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Nonunique stationary states in driven collisional systems with application to plasmas

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We study a driven particle system whose velocity distribution $f(v,t)$ satisfies a Boltzmann equation with a nonlinear collision term, and linear terms representing collisions with thermalized particles of another species having a specified Maxwellian distribution, and a driving force. We prove that when the nonlinear terms dominate, $f(v,t)$ is kept close to a Maxwellian distribution $M(v;u(t),e(t))$ with parameters $u(t)$ and $e(t)$ satisfying a system of nonlinear equations—the "hydrodynamic" equations. This result holds even when their stationary solution is nonunique, corresponding to a dynamical phase transition for f in such systems. We apply our results to a model of a partially ionized spatially homogeneous plasma in an external field E.

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Our understanding of nonequilibrium phenomena is very incomplete at the present time. In particular, there is no general microscopic theory of the nonequilibrium phase transitions observed in fluids, plasmas, chemical reactions, etc. Theories of such phenomena are at present based entirely on solutions of hydrodynamical type equations. These show how the great variety and complexity of nonequilibrium behavior can arise from the nonlinearities in the macroscopic equations [1]. It has not been possible however, so far, to derive these hydrodynamical equations, *in the interesting parameter ranges*, from the microscopic dynamics. All we have microscopically are molecular dynamic simulations of systems of particles ($\leq 10^6$) interacting via simple pair potentials, and the study via analytic means and/or computer simulations of highly simplified (lattice) model systems [2,3]. Lacking thus far are proofs of the existence of a nonequilibrium phase transition in any microscopic models of a physical system with Hamiltonian type dynamics.

Given the notorious difficulties encountered in deriving hydrodynamic equations from Hamiltonian dynamics even for systems with smooth macroscopic behavior [4] it seems reasonable to consider first the intermediate problem of starting with a kinetic description of the system using Boltzmann type equations [5]. Even for this level of microscopic description all the known proofs for the validity of hydrodynamic equations involving spatially nonuniform systems work only when these equations have unique smooth solutions [5]. To overcome this difficulty we consider here a spatially uniform system driven away from equilibrium by an externally imposed force. We prove, in simplified but still recognizable physical situations, that when the nonlinear collisions are sufficiently strong relative to the linear effects, the kinetic description closely tracks the macroscopic equations even when the driving is sufficiently strong for the latter to predict phase transitions. More precisely, we show that in this regime, the one particle velocity distribution function $f(v,t)$ is kept close to a Maxwellian $M(v;u(t),e(t))$ with parameters $u(t)$ and $e(t)$ satisfying a system of nonlinear equations, which are the "hydrodynamic" equations, and that this is true even when the stationary solutions of these equations are nonunique.

The methods developed to prove these results use the entropy production in collisions to control the distribution function. They apply to a wide class of spatially homogeneous cases and will hopefully be useful also for nonuniform systems. However, even in the spatially homogeneous settings considered here, expansion methods of the Chapman-Enskog type, usually the basic tool for establishing a connection between kinetic and hydrodynamic descriptions, are not applicable in the strongly driven range in which the nonuniqueness occurs.

Here we shall focus on a simple model inspired by some earlier work on a partially ionized plasma in a constant external electric field E [6]. An approximate description via self-consistent moments led there to a coupled set of nonlinear equations for the stationary electron current u and temperature T whose stationary solution yielded bistable behavior for certain ranges of E. The onset of this behavior can be understood as a transition, when the speed of the electrons increases with the field, from a low energy regime in which there is a strong coupling to the ions to a high energy regime where this coupling essentially vanishes. In the absence of electron–neutral-species collisions this leads to a runaway situation [7]. With neutral species present the stationary distribution would be smooth as E changes in the regime where one can neglect the nonlinear coupling induced by the electron-electron collisions. This is the case when the electron density is very low. One can then use the "electron swarm" approximation [8]. At higher densities the *e*-*e* collisions produce cooperative effects which can lead to instabilities.

In the present work we give a rigorous mathematical derivation of the validity of a macroscopic description and *ipso facto* of the existence of nonunique stationary states for a class of such driven kinetic models in which the collisions between the particles are "dominant" and prevent the distribution from deviating too much from a Maxwellian. This means that $f(v,t)$ has to stay close, in the function space of velocity distributions, to the manifold of Maxwellians parametrized by a mean velocity and temperature. This can lead under suitable conditions to the bifurcation of the unique stationary fixed point in this space valid for small E, to multiple stationary states for larger E. (At very large E the solution may again be unique.) For concreteness we shall refer from now on to our particles as electrons and use the general language of plasma physics even though the idealizations we make may not be justified in some situations.

Our starting point is a Boltzmann type equation [5–8] for the time evolution of the spatially homogeneous electron velocity distribution function $f(v,t)$

$$\frac{\partial f(v,t)}{\partial t} = -E\cdot\nabla f + Lf + \epsilon^{-1}Q(f), \tag{1}$$

where ∇ is the gradient with respect to v and the mass and charge of the electron have been set equal to unity. The linear term Lf represents collisions with the ions and neutral species; it is linear because we assume these strongly coupled massive components to have a specified time independent Maxwellian distribution (the generalization to the case where the ions are also out of equilibrium is straightforward). We have introduced a coupling parameter ϵ^{-1} in front of the nonlinear term $Q(f)$ representing e-e collisions. This is frequently done in kinetic theory [4]: its significance will become apparent later.

The effect of L is to bring f to equilibrium with the "thermal bath" represented by the massive particles, i.e., to a Maxwellian distribution M_n with zero mean velocity and an *a priori* specified temperature T_n (set here equal to unity) of the neutral species and ions; $M_n(v)\equiv(2\pi)^{-3/2}\exp[-v^2/2]$. In the absence of the external field E, $f(v,t)$ would approach $M_n(v)$, as $t\to\infty$, since the collisions between the electrons, represented by $Q(f)$, conserve momentum and energy and $Q(f)$ vanishes when f is *any* Maxwellian. When $E\neq 0$ the electric field drives f away from equilibrium with the ions and neutral species while $Q(f)$ tries to bring the distribution to a general Maxwellian $M(v;u,e)=(2\pi)^{-3/2}\exp[-(v-u)^2/2T]$ with the instantaneous value of momentum $u(t)\equiv\int_{\mathbb{R}^3}vf(v,t)d^3v$ and energy $e(t)\equiv\frac{1}{2}\int_{\mathbb{R}^3}v^2f(v,t)d^3v \equiv\frac{1}{2}u^2+\frac{3}{2}T$. Just how effective these collisions are in keeping $f(v,t)$ close to a Maxwellian is formally controlled by the parameter ϵ, which measures some effective mean time between electron-electron collisions. Our results apply when ϵ is "small enough." In physical terms we consider situations in which the e-e collisions dominate the electron–neutral-species interactions and the effects of the external field. This essentially requires that the electron density (or ionization fraction) not be too small and the electric field (in suitable units) not too large; see [6] for a discussion of appropriate physical situations. When the field is large we certainly have to worry about deviations from the Maxwellian in the tail of the distribution.

To carry out a mathematical proof one needs some conditions on the operators L and Q. We state the main properties we need and then give the simplest explicit example which still contains the essence of the phenomena. More physical and therefore more complicated models will be described elsewhere [9]. As already mentioned, the collision kernel Q is such that mass, momentum, and energy are conserved in a collision. Moreover, the entropy production singles out the class of Maxwellian distributions as the only one for which $Q(f)=0$. The operator L is assumed to conserve only the particle number, but the rates at which momentum and energy are changed may not be of the same magnitude: the latter being reduced by the ratio of electron to neutral masses for elastic collisions. The crucial conditions on L, beyond the conservation of mass, are that it is able to remove energy and momentum from the system at a rate sufficient to permit the establishment of a stationary state. At a more technical level, momentum bounds and smoothness conditions are required for L and Q [9]. All these conditions are satisfied for fairly realistic kinetic models; see also [10].

The *simplest* model having the desired mathematical properties which still keeps much of the essential of the physics is to choose for L a combination of two terms: (a) a relaxation term with constant frequency ν which conserves energy but makes the electron velocity isotropic (corresponding to the mass ratio of neutral species to electrons being infinite); (b) a Fokker-Planck term mimicking the energy loss in collisions with both neutral species and ions. To take into account the fact that the energy transfer to the ions decreases as the speed of the electrons increases we make the diffusion $D(v)$ in the Fokker-Planck term decrease with v to a constant nonzero value. This gives

$$Lf(\mathbf{v},t)=\nu[\bar{f}-f]+\nabla\cdot\left[D(v)M_n(v)\nabla\left(\frac{f(v)}{M_n(v)}\right)\right], \tag{2}$$

where $\bar{f}(|v|,t)$ is the sphericalized velocity distribution obtained from $f(v,t)$ by averaging over angles. For $D(v)$ we choose a form which will lead to explicit simple expressions for the hydrodynamic equations later

$$D(v)=a\exp(-b|v|^2/2)+c \tag{3}$$

for some strictly positive constants a, b, and c. For $Q(f)$ we take the Bhatnagar-Gross-Krook (BGK) model of the Boltzmann collision kernel [5],

$$Q(f)=M_f-f, \tag{4}$$

where for any velocity distribution f, M_f denotes the Maxwellian distribution with the same mean and variance as f.

Since $Q(f)$ drives f close towards the Maxwellian manifold M_f we should have, formally at least, that in the limit $\epsilon\to 0$, f will equal M_f for all time $t>0$. To keep track of the evolution of f we would then need only keep track of the moments $u(t)$ and $e(t)$. Our first theorem shows that this situation actually holds for small, but positive, values of ϵ.

Theorem 1. Let f be a solution of (1) with $f(v,0)=M_0(v;u(0),e(0))$ some arbitrary Maxwellian. Then there is a constant K depending only on ν, a, b, c, $|E|$, and $e(0)$ such that for all positive t,

$$\int_{\mathbb{R}^3}|f(v,t)-M_{f(\cdot,t)}(v)|d^3v\leq K\epsilon^{1/2}. \tag{5}$$

The requirement that $f(v,0)$ be Maxwellian is not essential, otherwise there is an initial layer, $t<t_0(\epsilon)$, with $t_0(\epsilon)\to 0$ as $\epsilon\to 0$, after which (5) is valid [9].

Our next problem is then to find the moments $u(t)$ and $e(t)$. Using the prescription $f=M_f$, which would be valid when "$\epsilon=0$," one easily obtains for the choice (2)–(4),

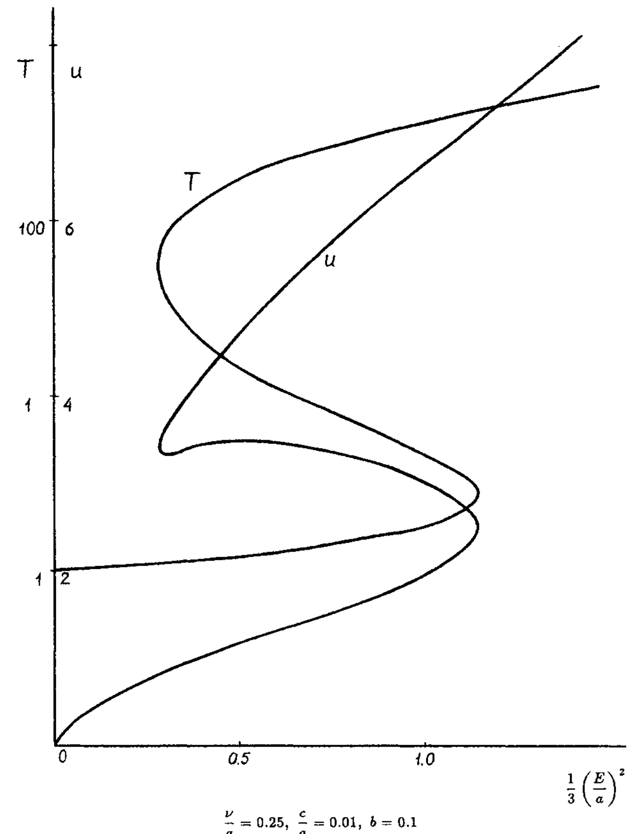

FIG. 1. Plot of electron temperature T and mean velocity u obtained from the solution of Eq. (6) as a function of the electric field.

$$\frac{du}{dt}=F(u,e)=E-u\left[\nu+c+a\,\exp(-w)\frac{1+b}{(1+b/\beta)^{5/2}}\right], \tag{6a}$$

$$\frac{de}{dt}=G(u,e)=Eu-c[2e(1-\beta)+\beta u^2] - \frac{a\,\exp(-w)}{(1+b/\beta)^{5/2}}\left[2e(1-\beta)+u^2\left(\beta-b\,\frac{1-\beta}{b+\beta}\right)\right], \tag{6b}$$

where $\beta^{-1}=T=\frac{2}{3}(e-\frac{1}{2}u^2)$, and $w=bu^2/2(1+bT)$. Solving (6) for the stationary values of u and e gives, for certain ranges of E, three such pairs, two stable, and one unstable; see Fig. 1.

For a small ϵ we prove that the moments $u_\epsilon(t)$ and $e_\epsilon(t)$ satisfy the equations $du_\epsilon/dt=F(u_\epsilon,e_\epsilon)+\epsilon^{1/4}\gamma(t)$ and $de_\epsilon/dt=G(u_\epsilon,e_\epsilon)+\epsilon^{1/4}\eta(t)$ with $\gamma(t)$ and $\eta(t)$ bounded uniformly in t. This shows that if $u(0)$ and $e(0)$ are inside a stable region of the (u,e) plane for a dynamical system described by the differential equations (6) then $u_\epsilon(t)$ and $e_\epsilon(t)$ will stay close to the solutions $u_0(t),e_0(t)$ of (6). Consequently, by Theorem 1, $f_\epsilon(v,t)$ will stay close to $M(v;u_0(t),e_0(t))$. Moreover, when there is a stable fixed point of (6), (u^*,e^*), then it will have a basin of attraction with a stable interior. Starting with an initial $u(0)$ and $e(0)$ in such a region $f(v;t)$ will stay close to $M(v;u^*,e^*)$ forever. This leads to the following result for the stationary solutions of (1).

Theorem 2. Let (u^*,e^*) be a stationary point of (6) and T^* the corresponding temperature. Then for ϵ small enough, there exists a unique stationary point in an ϵ neighborhood of $M(v;u^*,T^*)$, and there are no other stationary solutions of (1) that do not correspond to stationary solutions of (6).

Moreover, if (u^*,e^*) is a stable stationary solution of (6), then there is a neighborhood of $M(v;u^*,T^*)$ that is stable for (1). More precisely, given any $\delta>0$, there is an ϵ greater than zero such that if

$$\|f(v,0)-M(v,u^*,T^*)\|\leq\epsilon \tag{7}$$

then the $f(v,t)$ which solves (1) with the value of ϵ satisfies

$$\|f(v,t)-M(v;u^*,T^*)\|\leq\delta \tag{8}$$

for all $t\geq 0$. Likewise, the unstable stationary solutions of (6) can be shown to correspond to unstable stationary solutions of (1).

The detailed description of the stationary solutions follows by their almost explicit construction. In fact, one can show that the moments (u_ϵ,e_ϵ) of the stationary solution f_ϵ satisfy a closed equation of the form $F(u_\epsilon,e_\epsilon)+\epsilon\tilde{F}_\epsilon(u_\epsilon,e_\epsilon)=0$, $G(u_\epsilon,e_\epsilon)+\epsilon\tilde{G}_\epsilon(u_\epsilon,e_\epsilon)=0$, with suitable $\tilde{F}_\epsilon$ and $\tilde{G}_\epsilon$. An application of the implicit function theorem then yields (u_ϵ,e_ϵ) in an ϵ neighborhood of (u^*,e^*). These moments determine M_{f_ϵ} and hence f_ϵ itself, using the stationary equation. This construction is peculiar to the choice of the BGK collision kernel, but the results extend to more general collisions.

Our proof of Theorems 1 and 2, whose details will be presented elsewhere [9], has several ingredients. First we prove by direct calculations and "interpolation inequalities" some *a priori* bounds on the moments and smoothness of $f(v,t)$. We then prove an entropy production inequality to get strong bounds on the tendency of the BGK operator to keep f nearly Maxwellian.

To get an idea of how the latter works consider the time evolution of the system's "free energy" $A(t)=[e-T_n s]$

$$A(t)=\int[\tfrac{1}{2}v^2+\ln f]f(v,t)d^3v = \int \ln(f/M_n)f\,d^3v-\tfrac{3}{2}\ln 2\pi, \tag{9}$$

where T_n is the ion and neutral-species temperature which we have set equal to 1. Using the properties of L and Q we find after some manipulations

$$\frac{d}{dt}A(t)=E\cdot u-4\int D(v)M_n(v)[\nabla\sqrt{f/M_n}]^2d^3v - \frac{1}{\epsilon}\int \ln(f/M_f)[f-M_f]d^3v. \tag{10}$$

Combining (10) with other inequalities and bounds leads to the inequality

$$\int \ln(f/M_f)f(v,t)d^3v \leq \epsilon K, \tag{11}$$

where K is a constant. This shows that f has to stay close to M_f when ϵ is small.

As already mentioned, our methods allow us to treat more realistic collision kernels L and Q. In particular, we can choose for $Q(f)$ a real Boltzmann binary (linear) collision operator with suitable cross sections e.g., one appropriate for a Maxwell force law. We can even choose a combination of a Landau operator suitable for plasmas [7] and a Maxwell one.

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