equations for P_l and $\mathbf{Q}_l$ are then

$$P_l + \mathbf{v}_l \cdot \mathbf{Q}_l = 0$$

$$P_l + \mathbf{v}_n \cdot \mathbf{Q}_l = kA_l$$

$n \neq l$, which are easily solved by

$$P_l = \frac{2k}{3} A_l, \quad \mathbf{Q}_l = -\frac{2k}{3v^2} A_l \mathbf{v}_l.$$

In correspondence to given values of A_1, A_2 and A_3 we get then

$$f_l(\mathbf{x}, t) = C_l A_l / \left\{ C_l + \sum_{n=l+1}^{l+2} C_n exp[\gamma_{nl}(t + \mathbf{B}_{nl} \cdot \mathbf{x})] \right\}$$

where

$$\gamma_{nl} = p_n - p_l = P_n - P_l \tag{10}$$

$$\mathbf{B}_{nl} = (\mathbf{q}_n - \mathbf{q}_l)/(p_n - p_l) = (\mathbf{Q}_n - \mathbf{Q}_l)/(P_n - P_l). \tag{11}$$

All the f_l depend on the following 3 arguments only:

$$t + \mathbf{B}_{12} \cdot \mathbf{x}, \quad t + \mathbf{B}_{13} \cdot \mathbf{x}, \quad t + \mathbf{B}_{23} \cdot \mathbf{x}.$$

Furthermore, for each couple ij conditions (5) hold again. Then we can say that our solution represents the interaction of 3 solitons: 12, 13, and 23.

In order to understand the physical meaning of this solution, we fix a point x ($|\mathbf{x}| < \infty$) and study f_l as a function of t for $t \in \Re$. In the case $A_3 < A_2 < A_1$ we have

$$\lim_{t\to-\infty} f_1(\mathbf{x},t) = \lim_{t\to-\infty} f_2(\mathbf{x},t) = 0$$

$$\lim_{t\to-\infty} f_3(\mathbf{x},t) = A_3$$

$$\lim_{t\to+\infty} f_2(\mathbf{x},t) = \lim_{t\to+\infty} f_3(\mathbf{x},t) = 0$$

$$\lim_{t\to+\infty} f_1(\mathbf{x},t) = A_1.$$

The functions f_1 and f_3 are monotonically increasing and decreasing, respectively. Function f_2 increases, reaches a maximum and decreases. At $t \to -\infty$ we have only particles 3 at finite. Then all the three species are present and react among themselves. At $t \to +\infty$ only particles 1 survive.

4. Reaction $\mathcal{A} + \mathcal{A} \to \mathcal{B} + \mathcal{C}$.

Particles $\mathcal{M}$ $(\mathcal{M} = \mathcal{A}, \mathcal{B}, \mathcal{C})$ are endowed with the following 4 velocities in the plane

$$\mathbf{v}_{lM} = \mathbf{e}_l v_M \quad l = 1,2,3,4 \quad M = A, B, C$$

where

$$\mathbf{e}_1 = -\mathbf{e}_3 = \mathbf{i}$$

$$\mathbf{e}_2 = -\mathbf{e}_4 = \mathbf{j}.$$

The only possible events are the following

$$\mathcal{A}_l + \mathcal{A}_{l+2} \to \begin{cases} \mathcal{B}_1 + \mathcal{C}_3 \\ \mathcal{B}_3 + \mathcal{C}_1 \\ \mathcal{B}_2 + \mathcal{C}_4 \\ \mathcal{B}_4 + \mathcal{C}_2 \end{cases}$$

"head on" collisions, and

$$\mathcal{A}_l + \mathcal{A}_{l+1} \to \begin{cases} \mathcal{B}_l + \mathcal{C}_{l+1} \\ \mathcal{B}_{l+1} + \mathcal{C}_l \end{cases}$$

collisions "at angle".

Momentum conservation imposes

$$m_A v_A = m_B v_B = m_C v_C = \mathcal{P}.$$

Energy and mass conservation are expressed as follows:

$$\frac{\mathcal{P}^2}{2}(1/m_B + 1/m_C - 2/m_A) = \epsilon > 0 \tag{12}$$

$$2m_A = m_B + m_C.$$

Equation (12) fixes $\mathcal{P}$:

$$\mathcal{P} = 2\sqrt{\epsilon m_B m_C m_A}/|m_C - m_B|.$$

The equations for the number densities are then

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) f_l = -f_l[k f_{l+2} + h(f_{l+1} + f_{l+3})]$$

$l = 1, 2, 3, 4 \quad (l + 4 \to l)$, where k and h are the collision frequencies relevant, respectively, to the "head on" and "at angle" collisions.

Following the Osland–Wu approach we are led to

$$D\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) g_l - g_l \left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) D = -g_l[k g_{l+2} + h(g_{l+1} + g_{l+3})]$$

and

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) g_l = \alpha_l g_l \tag{13}$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) D = k g_{l+2} + h(g_{l+1} + g_{l+3}) + \alpha_l D \tag{14}$$

l=1,2,3,4, which are 8 equations in 5 unknowns.

We look for solutions of this kind

$$g_l(\mathbf{x}, t) = C_l A_l E_l(\mathbf{x}, t)$$

$$D(\mathbf{x}, t) = \sum_{l=1}^{4} C_l E_l(\mathbf{x}, t).$$

Conditions (3) and (4) hold (with $a_{nl} = k \ for \ l = n+2 \ and \ a_{nl} = h \ for \ l \neq n+2$) and we regard them as 16 equations for the 16 unknowns p_l, $\mathbf{q}_l$, α_l.

By eliminating p_l and $\mathbf{q}_l$ we get

$$\alpha_l + \alpha_{l+2} + kA_l = \alpha_{l+1} + \alpha_{l+3} + 2hA_l$$

l=1,2,3,4.

These equations are compatible only if $k = 2h$. This condition holds in the frame of the so called VHS (very hard sphere) model, which was studied by Ernst and Hendriks [7].

In this case we have

$$\alpha_1 + \alpha_2 = \alpha_3 + \alpha_4$$

and we can find P and $\mathbf{Q}$ such that

$$P + \mathbf{v}_l \cdot \mathbf{Q} = \alpha_l$$

l=1,2,3,4.

Now we set

$$p_l = P + P_l$$

$$\mathbf{q}_l = \mathbf{Q} + \mathbf{Q}_l$$

where P_l and $\mathbf{Q}_l$ are given by

$$P_l + \mathbf{v}_l \cdot \mathbf{Q}_l = 0 \tag{15}$$

$$P_l + \mathbf{v}_n \cdot \mathbf{Q}_l = a_{nl} A_l \tag{16}$$

$n \neq l$, which are easily solved as follows

$$P_l = \frac{k}{2} A_l$$

$$\mathbf{Q}_l = -\frac{k}{2v^2} A_l \mathbf{v}_l.$$

In correspondence to given values of A_1, A_2, A_3 and A_4 we have then

$$f_l(\mathbf{x}, t) = C_l A_l / \left\{ C_l + \sum_{n=l+1}^{l+3} C_n exp[\gamma_{nl}(t + \mathbf{B}_{nl} \cdot \mathbf{x})] \right\}$$

where γ_{nl} and $\mathbf{B}_{nl}$ are defined again as in (10) and (11).

All the f_l depend on the following 6 arguments only:

$$t + \mathbf{B}_{12} \cdot \mathbf{x}, \quad t + \mathbf{B}_{13} \cdot \mathbf{x}, \quad t + \mathbf{B}_{14} \cdot \mathbf{x}$$

$$t + \mathbf{B}_{23} \cdot \mathbf{x}, \quad t + \mathbf{B}_{24} \cdot \mathbf{x}, \quad t + \mathbf{B}_{34} \cdot \mathbf{x}.$$

For each couple nl, equations (5) hold and we can say that our solution represents the interaction of 6 solitons: 12, 13, 14, 23, 24, 34.

The condition $k = 2h$ can be dropped if we suppose that one of the f_l is 0. In this case the problem is similar to the three velocity one. For $f_1 = 0$, the equations for the number densities are

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) f_l = -f_l(kf_{l+2} + hf_3) \quad l = 2, 4$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_3 \cdot \nabla\right) f_3 = -hf_3(f_2 + f_4).$$

Following the Osland–Wu approach we get

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) g_l = \alpha_l g_l \quad l = 2, 3, 4$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_l \cdot \nabla\right) D = \alpha_l D + kg_{l+2} + hg_3 \quad l = 2, 4$$

$$\left(\frac{\partial}{\partial t} + \mathbf{v}_3 \cdot \nabla\right) D = \alpha_3 D + h(g_2 + g_4).$$

Looking for solutions of this kind

$$g_l(\mathbf{x}, t) = C_l A_l E_l(\mathbf{x}, t) \quad l = 2, 3, 4$$

$$D(\mathbf{x}, t) = \sum_{i=2}^{4} C_i E_i(\mathbf{x}, t),$$

we can set

$$p_l = P + P_l \quad \mathbf{q}_l = \mathbf{Q} + \mathbf{Q}_l$$

where

$$P + \mathbf{v}_l \cdot \mathbf{Q} = \alpha_l \quad l = 2, 3, 4.$$

The equations for P_l and $\mathbf{Q}_l$ are again (15) and (16), where $l = 2,3,4$ $n \neq l$. Their solution is

$$P_l = \frac{k}{2}A_l, \quad \mathbf{Q}_l = \frac{A_l}{v^2}[(h-k/2)\mathbf{v}_3 - k\mathbf{v}_l/2]$$

$l = 2,4,$

$$P_3 = hA_3, \quad \mathbf{Q}_3 = -\frac{hA_3}{v^2}\mathbf{v}_3.$$

The number densities are then given by

$$f_l(\mathbf{x},t) = C_lA_l/\left\{C_l + \sum_n C_n exp[\gamma_{nl}(t + \mathbf{B}_{nl}\cdot\mathbf{x})]\right\}$$

where $l = 2,3,4$ and

$$n = 3,4 \quad for \quad l = 2$$

$$n = 2,4 \quad for \quad l = 3$$

$$n = 2,3 \quad for \quad l = 4$$

[γ_{nl} and $\mathbf{B}_{nl}$ are still defined as in (10) and (11)].

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