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Nonunique Solutions of Kinetic Equations

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Two very hard particle models are solved and the nonuniqueness of the initial value problem for these (model) kinetic equations is explicitly demonstrated, when distribution functions decaying sufficiently slowly are permitted. The intimate connection between nonuniqueness and violation of conservation laws is made evident. The associated eigenvalue problems are solved. Finally, the general implications of these results for kinetic equations with transition rates that are increasing functions of the state variable, are stated in the form of a number of conjectures. They affect the solution of the Boltzmann equation for realistic intermolecular interactions when the collision rate $gI(g, \chi)$ is an increasing function of the relative velocity g.

KEY WORDS: Linear and nonlinear Boltzmann equation; initial value problem in kinetic theory; violation of mass or energy conservation; high energy tails of distribution functions; eigenfunctions with positive and negative eigenvalues.

1. INTRODUCTION

Rate equations or kinetic equations describe the time evolution of the probability distribution $F(x,t)$ over states x. A rate equation for a system of reacting polymers was recently discussed by Aizenman and Bak.[1] They found that the initial value problem only has a unique solution provided that the distribution function $F(x,t)$ decays faster than x^{-3} for large x, whereas existence of the conserved quantity (total mass in their case) only requires $F(x,t)$ to fall off faster than x^{-2}.

Closely related to this are results obtained by Cornille and Gervois,[2] who studied the eigenvalue problem associated with the linearized Boltzmann equation for hard spheres, and the corresponding linear problem for

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the case of self-diffusion (or neutron transport). Finally, Piasecki and Pomeau[3] very recently found exact solutions to the initial value problem associated with a hard sphere Rayleigh particle in a thermal bath at zero temperature. If velocity distribution functions, decaying sufficiently slowly for large velocities, are allowed, they showed that the solution of their initial value problem is not unique.

In this paper we shall discuss these problems in the context of the so-called very hard particle (VHP) models introduced by Ernst and Hendriks.[4–6] These are (mathematical) model Boltzmann equations that can be solved exactly. In Section 2 we demonstrate the intimate connection between the conservation laws and the nonuniqueness expected from the analogy with the Aizenman–Bak model. Section 3 gives the exact solution of the initial value problem for the linear case of self-diffusion. It is explicitly shown that for nonsingular distribution functions decaying faster than x^{-2}, where x stands for the energy variable, the solution of the initial value problem is unique. When distributions decaying like x^{-2} are allowed, the solution is no longer unique. In fact, an infinite number of solutions exist, parametrized by an arbitrary, time-dependent, total number of particles $N(t)$. In Section 4 we discuss the nonlinear model and arrive at similar conclusions except that nonuniqueness is now associated with x^{-3} decay, and is parametrized by an arbitrary, time-dependent, total energy $E(t)$. The associated eigenvalue problems are discussed in Section 5 and a set of eigenfunctions are found that have a continuous spectrum, live outside the standard Hilbert space of the Boltzmann problem, and violate one of the conservation laws. Our results, and those referred to above, have general implications for kinetic equations with transition rates that are increasing functions of the state variable. These implications are stated in Section 6 in the form of a number of conjectures.

2. CONSERVATION LAWS AND THE VHP MODEL

The problem at hand is a general one associated with kinetic equations with transition rates that are increasing functions of the state variable. However, in order to carry out explicit calculations, we shall specialize to a simple equation of the Boltzmann type, introduced by Ernst and Hendriks and called the vary hard particle (VHP) model.[6]

Let $F(x,t)$ be the distribution function for the energy x at time t. The VHP model is defined by the evolution equation

$$\partial_t F(x,t) = \int\int_0^\infty\int dx_1\, dx'\, dx'_1\, w(xx_1|x'x'_1)\left[F(x',t)F(x'_1,t) - F(x,t)F(x_1,t)\right] \tag{1}$$

where the transition rate $w(xx_1|x'x'_1)$ for a binary interaction $(x,x_1)\to(x',x'_1)$ is given as

$$w(xx_1|x'x'_1) = \delta(x + x_1 - x' - x'_1) \tag{2}$$

An alternative form of (1) is

$$\partial_t F(x,t) = \int_x^\infty du \int_0^u dy\left[F(y,t)F(u-y,t) - F(x,t)F(u-x,t)\right] \tag{3}$$

An exact solution of Eq. (3) in terms of the initial distribution $F(x,0)$ was given by Ernst and Hendriks.[5]

The purpose of the present analysis is to show the following: (i) The Ernst–Hendriks solution is indeed the unique solution, *if* one restricts the class of allowed functions $F(x,t)$ to nonsingular ones (to be defined below) which, for all $t \geqslant 0$ and large x, decay faster than x^{-3} (i.e., at least as fast as $x^{-3-\epsilon}$, where $\epsilon > 0$); (ii) If, however, functions decaying asymptotically like x^{-3} (or slower) are permitted, infinitely many solutions to the initial value problem exist. Analogous statements will be proved for the linear VHP-model for self diffusion, where nonuniqueness is associated with decay like x^{-2} rather than x^{-3}.

This nonuniqueness is intimately connected with the conservation laws of the models. Before we enter into a detailed discussion of explicit solutions, we shall indicate this connection by reexamining the standard proofs of the conservation laws for the number of particles $N(t)$ and the energy $E(t)$ defined by

$$N(t) = \int_0^\infty dx\, F(x,t); \qquad E(t) = \int_0^\infty dx\, xF(x,t) \tag{4}$$

We assume $N(t)$ and $E(t)$ to be finite. Taking the appropriate moments of (3) and freely interchanging the order of integrations, one finds that

$$\dot{N} = 2E \cdot N - 2E \cdot N \tag{5}$$

$$\dot{E} = \Sigma \cdot N + E^2 - \Sigma \cdot N - E^2 \tag{6}$$

where

$$\Sigma(t) = \int_0^\infty dx\, x^2 F(x,t)$$

Since $N(t), E(t) < \infty$ all quantities in (5) are well defined, $\dot{N} = 0$ and thus $N(t) = N = \text{const}$. If, in addition, $F(x,t)$ decays faster than x^{-3} for large x, Σ is also well defined, and $E(t) = E = \text{const}$. This constitutes the standard proof of the conservation laws. If, however, $F(x,t) \simeq x^{-3}$, Σ does not exist, the expression for $\dot{E}$ is of the form "$\infty \cdot 0$", and a closer inspection of the steps leading to (6) becomes necessary. One easily shows that in the marginal case of $F(x,t) \simeq x^{-3}$, $\dot{E}$ can take any desired value. Such solutions correspond to an influx of energy from infinite energies at an (arbitrary) rate $\dot{E}(t)$.

In the above argument it was taken for granted that in the computation of time derivatives of conserved quantities, (N and E here) the operations $\partial/\partial t$ and $\int^\infty dx$ commute. This amounts to a regularity condition on $F(x,t)$. Whenever we restrict ourselves to nonsingular $F(x,t)$, the implication is that this regularity condition is met.

Similar statements can be made about the VHP model for a tagged particle in a bath of similar particles in thermal equilibrium. One derives the kinetic equation for this model from (3) by replacing $F(u-x,t)$ and $F(u-y,t)$ by the equilibrium distributions e^{-u+x} and e^{-u+y}, respectively. That is,

$$\partial_t F(x,t) = \int_x^\infty du\, e^{-u} \int_0^u dy \left[e^y F(y,t) - e^x F(x,t) \right] \tag{7}$$

or

$$(\partial_t + x + 1) F(x,t) = \int_x^\infty du\, e^{-u} \int_0^u dy\, e^y F(y,t) \tag{8}$$

Note that this equation can also be interpreted as describing a Rayleigh particle of mass M and with VHP interactions with an equilibrium bath of particles with mass m. It is easy to show that the only effect of a larger mass is to rescale the time to $\tau = tm/M$.

In the case of the linear VHP model, only $N(t)$ is a conserved quantity and integration over (8) yields

$$\dot{N} = E + N - E - N$$

If $E(t) < \infty$, i.e., if $F(x,t)$ decays faster than x^{-2}, $\dot{N} = 0$ and particle conservation is proved. In the marginal case when $F(x,t) \simeq x^{-2}$, E does not exist. Such solutions correspond to an influx of particles from infinite energies at an (arbitrary) rate $\dot{N}(t)$, as shown explicitly in Section 3.

In the next section we shall give an explicit solution of (8) in the general case when functions $F(x,t)$ decaying like x^{-2} (or slower) are allowed and, correspondingly, time-dependent $N(t)$ are permitted. We return to the nonlinear equation in Section 4.

3. EXPLICIT SOLUTIONS FOR THE LINEAR VHP MODEL

The kinetic equation (8) can be solved in terms of the Laplace transform of $F(x,t)$ in the energy variable, defined as

$$G(z,t) = \int_0^\infty dx\, e^{-zx} F(x,t) \tag{9}$$

Laplace transformation of (8) yields the first-order partial differential equation

$$G_t(z,t) - G_z(z,t) + \left[1 + \frac{1}{z(z+1)}\right]G(z,t) = \frac{1}{z}G(0,t) \tag{10}$$

where G_t and G_z are partial derivatives. As a result of the discussion of the previous section, we shall allow the number of particles to depend on time, stipulating the initial value to be unity:

$$G(0,t) = N(t), \qquad N(0) = 1 \tag{11}$$

The solution of (10) may be obtained by a transformation of variables

$$\begin{gathered} z = x, \qquad z + t = u \\ G(z,t) = G(x, u-x) \equiv y_u(x) \\ N(t) = G(0,t) = G(0, u-x) \equiv n_u(x) \end{gathered} \tag{12}$$

In these variables, Eq. (10) reduces to the following ordinary differential equation, u playing the role of a hidden parameter

$$y_u' - \left[1 + \frac{1}{x(x+1)}\right]y_u + \frac{n_u(x)}{x} = 0 \tag{13}$$

The general solution of (13) contains one integration constant which can be an arbitrary function $A(u)$ of u:

$$y_u(x) = \frac{xe^x}{x+1}A(u) + \frac{xe^x}{x+1}\int_\infty^x dy\, n_u(y)\frac{d}{dy}\left(\frac{e^{-y}}{y}\right)$$

In terms of the original variables the solution becomes,

$$G(z,t) = \frac{ze^z}{z+1}A(z+t) + \frac{ze^z}{z+1}\int_\infty^z dy\, N(z+t-y)\frac{d}{dy}\left(\frac{e^{-y}}{y}\right) \tag{14}$$

The arbitrary function A can be determined in terms of the Laplace transform of the initial energy distribution $F(x,0) = F_0(x)$

$$G(z,0) \equiv G_0(z) = \frac{ze^z}{z+1}A(z) + \frac{ze^z}{z+1}\int_\infty^z dy\, N(z-y)\frac{d}{dy}\left(\frac{e^{-y}}{y}\right) \tag{15}$$

Substitution of (15) into (14) gives, after a partial integration

$$\begin{aligned} G(z,t) = {} & \frac{N(t)}{z+1} + \frac{ze^{-t}}{(z+1)(z+t)}\left[(z+t+1)G_0(z+t) - 1\right] \\ & - \frac{ze^{-t}}{z+1}\int_0^t d\tau \frac{e^\tau}{z+t-\tau}\dot{N}(\tau) \end{aligned} \tag{16}$$

The general solution for $F(x,t)$ follows from (16) by Laplace inversion as

$$F(x,t) = N(t)e^{-x} - \frac{d}{dx}\left[e^{-(x+t)}\int_0^x dy\, e^{-yt}\Phi(y)\right] \tag{17a}$$

and is valid for all $t \geqslant o$. Here

$$\Phi(y) = \frac{d}{dy}\left[e^y\int_y^\infty du\, F_0(u)\right] + \int_0^t d\tau\, e^{y+y\tau+\tau}\dot{N}(\tau) \tag{17b}$$

and $N(t)$ is an arbitrary continuous function of t. If $N(t)$ would have a discontinuity at $t = t_a$, then $F(x,t)$ in (17) is not a solution at $t = t_a$.

The solution (17) explicitly displays the nonuniqueness of the initial value problem (8). For *any* given continuous function $N(t)$ with $N(0) = 1$, (17) solves the kinetic equation (8) for all $t \geqslant 0$ with the prescribed initial distribution $F(x,0) = F_0(x)$.

On the other hand it is clear that the only source of nonuniqueness in (17) is the variation in time of $N(t)$. The kinetic equation, however, gives a statistical description of a collision dynamics which conserves the number of particles. Thus solutions with a time-dependent $N(t)$, although mathematically permitted, are clearly unacceptable from a physical point of view.

The explicit solution also shows the intimate connection, discussed in Section 2, between a time-dependent $N(t)$ and high energy tails of the form x^{-2}. This connection is most easily found from an analysis of (16) for small z. For the moment, we shall assume that when z becomes small, $G_0(z) - 1 \simeq z^{\alpha-1}$, with $\alpha - 2 \geqslant \epsilon > 0$. From (16) one then finds

$$G(z,t) \simeq N(t) + \dot{N}(t)z\ln z + \mathcal{O}(z). \tag{18}$$

This singularity in $G(z,t)$ at $z = 0$ corresponds to an asymptotic decay of $F(x,t)$ for large x of the form

$$F(x,t) \simeq \dot{N}(t)/x^2 \qquad (x \gg 1). \tag{19}$$

As $F(x,t)$ is a distribution function, $\dot{N}(t) \geqslant 0$. A time dependent $N(t)$ therefore implies high energy tails decaying like x^{-2}.

The reason why solutions with a large x-behavior of the form $a(t)/x^2$ do not obey the law of number conservation can also be understood by considering the flux $\dot{N}(x_0,t)$ in the total number of particles with energy $x \leqslant x_0$ where $N(x_0) = \int_0^{x_0} dx\, F(x,t)$. It can be easily deduced from (8) that

$$\dot{N}(x_0) = x_0\int_{x_0}^\infty dy\, F(y) - e^{-x_0}\int_0^{x_0} dy\, e^y F(y) \tag{20}$$

If x_0 is sufficiently large, it follows that $\dot{N}(x_0,t) = a(t)\{1 + \mathcal{O}(x_0^{-2})\}$, that is there is an influx of particles coming from infinite energies. The coefficient $a(t)$ in the high energy tail equals the total flux $\dot{N}(t)$ of particles into the system.

Finally, we shall discuss the time evolution of the term in (16) containing the initial distribution $G_0(z)$, i.e., $F_0(x)$. Assume that $F_0(x)$ has an algebraic tail of the form $F_0(x) \simeq x^{-\alpha}$ with $\alpha > 2$. For simplicity, let α be noninteger. The singularity with Re$z < 0$, closest to $z = 0$—which determines the large-x behavior of $F(x, t)$—yields a dominant contribution

$$G(z, t) \simeq e^{-t} z (z + t)^{\alpha - 2} \tag{21}$$

as follows from (16) for finite t (with $t < 1$).

Laplace inversion of (21) yields terms that for any finite time are bounded by (essentially) $\exp[-(x + 1)t]$. [Integer α's (including $\alpha = 2$!) introduce logarithmic terms in (21), but do not alter this conclusion]. That is, even for $\alpha = 2$ the second term in (16), evolving from $F_0(x)$, gives exponentially decaying energy distributions for finite t. The corresponding contribution $[N_0(t) - 1]$ to $N(t)$ is highly singular at $t = 0$. Although $N_0(t) - 1$ remains constant $(= 0)$, and $\dot{N}_0(t = 0) = 0$, higher time derivatives diverge at $t = 0$. With $n + 1 \leqslant \alpha < n + 2$, the first n derivatives of $N(t) - 1$ remain zero, while all higher time derivatives diverge at $t = 0$.

In summary, we conclude the following: (i) Restriction of allowed functions to nonsingular ones decaying faster than x^{-2} for $x \gg 1$, ensures a unique solution of the initial value problem (8). This restriction also guarantees the validity of the conservation law, $N(t) = \text{const}$. (ii) If functions decaying like x^{-2} are permitted, infinitely many solutions of the initial value problem (8) exist, parametrized by the arbitrary continuous nondecreasing function $N(t)$. The coefficient in front of the x^{-2} tail is $\dot{N}(t)$. (iii) Initial algebraic decays, $F_0(x) \simeq x^{-\alpha}$ $(\alpha > 2)$, will for any finite time be changed into exponential decays, (essentially bounded by $\exp[-(x + 1)t]$).

4. THE NONLINEAR VHP MODEL

We now return to the nonlinear VHP model defined by the kinetic equation (3). In terms of the Laplace transform in the energy variable, $G(z, t)$, the number of particles and the energy are given as

$$G(0, t) = N(t) = 1$$

$$G_z(0, t) = -E(t); \qquad (E(0) = 1) \tag{22}$$

Since we shall always work with distribution functions for which the energy $E(t)$ exists, Eq. (5) guarantees conservation of the number of particles. Thus, with finite $E(t)$, no solution of (3) exists which has a time-dependent $N(t)$. We can therefore put $N(t) = 1$ for this model.

A Laplace transformation of (3) yields a first-order partial differential equation for $G(z, t)$:

$$G_t - G_z + E(t) G = (1/z)(1 - G^2) \tag{23}$$

When we include distribution functions decaying like x^{-3} for large energies, $E(t)$ is not necessarily a constant. The problem is thus to solve (23) with an arbitrary function $E(t)$. By a variable transformation analogous to (12), Ernst and Hendriks[5] were able to find the complete solution of (23) for the case $E(t) = 1$. For arbitrary $E(t)$, we have only been able to find a perturbative solution. In the following we shall restrict ourselves to the linearized version of (23).

4.1. The Linearized Case

We assume the system to be close to the equilibrium state with a total energy $E = 1$, and linearize around the corresponding distribution, e^{-x}:

$$\begin{aligned} F(x,t) &= e^{-x} + f(x,t) \\ G(z,t) &= \frac{1}{z+1} + g(z,t) \end{aligned} \tag{24}$$

with

$$\begin{aligned} \int_0^\infty dx\, f(x,t) &= g(0,t) = 0 \\ \int_0^\infty dx\, xf(x,t) &= -g_z(0,t) = E(t) - 1 \equiv \epsilon(t) \end{aligned} \tag{25}$$

With f, g, and ϵ treated as small quantities, Eq. (23) linearizes to

$$g_t - g_z + \left[1 + \frac{2}{z(z+1)}\right] g = -\frac{\epsilon(t)}{z(z+1)} \tag{26}$$

which should be solved subject to the initial conditions $g(z,0) = g_0(z)$ [and $\epsilon(0) = 0$)].

In this form the problem becomes similar to Eq. (10), and the same technique used to solve the linear model in Section 3 gives the following solution for (26) for all $t \geqslant 0$:

$$\begin{aligned} g(z,t) = &-\frac{z\epsilon(t)}{(z+1)^2} + \frac{z^2(z+t+1)^2}{(z+1)^2(z+t)^2} g_0(z+t) \\ &+ \frac{z^2 e^{-t}}{(z+1)^2} \int_0^t d\tau \frac{e^\tau}{z+t-\tau} \dot{\epsilon}(\tau) \end{aligned} \tag{27}$$

This result is completely analogous to (16) and its Laplace inversion to (17). It satisfies the initial condition $g(z,0) = g_0(z)$, $\epsilon(0) = 0$, and contains the arbitrary continuous function $\epsilon(t)$. The discussion at the end of Section 3 applies also to this case with one slight modification. The last term in (27) gives a dominant singularity for small z of the form

$$g(z,t) \simeq -\dot{\epsilon}(t) z^2 \ln z + \mathcal{O}(z^2) \tag{28}$$

corresponding to a high-energy tail

$$f(x,t) \simeq 2\dot{\epsilon}(t)/x^3 \qquad (x \gg 1) \tag{29}$$

implying $\dot{\epsilon}(t) \geqslant 0$. A unique solution to the initial value problem and conservation of the energy is therefore guaranteed in this case if one restricts the allowed functions to those decaying faster than x^{-3} for high energies. Initial algebraic decays $F_0(x) \simeq x^{-\alpha}$ with $\alpha > 2$ [$E(t) < \infty$!] will be changed into exponential decays for finite times.

4.2. The Nonlinear Case

It is obvious a priori that the nonlinear equation (23) is similar to its linearized version with respect to the nonuniqueness problem. For any given $E(t)$, the solution of the first-order partial differential equation will contain an arbitrary function of the argument $(z + t)$. This function is determined by the initial distribution $F(x,0) = F_0(x)$, but the arbitrariness associated with $E(t)$ remains. Consequently, when a time-dependent energy is permitted, an infinite number of solutions of the nonlinear kinetic equation exists.

Even without knowing the explicit form of the solution, one can discuss its high-energy tail. This is most conveniently done by solving (23) for small z. To this end we introduce

$$G(z,t) = 1 - zE(t) + \Delta(z,t) \tag{30}$$

when $E(t)$ is a continuous function of t.

From (22) one concludes that $\Delta(z,t)$ vanishes faster than linearly in z as $z \to 0$. Insertion of (30) into (23) yields, to dominant order in z,

$$z \frac{d\Delta}{dz} - 2\Delta + z^2 \dot{E}(t) = 0 \qquad (z \to 0) \tag{31}$$

which implies that

$$\Delta(z,t) \simeq -\dot{E}(t) z^2 \ln z \qquad (z \to 0) \tag{32}$$

The high-energy asymptotics of $F(x,t)$ follows from (32) as

$$F(x,t) \simeq 2\dot{E}/x^3 \qquad (x \gg 1) \tag{33}$$

which is precisely the same result as for the linearized problem.

Thus, also for the nonlinear problem a unique solution (which conserves energy) is guaranteed if one restricts the allowed functions $F(x,t)$ to those decaying faster than x^{-3}. This solution (with $E = 1$) was found by Ernst and Hendriks to be

$$G(z,t) = \frac{\phi(z+t) + (z-1)e^{-t}}{(z+1)\phi(z+1) - e^{-t}}$$

where $\phi(z)$ is determined from the requirement that $G(z,0) = G_0(z)$.

5. THE EIGENVALUE PROBLEM

Eigenvalues and eigenfunctions are important tools in analyzing linear or linearized kinetic equations. It is therefore of interest to study the models discussed in the two previous sections from this point of view. In order to do so, we write the linear Boltzmann equation (7) and the linearized version of (3) as

$$\partial_t F = -\Omega F \tag{34}$$

and study solutions of the form $F(x,t) = F_\lambda(x)e^{-\lambda t}$. This leads to the eigenvalue problem

$$\Omega F_\lambda = \lambda F_\lambda \tag{35}$$

In the Hilbert space defined by the inner product

$$(A,B) = \int_0^\infty dx\, e^x A(x)B(x) \tag{36}$$

the Boltzmann operator Ω is self adjoint, i.e., $(A,\Omega B) = (\Omega A, B)$, and non negative-definite, i.e., $(A,\Omega A) \geqslant 0$.

For our models we shall explicitly demonstrate the following results: The eigenfunctions in this function space are orthogonal and form a complete set of basis functions. The spectrum consists of an isolated eigenvalue at $\lambda = 0$ and a continuum for $\lambda \geqslant 1$. In addition, there exist eigenfunctions *outside* this Hilbert space with a continuous spectrum for $\lambda < 1$ ($\lambda \neq 0$). These eigenfunctions violate a conservation law, as found for the hard sphere case by Cornille and Gervois.[2]

5.1. The Linear VHP Model

It is convenient to start from Eq. (10). With $G(z,t) = G_\lambda(z)\exp(-\lambda t)$ gives the ordinary differential equation

$$-G_\lambda'(z) + \left[1 - \lambda + \frac{1}{z(z+1)}\right]G_\lambda(z) = \frac{1}{z}G_\lambda(0) \tag{37}$$

where a prime denotes differentiation with respect to z. The solution reads

$$G_\lambda(z) = C\frac{z}{z+1}e^{(1-\lambda)z} + G_\lambda(0)\frac{z}{z+1}\int_z^\infty dy\,\frac{y+1}{y^2}e^{-(1-\lambda)(y-z)} \tag{38}$$

where C is an arbitrary normalization constant. In order for $G_\lambda(z)$ to be the Laplace transform of an $F_\lambda(x)$, it must be bounded for large positive z. Equation (38) offers two possibilities only:

(i) $\lambda \geqslant 1$: $C \neq 0$, $G_\lambda(0) = 0$
(ii) $\lambda < 1$: $C = 0$, $G_\lambda(0) \neq 0$

For $\lambda \geqslant 1$ inverse Laplace transformation of (38) with $C = 1$ yields

$$F_\lambda(x) = \delta(x+1-\lambda) - e^{-x-1+\lambda}\Theta(x+1-\lambda), \qquad \lambda \geqslant 1 \tag{39}$$

where $\delta(x)$ is the Dirac function and $\Theta(x)$ the step function. For $\lambda < 1$ Laplace inversion with $G_\lambda(0) = 1$ gives

$$F_\lambda(x) = e^{-x} + \lambda\frac{d}{dx}\int_0^x dy\,\frac{e^{-y}}{x-y+1-\lambda}, \qquad \lambda < 1 \tag{40}$$

Among all the eigenfunctions with $\lambda < 1$, only the one with $\lambda = 0$, i.e., $F_0(x) = e^{-x}$, belongs to the Hilbert space (36). This follows from the fact that the asymptotics of the last term in (40) for large x is

$$F_\lambda(x) \simeq -\frac{\lambda}{x^2} + \mathcal{O}(x^{-3}) \tag{41}$$

in agreement with (19).

It is evident that the eigenfunctions outside Hilbert space give time-dependent contributions to the number of particles. For arbitrary $\lambda < 1$, the second term in (40) integrates to zero and the first term gives

$$N_\lambda(t) = e^{-\lambda t}\int_0^\infty dx\,F_\lambda(x) = e^{-\lambda t}$$

In other words, the eigenfunctions outside Hilbert space violate particle conservation.

The functions $F_0(x)$ and $F_\lambda(x)$ with $\lambda \geqslant 1$ form a complete orthogonal set of basis functions in the Hilbert space (36) and one easily verifies the orthogonality relation

$$\begin{aligned} &\int_0^\infty dx\,e^x F_0(x)F_\lambda(x) = 0 \\ &\int_0^\infty dx\,e^x F_\lambda(x)F_{\lambda'}(x) = e^{\lambda-1}\delta(\lambda-\lambda') \end{aligned} \qquad (\lambda, \lambda' \geqslant 1)$$

and the completeness relation

$$e^x F_0(x)F_0(x') + \int_1^\infty d\lambda\,e^{x+1-\lambda}F_\lambda(x)F_\lambda(x') = \delta(x-x')$$

5.2. The Linearized VHP Model

Next we turn to the eigenvalue problem for the linearized VHP model. The complete solution is obtained only if one does not impose any a priori conditions on the eigenfunctions, such as (21). Then $G(z,t)$ satisfies the equation

$$G_t - G(0)G_z - G_z(0)G = \frac{1}{z}\left[G^2(0) - G^2\right] \tag{42}$$

The eigenvalue equation is obtained when one puts

$$G(z,t) = \frac{1}{z+1} + e^{-\lambda t}g_\lambda(z) \tag{43}$$

and linearizes in $g_\lambda(z)$:

$$g'_\lambda - \left[1 - \lambda + \frac{2}{z(z+1)}\right]g_\lambda = \left[\frac{1}{(z+1)^2} - \frac{2}{z}\right]g_\lambda(0) - \frac{1}{z+1}g'_\lambda(0) \tag{44}$$

The prime denotes differentiation with respect to z.

As explained in Section 2, internal consistency dictates that the solutions of (42) and (44) must conserve the number of particles. Putting $z = 0$ in (43) one must therefore distinguish between two cases:

(a) $\lambda \neq 0, \quad g_\lambda(0) = 0$

(b) $\lambda = 0, \quad g_\lambda(0) \neq 0$

The general solution of (44) in case (a) is readily found to be

$$g_\lambda(z) = \left(\frac{z}{z+1}\right)^2 e^{(1-\lambda)z}\left[C + g'_\lambda(0)\int_z^\infty dy\,\frac{y+1}{y^2}e^{-(1-\lambda)y}\right] \tag{45}$$

where C is an arbitrary constant. By the same arguments as for the linear model, the case (a) splits into two distinct possibilities:

(a1) $\lambda \geqslant 1: \quad C \neq 0, \quad g'_\lambda(0) = 0$

(a2) $\lambda < 1: \quad C = 0, \quad g'_\lambda(0) \neq 0$

For $\lambda \geqslant 1$, inverse Laplace transformation of (45) yields (with $C = 1$)

$$f_\lambda(x) = \delta(x+1-\lambda) + e^{-x-1+\lambda}(x-1-\lambda)\Theta(x+1-\lambda) \qquad (\lambda \geqslant 1) \tag{46}$$

For $\lambda < 1$ one finds from (45), with $g'_\lambda(0) = -1$ after some calculation

$$f_\lambda(x) = (x-1)e^{-x} - \lambda\left(\frac{d}{dx}\right)^2\int_0^x dy\,\frac{ye^{-y}}{x-y+1-\lambda} \qquad (\lambda < 1) \tag{47}$$

For large x, the eigenfunctions $f_\lambda(x)$ with $\lambda < 1$ decay like $-2\lambda/x^3$ [in agreement with (29)] and do not belong to the Hilbert space (36) (except for $\lambda = 0$). Furthermore, $\int_0^\infty dx\, f_\lambda(x)$ vanishes, whereas $\int_0^\infty dx\, x f_\lambda(x) \neq 0$, so that these eigenfunctions violate energy conservation. Notice that negative eigenvalues are allowed. This is not in conflict with the H-theorem since the non negative-definite character of Ω can only be proved for functions belonging to the Hilbert space (36).

Finally, we consider the case (b) where $\lambda = 0$. The corresponding differential equation (44) contains two arbitrary constants, $g_0(0)$ and $g_0'(0)$. The two independent solutions can be chosen to be

$$f_0^{(1)}(x) = e^{-x}, \qquad f_0^{(2)}(x) = (x-1)e^{-x} \tag{48}$$

The two solutions (48) together with the $f_\lambda(x)$ of (46) with $\lambda \geqslant 1$, form a complete and orthogonal basis for the Hilbert space (36).

6. CONJECTURES

In this section we summarize the general arguments of Section 2, the explicit results in Sections 3 and 4, and certain results obtained by others, in a form of a few conjectures on kinetic equations for models with transition rates that are increasing functions of the state variable.

To be specific, we shall consider the Boltzmann equation for a d-dimensional dilute gas in an isotropic and spatially uniform state:

$$\partial_t f(v,t) = \int d\mathbf{w} \int d\hat{n}\; gI(g,\chi)\left[f(v',t)f(w',t) - f(v,t)f(w,t)\right] \tag{49}$$

Here $I(g,\chi)$ is the differential cross section for the collision $(\mathbf{v},\mathbf{w}) \to (\mathbf{v}',\mathbf{w}')$ in terms of the relative velocity $g = |\mathbf{w} - \mathbf{v}|$ and the scattering angle χ. The unit vector $\hat{n}$ is defined by $\hat{n} = \hat{g}'$ such that $\hat{n} \cdot \hat{g} = \cos\chi$.

We shall specify the model further by assuming that the interaction potential has the form const $\cdot\, r^{-n}$. In that case one has[7,6]

$$gI(g,\chi) = g^\gamma \alpha(\chi) \tag{50}$$

with

$$\gamma = 1 - 2(d-1)/n \tag{51}$$

Maxwell molecules are defined in all dimensions as having velocity-independent collision rates, i.e., $\gamma = 0$ or $n = 1/2(d-1)$. Hard d-dimensional spheres correspond to $n \to \infty$, i.e., $\gamma = 1$. For molecules "harder" than Maxwell molecules $0 < \gamma \leqslant 1$. The VHP model cannot be derived from any Hamiltonian and corresponds to $\gamma = 2$ (hence its name).

The number of particles and the energy (in suitable units) are defined as

$$N(t)=\int d\mathbf{v}\, f(v,t)=\int d\hat{v}\int_0^\infty dv\, v^{d-1}f(v,t) \tag{52}$$

$$E(t)=\int d\mathbf{v}\, \frac{1}{2}v^2 f(v,t)=\frac{1}{2}\int d\hat{v}\int_0^\infty dv\, v^{d+1}f(v,t) \tag{53}$$

In order to prove that energy is conserved, i.e., that $\dot{E}=0$, one must calculate the difference of two integrals of the form

$$\int d\mathbf{v}\, v^2\int d\mathbf{w}\int d\hat{n}\, \alpha(\chi)|\mathbf{w}-\mathbf{v}|^\gamma f(v,t)f(w,t) \tag{54}$$

Disregarding the well-understood problem[7] of separating the two integrals due to the form of $\alpha(\chi)$ at small scattering angles, one arrives by simple power counting at v-integrals of the type

$$\int^\infty dv\, v^{d-1+2+\gamma}f(v,t) \tag{55}$$

The interchange of the order of integrations used in the standard proof of $\dot{E}=0$ requires that the integral (55) converges, i.e., that $f(v,t)$ decays faster than $1/v^{d+2+\gamma}$. For positive γ this is a more stringent requirement than that necessary for the existence of the energy (53). The problem therefore seems to contain all the features discussed in Sections 2–4, and one is led to the following conjectures:

(1) For nonsingular velocity distributions $f(v,t)$ that decay faster than $1/v^{d+2+\gamma}$ both N and E are conserved quantities and the initial value problem has a unique solution.

(2) When distributions decaying like $1/v^{d+2+\gamma}$ are allowed, there exist an infinite number of solutions of the initial value problem, parametrized by the arbitrary function $E(t)$.

(3) Similar statements can be made about the self-diffusion or Rayleigh particle problem with $(d+\gamma)$ replacing $(d+2+\gamma)$ and $N(t)$ replacing $E(t)$.

(4) There exists a continuous spectrum of eigenfunctions with $-\infty<\lambda<\lambda_0$, excluding $\lambda=0$, where λ_0 is a model-dependent positive constant. For $\gamma>0$, the corresponding eigenfunctions, decaying for large v like $1/v^{d+2+\gamma}$ (like $1/v^{d+\gamma}$ in the self-diffusion or Rayleigh particle problem) violate the law of energy conservation (particle conservation in the self-diffusion case). Furthermore, these eigenfunctions do not belong to the standard Hilbert space in which the linearized collision operator is self-adjoint and positive definite.

(5) For particles softer than Maxwell molecules ($\gamma < 0$), the solution of the initial value problem is unique, and the conservation laws hold, provided only that the relevant conserved quantity exists.

In this paper we have shown these conjectures to be true for the VHP model, which describes a two-dimensional ($d = 2$) gas with a collision rate $gI(g\chi) \sim g^2$ ($\gamma = 2$). The conjectures are also supported by results on the eigenvalue problem for hard sphere systems obtained by Cornille and Gervois,[2] and the (negative) results for arbitrary γ by Hauge and Praestgaard.[8]

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