ENTROPY AND KINETIC THEORY FOR A CONFINED GAS

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1. Introduction. A well-known theorem in the classical kinetic theory for a gas states that the entropy is an increasing function of time. However, in order to obtain this theorem for a *confined* gas, some assumption about molecular response to the container wall is required. For example, it is enough to suppose that the wall reflects the molecules specularly [4].

The need for a "wall hypothesis" in the entropy theorem certainly comes as no great surprise. After all, entropy is a measure of chaos in the system of molecules which compose the gas. It may be that the wall contributes to a greater chaos among the molecules. But it is also conceivable that the wall somehow orders the behavior of the molecules and supplies information to the gas. We might well ask, when does the presence of the wall lead to greater disorganization among the molecules and when does it lead to greater organization?

Unfortunately, the answer to this question is not obvious from previous versions of the entropy theorem. The difficulty lies in the term which represents the wall's contribution to entropy growth. The question we are asking is, when is this "wall term" positive and when is it negative? In the proof of a typical entropy theorem, the wall term is made positive or zero only by invoking some kind of *ad hoc* hypothesis about the wall, for example, that it reflects molecules specularly. Authors give sufficient, but not necessary, conditions for the wall term to be positive. Perhaps Cercignani [2] describes the state of research most honestly. In assessing the general relation between boundary conditions and increasing entropy, he says simply (p. 58), "no investigation has been done on this subject, to the best of my knowledge."

This paper contains a new version of kinetic theory in which a general wall hypothesis is incorporated into the model from the beginning. In this context we develop the entropy theorem further and produce a new theorem in which the sign of the wall term is shown to depend only on simple properties of wall-molecule interactions. Both necessary and sufficient conditions are given for the wall term to be positive. Explicit examples are constructed in which the entropy is a strictly *decreasing* function for all time because the wall steadily provides information to the system of molecules. Furthermore, it is shown that this entropy decrease can even occur in gas flows for which the most common of all boundary conditions—no slip—applies at the wall.

In order to add a wall hypothesis correctly to the axioms of kinetic theory, it is necessary to re-state the theory as a whole. For this reason we are forced to consider just what constitutes an axiomatic kinetic theory. This is partly a philosophical problem, but we cannot avoid it. In this paper we view a kinetic theory as having three components: input data, axioms, and motivation. Each item of data is a well-defined mathematical object from analysis, for example, a number, a set, or a function. The axioms take the form of an initial value problem for some probability distribution on possible states of the gas. The problem is constructed in a definite way from the input data, and the solution to the problem is interpreted as a description of the evolution of the probable state of the gas from its probable initial state. Motivation for the data and axioms is, of course, unnecessary to the mathematics but essential to the physics. We need to know how to identify the input data and the output probability function with aspects of physical experience. The motivational arguments tell us this, guide us in our choice of axioms, and give significance to our theorems.

There are historically at least two distinct ways to construct a molecular model for a gas. (Here "molecule" means "point mass"). The first, which we refer to as "model 1", assumes that the molecules, experiencing various forces of attraction and repulsion, move according to Newton's laws. Among the input data for this model are, for example, the functions which represent these forces. The basic axiom in the model is called *conservation of probability*. It describes the evolution in time of a probability distribution F over all possible states of the system of molecules.

The second approach to a molecular theory of a gas, which we call "model 2", is quite different. In this case, a probability distribution f describes, not the probable state of the entire system of molecules, but that of a single "typical" molecule. The many-body problem which underlies model 1 is forgotten, and only certain stylized pairwise molecular interactions are considered. A function which represents these interactions is part of the input data. In this case, the axiom which governs the evolution in time of the function f is called the *Maxwell-Boltzmann equation*.

In this paper, the assumption made about molecular reaction to the container wall (in both models 1 and 2) is conceptually simple, and it is not new. It was proposed and studied for a model 1 gas in an earlier work [6] by M. Shinbrot and myself. We supposed that when a molecule encounters the wall, it is "reflected", that is, its incident velocity is instantaneously converted to a reflected velocity by a definite rule called a "reflection law".

Interestingly, this is not so very different from the kind of assumption made about molecular interactions in the *interior* of the gas when defining the Maxwell-Boltzmann axiom. Here, when two molecules interact, their incident velocities are assumed to be converted instantaneously to scattered velocities by a definite rule called (in this paper) a "collision law". (For an example of this approach, see [9].) Thus, to specify a reflection law at the boundary is

quite analogous to specifying a collision law in the interior of a gas. Each assumption can have equal status in the theory, and can enter as part of the input data.

Model 2 as it appears in this paper differs in several aspects from its usual version in other works. A typical treatise on model 2 begins with a discussion of the mechanics of two-molecule collisions. The results of this discussion are then used in stating the Maxwell-Boltzmann equation. In this paper, we define a more general kind of collision law, one which need *not* conserve energy or momentum. The Maxwell-Boltzmann equation can be stated at once, and the discussion of molecular mechanics can be included as a theorem about three-dimensional collision laws with certain special properties. Furthermore the formulation given here easily extends to arbitrary dimensions so that one item of input data can be k, the dimension of the space in which the molecules are free to move. This allows us to search for examples of the theory in one and two dimensions. As we see in § 7, some insights gained when $k = 1$ have extensions to the case $k = 3$.

Since the models for a gas posed here are variations on earlier work, we should ask if they are somehow reasonable or "coherent". One method of judging comes from the motivational arguments. If there seems to be a "good physical reason" for the axioms, we feel somewhat secure in choosing them. However, we can impose more rigid mathematical requirements. Let G represent F or f at the time t, and let G_0 represent G when $t = 0$. Write $\int G$ for the integral of G over all possible states for fixed t. Then minimal requirements for our axioms would seem to be:

(1.1) For any G_0 in a suitable class of functions, the initial value problem posed for G is uniquely solvable.

(1.2) If $G_0 \geqq 0$ and $\int G_0 = 1$, then $G \geqq 0$ and $\int G = 1$.

In a sense, if the model gives us this much, it is enough. As long as we know the initial probable state of the gas, our axioms tell us its probable state for any time $t > 0$. Furthermore, the solution to the initial value problem is indeed a probability distribution. If the model conforms to (1.1) and (1.2), it predicts; and that is what a model should do. But we surely also hope that what the model predicts is in accord with the normal macroscopic behavior of a gas. This behavior is determined by differential equations and boundary conditions in the density, velocity, stress, etc., of the gas. So we might also expect that

(1.3) The model prescribes differential equations and boundary conditions for the macroscopic properties of the gas.

As the discussion so far suggests, this paper contains more than a simple statement of kinetic theory and the proof of an entropy theorem. The very act of stating a kinetic theory poses mathematical and philosophical problems which we must address. These guide the organization of the material which follows.

In §§ 2-3 models 1 and 2 (and a third intermediate model, which we call model 1 1/2) are given, along with their motivational arguments. Then in § 4

we begin to weigh our models against criteria (1.1)–(1.3). Part of the discussion of (1.3) depends on special properties of reflection and collision laws. These are discussed in § 5. We also show in that section that our definition of a collision law is compatible with the classical one. In § 6 we state the entropy theorem and show that the sign of the wall term is determined by a simple condition on the reflection law alone. Finally, in § 7 we give examples in which the entropy is strictly decreasing for all time, and we interpret physically the process by which they occur. Although the examples are one-dimensional, they have extensions to theorems for three-dimensional gases.

In our discussion of criteria (1.1)–(1.3), we do not pretend to deal seriously with some of the deeper mathematical questions. For example, we do not prove the positivity requirement $G \geqq 0$ in (1.2) for model 2. Even (1.1) poses well-known unsolved problems. However, we do give in § 7 special circumstances in which unique solutions exist for *all* time, and we also show that there are circumstances in which solutions are unique for *no* time.

An underlying feature of all models proposed in this paper is that the motion of the molecules by themselves is *deterministic*. However, their initial state is not known precisely, and consequently neither is their state for any later time. Thus we use probability only to describe our knowledge of the state of the *system* of molecules, not to describe *individual* molecular interactions with each other or the wall. It is possible to state a variation of model 2 in which the reflection and collision laws are stochastic rather than deterministic. Such a model includes the diffuse reflection law at the wall originally proposed by Maxwell [5] and used by many authors since. This model will be discussed in a future work.

2. A confined gas: model 1. We begin the body of this paper with a brief discussion of a model for a confined gas based on the axiom of conservation of probability. This material will serve us later in three ways. First, we can use it to derive a boundary condition for another model based on the Maxwell-Boltzmann equation. Second, we can make a clear distinction between the assumptions in these two models and point out yet another model (called model 1 1/2) which lies logically between them. And third, we can exhibit cases in which models 1 1/2 and 2 agree. To do this requires a precise statement of what it means for molecules to be indistinguishable. That, too, is given here. Much of the material in this section appears in greater detail in [6]. The concept of indistinguishability is discussed in the context of the Liouville equation for an unconfined gas in [7].

Model 1 requires for its construction six pieces of input data. These are (1) an integer $k \geqq 1$, (2) an integer $N \geqq 1$, (3) a scalar $m > 0$, (4) a domain $D \subset R^k$ with differentiable boundary, (5) a set of functions $q_i : D^N \to R^k$, $i = 1, \ldots, N$, and (6) a function $A : \partial D \times R^k \to R^k$. There is a restriction on the set of N functions q_i. Let Γ_N be the group of permutations on N objects. If $P \in \Gamma_N$ and if $\{x_i\}_{i=1}^N$ is an ordered set of k-vectors, let $\{x_{Pi}\}_{i=1}^N$ represent

the set permuted by P. Then we require that

(2.1) $\{q_{Pi}(x_1, \ldots, x_N)\}_{i=1}^{N} = \{q_i(x_{P1}, \ldots, x_{PN})\}_{i=1}^{N},$

for every $P \in \Gamma_N$. There is also a restriction on the function A. If $x \in \partial D$, with $n(x)$ the outward unit normal vector at x, and if $v \in R^k$, then we require that

(2.2) $n(x) \cdot A(x, v) \leqq 0$ when $n(x) \cdot v \geqq 0$.

We assume that A is continuous on ∂D and that $A(x, .)$ is a differentiable bijection between the sets $\{v \in R^k : n(x) \cdot v \geqq 0\}$ and $\{v \in R^k : n(x) \cdot v \leqq 0\}$.

These items of input data can be interpreted physically as follows. N is the number of identical point molecules, m is the mass of each one, and k is the dimension of the space in which they are free to move. D is the domain in which the gas is confined. The force on the ith molecule is $q_i(x_1, \ldots, x_N)$, where x_j is the position of the jth molecule. This force is to account for external fields, as well as the influence of the molecules on each other. The restriction (2.1) is a rigorous statement that, if the positions of the molecules are permuted, then the corresponding forces between them are likewise permuted. In short, the molecules are identical, not only in mass, but also in their effect on each other. Finally, the object A is the "reflection law" described in § 1. The condition (2.2) requires that A should transform "incident velocities" (for which $n \cdot v \geqq 0$) into "reflected velocities" (for which $n \cdot v \leqq 0$).

In order to construct a model for a gas from these six pieces of data, imagine that the system of molecules is in motion. At time t suppose that the ith molecule has position $x_i(t)$ and velocity $v_i(t)$. If $x_i(t) \in \partial D$, then $v_i(t)$ is ambiguous; for the sake of convention, assign the reflected (as opposed to the incident) value. Then for some time interval (t_1, t_2), the function

(2.3) $\zeta(t) = \{x_1(t), \ldots, x_N(t), v_1(t), \ldots, v_N(t)\}$

describes the motion of the entire system of molecules. The range of this function lies in the set

$$S = \{(x_1, \ldots, x_N, v_1, \ldots, v_N): x_i \in \bar{D}, v_i \in R^k, n(x_i) \cdot v_i \leqq 0$$
$$\text{if } x_i \in \partial D\}$$

The members of S are called *states* of the system of molecules. Notice that a state always refers to the condition after reflection. The motion of the system is, of course, determined by Newton's equations and the reflection law. In the notation we have set out, these take the form

(2.4) $\dfrac{dx_i}{dt} = v_i, \quad \text{if } x_i(t) \in D;$

(2.5) $\dfrac{dv_i}{dt} = \dfrac{1}{m} q_i(x_1, \ldots, x_N), \quad \text{if } x_i(t) \in D;$

(2.6) $v_i(t) = A\left(x_i(t), \lim_{\tau \to t-0} v_i(\tau)\right), \quad \text{if } x_i(t) \in \partial D.$

Using only the six pieces of input data for model 1, we can now state the completely formal

Definition. A *trajectory* is a function $\zeta : (t_1, t_2) \to S$ of the form (2.3) for which two conditions hold. First, ζ is continuous form the right, and second, the components of ζ satisfy (2.4)–(2.6). If $\zeta : R^1 \to S$, the trajectory is said to *exist for all time*.

In principle, the initial point of a trajectory should uniquely determine the trajectory. The ordinary differential equations (2.4)–(2.5) determine the motion until, for some i, $x_i(t) \in \partial D$. Then (2.6) applies, and, afterwards, the motion continues according to (2.4)–(2.5). Thus, at least in principle, the definition allows us to determine $\zeta(t)$ from $\zeta(0)$. We call this function the *trajectory map* Ψ. It is defined by the formula

$$\Psi(t, \zeta(0)) = \zeta(t).$$

If trajectories always exist for all time, then

(2.7) $\Psi : R^1 \times S \to S.$

For the remainder of this section, we assume (2.7). The questions of existence and uniqueness are raised again in §§ 4 and 7.

The trajectory map has three elementary properties which concern us here. The first and second are

(2.8) $\Psi(0, \zeta) = \zeta$

(2.9) $\Psi(t_2, \Psi(t_1, \zeta)) = \Psi(t_1 + t_2, \zeta).$

To state the third, we need some notation. If $P \in \Gamma_N$ and $\zeta = (x_1, \ldots, x_N, v_1, \ldots, v_N)$, let

$$P\zeta = (x_{P1}, \ldots, x_{PN}, v_{P1}, \ldots, v_{PN}).$$

Then, for every $P \in \Gamma_N$,

(2.10) $P\Psi(t, \zeta) = \Psi(t, P\zeta).$

The proofs of these three properties are straightforward from the definitions. In particular, to prove (2.10) it is necessary to use (2.1). Notice that, in words, (2.10) says that permuting the initial positions and velocities of the molecules results in the same permutation of their positions and velocities for all time. This is the result of the "identical effect" which the molecules have on each other. A consequence of (2.8)–(2.9) is that, for each $t \in R^1$, the trajectory map has an inverse

$$\Psi^{-1}(t, \cdot) = \Psi(-t, \cdot) : S \to S.$$

One step remains in formulating model 1 for a gas. Notice that the input information has so far been used (in principle) to determine a trajectory map

Ψ satisfying (2.7)–(2.10). However, the state ζ of the system at any time t can never be known exactly when N is extremely large. We assume instead that it is known probabilistically in terms of a distribution function $F(t, \zeta)$, $\zeta \in S$. Thus, if $V \subset S$, then $\int_V F(t, \zeta)d\zeta$ represents the probability that the system of molecules will occupy a state in V at time t. The basic hypothesis which we make for F is the axiom of *conservation of probability*:

$$(2.11) \quad \int_{\Psi(t, V)} F(t, \zeta)d\zeta = \int_V F(0, \zeta)d\zeta$$

for every measurable $V \subset S$. The motivation for this axiom is quite simple. In (2.11) we merely require that the *probable* evolution of the system, as described by F, is compatible with its *actual* evolution, as described by Ψ.

Viewed mathematically, (2.11) is essentially an evolution equation for F, as demonstrated in

THEOREM 2.1. *Let* $F_0 \colon S \to [0, +\infty)$. *Then there is a function* $F \colon R^1 \times S \to [0, +\infty)$ *which satisfies* (2.11) *and*

$$(2.12) \quad F(0, \zeta) = F_0(\zeta).$$

For each t, this function is unique up to sets of measure zero in S, and is given by

$$(2.13) \quad F(t, \zeta) = F_0(\Psi^{-1}(t, \zeta)) \left| \frac{\partial \Psi^{-1}}{\partial \zeta}(t, \zeta) \right|.$$

The elementary proof of this theorem involves a change of variable in the right-hand side of (2.11) and the argument that the set $\Psi(t, V)$ is arbitrary. For details, see [6].

We are interested in gases composed of identical point molecules. Thus the probability distribution F should somehow contain the information that the molecules are "indistinguishable". This concept is made precise in the

Definition. The molecules of the gas are said to be *indistinguishable* at time t, if, for every $P \in \Gamma_N$, $F(t, P\zeta) = F(t, \zeta)$. In particular, the molecules are *initially indistinguishable* if

$$(2.14) \quad F_0(P\zeta) = F_0(\zeta)$$

for every $P \in \Gamma_N$.

In other words, "indistinguishability" means that a mere permutation of the positions and velocities of the N molecules does not alter the probability for states of the system. An immediate consequence of this definition is

THEOREM 2.2. *If the molecules of the gas are initially indistinguishable, they are indistinguishable for all time.*

Proof. Let $P \in \Gamma_N$. By definition of $P\zeta$ for $\zeta \in S$, P can be regarded as a function $P \colon S \to S$. Furthermore, $|\partial P/\partial \zeta| = 1$. Holding t fixed, we can write (2.10) in the form

$$(2.15) \quad P \circ \Psi = \Psi \circ P,$$

where it is understood that $\Psi: S \to S$. Applying the chain rule to (2.15) gives

$$\left|\frac{\partial P}{\partial \zeta}\,(\Psi(\zeta))\right|\left|\frac{\partial \Psi}{\partial \zeta}\right| = \left|\frac{\partial \Psi}{\partial \zeta}\,(P\zeta)\right|\left|\frac{\partial P}{\partial \zeta}\right|,$$

that is, expressing the dependence on t again,

$$(2.16) \quad \left|\frac{\partial \Psi}{\partial \zeta}\,(t, \zeta)\right| = \left|\frac{\partial \Psi}{\partial \zeta}\,(t, P\zeta)\right|.$$

It follows that

$$
\begin{aligned}
F(t, P\zeta) &= F_0(\Psi(-t, P\zeta))\left|\frac{\partial \Psi}{\partial \zeta}\,(-t, P\zeta)\right|, \text{ by } (2.13), \\
&= F_0(P\Psi(-t, \zeta))\left|\frac{\partial \Psi}{\partial \zeta}\,(-t, \zeta)\right|, \text{ by } (2.10) \text{ and } (2.16), \\
&= F_0(\Psi(-t, \zeta))\left|\frac{\partial \Psi}{\partial \zeta}\,(-t, \zeta)\right|, \text{ by } (2.14), \\
&= F(t, \zeta), \text{ by } (2.13).
\end{aligned}
$$

This proves Theorem 2.2.

Theorem 2.2 shows that it is reasonable both physically and mathematically to assume that F_0 satisfies (2.14). This we will do. One measure of the usefulness of this hypothesis is seen in the following definition. Let

$$(2.17) \quad f(t, x, v) = \int_{D^{N-1} \times R^{k(N-1)}} F(t, x_1, \ldots, x_N, v_1, \ldots v_N)dx_2 \ldots dx_N$$
$$\times dv_2 \ldots dv_N,$$

where $x = x_1$ and $v = v_1$. This is a probability distribution on the set

$$T_r = \{(x, v) : x \in \bar{D}, v \in R^k, n(x) \cdot v \leqq 0 \text{ if } x \in \partial D\}$$

of reflected states (x, v) for the first molecule. Because of (2.14) and theorem 2.2, the distribution f is the same as a similar one defined for the jth molecule. (Let P be the permutation which corresponds to exchanging the 1st and the jth molecules.) Thus we are justified in (2.17) with selecting one molecule as typical and letting it speak for all.

Let $T = \bar{D} \times R^k$ be the set of all possible states (x, v), incident or reflected, for a given molecule. Notice that $T = \bar{T}_r$. With these definitions, we now state an important fact about f in

THEOREM 2.3. *If $f(t, \cdot)$ is continuous on T_r with a continuous extension to T, if $x \in \partial D$, and if $v \in R^k$ with $n(x) \cdot v \geqq 0$, then*

$$(2.18) \quad n(x) \cdot vf(t, x, v) = -n(x) \cdot A(x, v)\left|\frac{\partial A}{\partial v}\,(x, v)\right|f(t, x, A(x, v)).$$

This theorem is proved in [6]. Its proof involves the computation of $|(\partial \Psi^{-1}/\partial \zeta)(t, \zeta)|$ and the use of (2.13). The reason for presenting Theorem 2.3 here will become obvious in § 3. An important part of the construction of model 2 will be motivated by it.

In terms of f we can define the macroscopic properties of the gas in the usual fashion common to all kinetic models. Let $M = mN$ be the total molecular mass, and let $\int$ represent $\int_{R^k} \ldots dv$; where $v = \{v^i\}_{i=1}^k$. Then, by definition,

(2.19) $\rho = M \int f$,

(2.20) $\rho s^i = M \int v^i f, s = \{s^i\}_{i=1}^k$,

(2.21) $\sigma^{ij} = M \int (v^i - s^i)(v^j - s^j) f, \sigma = \{\sigma^{ij}\}_{i,j=1}^k$,

(2.22) $p = \dfrac{1}{k} \displaystyle\sum_{i=1}^k \sigma^{ii}$,

(2.23) $\rho \epsilon = \tfrac{1}{2} k p = \tfrac{1}{2} M \int |v - s|^2 f$,

(2.24) $\tau^i = \tfrac{1}{2} M \int |v - s|^2 (v^i - s^i) f, \tau = \{\tau^i\}_{i=1}^k$,

where ρ is the density, s the velocity, σ the stress tensor, p the pressure, ϵ the internal energy (per unit mass), and τ the heat flow vector for the gas. All these definitions are motivated physically in [3].

This completes the basic construction of model 1 for a gas. In summary, six pieces of input data are used to formulate a modified system of ordinary differential equations (2.4)–(2.6) which then determine (in principle) a trajectory map Ψ satisfying (2.7)–(2.10). This is used, in turn, to state an initial value problem (2.11), (2.12), and (2.14) for F. The solution to this problem is (2.13). Because of Theorem 2.2, it can be used to define (unambiguously) the macroscopic properties of the gas.

Notice that the forces $\{q_i\}_{i=1}^N$ and the reflection law A are used only to determine Ψ. Thus an alternate model, which still incorporates conservation of probability, can be formulated using only five objects: k, N, m, D, and a function Ψ satisfying (2.7)–(2.10). The initial value problem (2.11), (2.12), and (2.14) for F can still be posed, Theorems 2.1 and 2.2 are still valid, and the definitions (2.19)–(2.24) can still be formulated. In this scheme, Newton's laws are ignored altogether and the rule Ψ for determining trajectories is taken as one of the primitives. This description of a gas we call model 1 1/2.

3. A confined gas: model 2. In this section we pose a model for a confined gas based on the Maxwell-Boltzmann equation. Although some authors seem to feel that this equation can be derived from model 1, the fact is that no one has ever obtained it in this way by a rigorous process of approximation. (See [8, p. 155], and [2, p. 23].) Nevertheless, it *is* possible to obtain a boundary condition for model 2 rigorously from model 1. Furthermore, this same boundary condition can also be obtained by a motivational argument which closely

parallels the motivation for the Maxwell-Boltzmann equation itself. To see how this can be done, we must reformulate model 2 from the beginning. We also introduce into model 2 all the features described in § 1.

Seven pieces of input data are required for model 2. These are (1) an integer $k \geqq 1$, (2) a scalar $m > 0$, (3) a domain $D \subset R^k$ with a differentiable boundary, (4) a function $q : D \rightarrow R^k$, (5) a function $A : \partial D \times R^k \rightarrow R^k$, (6) a number $r \in [0, +\infty]$, the extended positive real number line, where $r = 0$ if $k = 1$, and (7) a function $B : Z \rightarrow Z$, where

$$Z = \{(y, v_1, v_2) : y, v_1, v_2 \in R^k; |y| \leqq r; y \cdot (v_2 - v_1) = 0\}$$

is a subset of R^{3k}. To describe the macroscopic properties of the gas, we also need (8) a scalar $M > 0$.

The restrictions of § 2 again apply to A, in particular (2.2). We also impose two principal requirements on B, namely,

(3.1) $B^2 = I$, and

(3.2) $B \circ B_e = B_e \circ B$,

where I is the identity function and B_e is the "exchange law"

$$B_e(y, v_1, v_2) = (-y, v_2, v_1), \quad (y, v_1, v_2) \in Z.$$

Notice that the set Z is all or part of the $(3k - 1)$-dimensional surface in R^{3k} whose equation is $y \cdot (v_2 - v_1) = 0$. This surface carries the induced measure from R^{3k}. Thus B maps a $(3k - 1)$-dimensional measure space onto itself. We assume the map is absolutely continuous, so that it possesses a Jacobian. (However, we cannot automatically conclude from (3.1) as some authors seem to do, that this Jacobian has magnitude 1. B may map a part Z_1 of Z expansively onto another part Z_2, and map Z_2 contractively onto Z_1.)

The mathematical objects listed above correspond, of course, to various physical aspects of the gas. The first three are familiar from model 1. Thus D is the domain which confines the gas in a space of dimension k, and m is the mass of a molecule. When we need it, the eighth object M is the total mass of all molecules. The function A is again a reflection law. For $x \in D$, $q(x)$ is the force due to external fields (gravity, for example) on a single molecule at position x.

The essentially new objects are B and r, the "collision law" and its "cut-off point". In order to give significance to these two objects, imagine that molecular interactions are rare in the life of a molecule and that it is enough to consider only pairwise interactions. Picture an interaction as an instantaneous event in which the "incident velocities" v_1 and v_2 of two molecules are suddenly converted to "scattered velocities" v_1 and v_2. Such an event is called a "collision". We imagine that the molecules approach each other on straight-line trajectories before colliding. As an approximation, suppose that collision occurs at the moment when the two molecules, moving in straight lines, are

closest to each other. (If the collision law is determined by a force law between molecules, the moment of interaction may be slightly different. But, even in this case, the approximation is always made in the motivational argument for the Maxwell-Boltzmann equation.) Let x_1 and x_2 be the positions of the two molecules at this moment. Then one can show that $(x_2 - x_1) \cdot (v_2 - v_1) = 0$. Thus, at the moment of closest approach, the relative velocity is perpendicular to the relative displacement.

With this scheme of things in mind, we can now interpret B and r. Let us write

$$(3.3) \quad (y', v_1', v_2') = B(y, v_1, v_2), \, y \cdot (v_2 - v_1) = 0, |y| \leqq r.$$

In this equation, think of (v_1, v_2) as incident velocities, (v_1', v_2') as scattered velocities, and y as the displacement of the second molecule relative to the first at the moment of collision. We refer to the variable y as the "impact parameter", for the collision law. Notice that, for physical reasons, (v_1', v_2') should be allowed to depend both on the orientation of y and its magnitude. Thus, if molecule 2 approaches molecule 1 from above, it may be scattered upwards (think of a repulsive force between molecules), while if it approaches from below, it may be scattered downwards. Similarly, if $|y|$ is small, we might expect the incident velocities to be changed considerably by collision. But, if $|y|$ is large, the molecules should, more or less, ignore each other, so that $(v_1, v_2) \approx (v_1', v_2')$. In fact, for $|y|$ larger than a certain distance r, the molecules may have no effect on each other at all. The parameter r in the model allows us to express this possibility. If $r = +\infty$, then the molecules influence each other at arbitrarily large distances of interaction.

We have interpreted every entry in equation (3.3) except y'. The significance of this variable can be seen through the hypothesis (3.1) for B. It follows from (3.1) and (3.3) that

$$(3.4) \quad B(y', v_1', v_2') = (y, v_1, v_2).$$

In (3.4), (v_1', v_2') are now *incident* velocities and (v_1, v_2) are *scattered* velocities. Thus y' is a value of the impact parameter which makes it possible to return to velocities (v_1, v_2) starting from velocities (v_1', v_2'). In effect, (3.1) says that for every collision there is another which reverses the process. A full knowledge of B includes the knowledge of y' as a function of $(y, v_1, v_2) \in Z$, that is, the knowledge of at least one way in which a given collision can be reversed.

It remains only to interpret the hypothesis (3.2) for B. Notice that reversing v_1 and v_2 and replacing y by $-y$ exchanges, in effect, the roles of molecules 1 and 2. Thus (3.2) says that exchanging the molecules before the collision is the same as exchanging them after: the collision law does not detect the switch. This hypothesis is obviously related to the notion developed in § 2 that the molecules are identical in their effect on each other, or indistinguishable. In the notation of (3.3), we can write (3.2) in the form

$$(3.5) \quad (-y', v_2', v_1') = B(-y, v_2, v_1).$$

As suggested in § 1, the object B defined in this section, that is, a function from Z to Z satisfying (3.1) and (3.2), differs from the usual object taken as a primitive in most treatments of the Maxwell-Boltzmann version of kinetic theory. (In fact, most treatments do not specify a clear primitive. See, however, [**9**].) Usually one starts by assuming conservation of energy and momentum, along with a few geometric requirements implicit in how the pictures are drawn, and then one obtains something akin to (3.1)–(3.2). In § 5, we will see rigorously how this can be done. However, (3.1) and (3.2) are sufficient to develop a "coherent" kinetic theory and to obtain an entropy theorem. We do not need to require conservation. For example, our theory admits the rather curious "reverse" scattering law

$$(3.6) \qquad B_r(y, v_1, v_2) = (y, -v_1, -v_2).$$

Notice that B_r maps Z to Z and satisfies (3.1)–(3.2); yet B_r does not conserve momentum. In a model with $B = B_r$, molecules simply reverse velocities in their trajectories whenever they collide.

We now have seven mathematical objects (excluding M) before us, each with a certain physical significance. How can we construct a kinetic theory from them? In case $q = 0$, we seem almost to have enough mechanical rules (A and B, instead of A and Newton's laws) to construct a trajectory map Ψ. (For interactions of three or more molecules, we may assume, for example, that the molecules ignore each other). Using this knowledge of Ψ, we can then continue along the lines of model 1 1/2. In fact, the Maxwell-Boltzmann equation is *motivated* by just this idea, but the resulting axiom is quite different from conservation of probability. In order to make this clear, we first state the axioms entirely formally in terms of the seven pieces of input data.

To do this and to do many other things in this paper, we need some additional notation. First, define the velocities

$$(3.7) \qquad w = v_2 - v_1, w' = v_2' - v_1'$$

of the second molecule relative to the first. Also, if $x \in \partial D$, let

$$(3.8) \qquad v^* = A(x, v), n(x) \cdot v \geqq 0, n(x) \cdot v^* \leqq 0.$$

Functions are frequently evaluated at the velocities v_1, v_2, v_1', v_2', and v^*. If $f(t, x, v) : R^1 \times \bar{D} \times R^k \to R^1$, then, for given $(t, x) \in R^1 \times D$ and $(y, v_1, v_2) \in Z$, define

$$(3.9) \qquad f_i = f(t, x, v_i), f_i' = f(t, x, v_i'); i = 1, 2.$$

Similarly, if $x \in \partial D$ and $n(x) \cdot v \geqq 0$, define

$$(3.10) \quad f^* = f(t, x, v^*).$$

We have frequent need for various kinds of integrals. These are

$$(3.11) \quad \int = \int \ldots dv, \int_i = \int_{R^k} \ldots dv_i, \int_i' = \int_{R^k} \ldots dv_i' \text{ for } i = 1, 2.$$

Also, if $x \in \partial D$, let

$$(3.12) \quad \int_{-} = \int_{n(x) \cdot v < 0} \ldots dv, \quad \int_{+} = \int_{n(x) \cdot v > 0} \ldots dv.$$

Next define the $(k-1)$-dimensional disc

$$(3.13) \quad \Delta(r, v_1, v_2) = \{ y \in R^k : y \cdot (v_2 - v_1) = 0, |y| \leq r \},$$

and let

$$(3.14) \quad \int_{\Delta} = \begin{cases} \int \int_{y \in \Delta(r, v_1, v_2)} \ldots dS(y), & k \geq 2 \\ 1, & k = 1 \end{cases},$$

$$\int_{\Delta}' = \begin{cases} \int \int_{y \in \Delta(r, v_1', v_1')} \ldots dS(y), & k \geq 2 \\ 1, & k = 1 \end{cases},$$

where $dS(y)$ is an element of $(k-1)$-dimensional area on Δ.

Certain Jacobians are also of interest, namely

$$(3.15) \quad J'(y, v_1, v_2) = \left| \frac{\partial(y', v_1', v_2')}{\partial(y, v_1, v_2)} \right|, \quad (y, v_1, v_2) \in Z,$$

and, for $x \in \partial D$,

$$(3.16) \quad J^*(x, v) = \left| \frac{\partial v^*}{\partial v} \right|, \quad n(x) \cdot v \geq 0.$$

In (3.15), it is important to remember that J' is *not* the Jacobian of a map from R^{3k} to R^{3k}, but of the map B from the $(3k-1)$-dimensional measure space Z to itself, as described earlier.

The operator

$$(3.17) \quad \mathscr{E}f(t, x, y, v_1, v_2) = |w'| f_1' f_2' J' - |w| f_1 f_2, \quad (y, v_1, v_2) \in Z,$$

is now well-defined for functions $f : R^1 \times \bar{D} \times R^k \to R^1$. In case $k = 1$, we always take $r = 0$, so that $\mathscr{E}f$ does not depend on y. Notice from (3.5) and (3.17) that

$$(3.18) \quad \mathscr{E}f(t, x, y, v_1, v_2) = \mathscr{E}f(t, x, -y, v_2, v_1), \quad (y, v_1, v_2) \in Z.$$

Next define the integral operator

$$(3.19) \quad \mathscr{C}f(t, x, v_1) = \int_2 \int_{\Delta} \mathscr{E}f,$$

and the differential operator

$$(3.20) \quad \mathscr{D}f(t, x, v) = \partial_t f + \nabla_x \cdot (vf) + \nabla_v \cdot \left(\frac{q}{m} f \right),$$

where $\nabla_x \cdot$ and $\nabla_v \cdot$ refer to divergences with respect to x and v.

Finally, if $f_0 : \bar{D} \times R^k \to [0, +\infty]$, consider the following initial boundary value problem for a function $f : R^1 \times \bar{D} \times R^k \to R^1$:

(3.21) $\mathscr{D}f_1 = \mathscr{C}f, x \in D$

(3.22) $n(x) \cdot vf = -n(x) \cdot v^*J^*f^*, x \in \partial D, n(x) \cdot v > 0$

(3.23) $f(0, x, v) = f_0(x, v)$.

The notation leading to these axioms is somewhat elaborate, but it can be summarized in a few words. We designate scattered velocities by v_1' and v_2', relative velocities by w and w', and reflected velocities by v^*. This notation is given in (3.3) and (3.7)–(3.8). Equations (3.9)–(3.16) express (i) functions evaluated at various velocities, (ii) integrals over various domains, and (iii) the Jacobians for the reflection and scattering laws. Finally (3.17)–(3.20) define the operators in terms of which the initial boundary value problem (3.21)–(3.23) for f is posed.

In (3.21) it is necessary, of course, to know that the integrals (3.19) converge. We always assume that f tends to zero fast enough as $|v| \to +\infty$ (and, if $r = +\infty$, that $\mathscr{C}f$ tends to zero fast enough as $|y| \to +\infty$) so that $\int_2 \int_\Delta \mathscr{C} f$ converges. We do not pursue here the important related question: if f_0 has this property, does the solution f to (3.21)–(3.23) also have this property for every t?

From a purely formal point of view, seven pieces of input data have been used to pose the problem (3.21)–(3.23) for a function f. These equations are for model 2 what (2.11), (2.12), and (2.14) are for model 1: an initial value problem designed from the initial data to determine the evolution of probability for states of the system of molecules. The function f has the same interpretation in model 2 as it did in model 1. In terms of f we define the macroscopic properties of the gas (2.19)–(2.24), just as before. Notice that in model 2 we use the eighth piece of information $M > 0$ only for this step.

Axioms (3.21)–(3.23) are now well-defined formally, but it remains to give the motivation for them. This is essential here for two reasons. First, as a result of our very general definition of a collision law, the operator $\mathscr{C}$ in (3.17) does not have quite the form that appears in the literature. This leads to modified version (3.21) of the Maxwell-Boltzmann equation. Second, (3.22) is a new boundary condition for (3.21). Thus both axioms (3.21) and (3.22) are new, and some justification is required for them.

One motivation for (3.22) is theorem 2.3; notice that (2.18) and (3.22) are the same. Since (3.22) is a theorem in model 1, it seems reasonable as an axiom in model 2. But we can go even further than this. We can state a motivation for (3.22), given A, along precisely the same lines as the motivation for (3.21), given B. Both arguments will now be presented.

We begin with the motivation for (3.21). First notice that, in a coordinate system moving with molecule 1, molecules 1 and 2 collide at the moment

when number 2 reaches the $(k - 1)$-dimensional plane through number 1 perpendicular to the oncoming relative velocity w of number 2. If $r < +\infty$, then the plane is replaced by a $(k - 1)$-dimensional disc of radius r centered at x, the position of molecule 1 at the moment of interaction. Let us call this disc Δ_x. Using the notation of (3.13), we can write

$$(3.24) \quad \Delta_x = \{x + y; y \in \Delta(r, v_1, v_2)\},$$

where, as usual, v_i is the velocity of molecule i $(i = 1, 2)$.

When molecule 2 collides with molecule 1, number 1 (which is typical of all) suddenly jumps from one part of state space $T = \bar{D} \times R^k$ to another. Probability should be lost or gained accordingly in the affected regions of T. (Note that this statement refers tacitly to the idea of conservation of probability). We can ask, at what time rate is probability lost or gained in some part of T due to molecular collisions?

To answer this question, we compute the probability that some molecule, say number 2, collides with number 1 during the time interval $(t, t + dt)$. Notice that, if number 2 does so, it must reach a point on the appropriate disc Δ_x during this time; that is, it must be within the perpendicular distance $|w|dt$ of Δ_x. To strike a patch of surface $dS(z)$ around the point $z \in \Delta_x$, it must lie in a cylinder with base $dS(z)$ and volume $|w|dt\, dS(z)$. Thus, given that molecule 1 occupies a state at or near (x, v_1) at time t, the probability P that some molecule interacts with it during $(t, t + dt)$ is

$$(3.25) \quad P = dt \int_{v_2 \in R^k} \int_{z \in \Delta_x} |w|\, f(t, z, v_2) dS(z) dv_2.$$

In (3.25), x is fixed. We can let $z = x + y$ and take advantage of (3.24) to write

$$(3.26) \quad P = dt \int_{v_2 \in R^k} \int_{y \in \Delta(r, v_1, v_2)} |w|\, f(t, x + y, v_2) dS(y) dv_2.$$

A standard approximation is always made in (3.26). It is assumed that when collisions occur, the molecules are close enough that $f(t, x + y, v_2) \approx f(t, x, v_2)$. This approximation is a little strange when $r = +\infty$, but it is always made. Thus (3.26) becomes

$$(3.27) \quad P = dt \int_2 \int_\Delta |w|\, f_2.$$

When $k = 1$, molecules always collide head-on, so, in effect, $r = 0$ and there is no dependence on y. However, in the argument leading to (3.25), the relevant one-dimensional cylinder has volume $|w|\, dt$. No cylinder "base" enters the

discussion, and (3.27) takes the form

$$P = dt \int_2 |w| f.$$

This motivates the definition (3.14) for $\int_\Delta$ when $k = 1$.

The probability P is a conditional probability. In computing it, one assumes that molecule 1 has a state at or near (x, v_1) at time t. Let $[x, dx; v_1, dv_1]$ represent a box of volume $dx\, dv_1$ around the point $(x, v_1) \in T$. Then

$$Q = f_1\, dx\, dv_1$$

is the probability that molecule 1 is in $[x, dx; v_1, dv_1]$ at time t. If we assume P and Q are probabilities of independent events (this assumption that the probable states of different molecules are independent is called "molecular chaos" [4]), then

$$(3.28) \quad PQ = dt\, dx\, dv_1 \int_2 \int_\Delta |w| f_1 f_2$$

is the probability that molecule 1 is located in the box $[x, dx; v_1, dv_1]$ at time t and then collides with another molecule during the time interval $(t, t + dt)$. In this case, molecule 1 is lost to the region around (x, v_1) in T.

Of course, molecule 1 might also *enter* the box $[x, dx; v_1, dv_1]$ by colliding with another molecule during the interval $(t, t + dt)$. The probability R that this will happen is, by the same reasoning which led to (3.28),

$$(3.29) \quad R = dt\, dx\, dv_1' \int_2' \int_\Delta' |w'| f_1' f_2',$$

where we use the fact that $B^{-1} = B$ by (3.1). Notice that the right-hand side of (3.29) contains the differential element $dS(y')dv_1'dv_2'$. Because $y' \cdot (v_2' - v_1') = 0$ throughout the element, we may regard $dS(y')dv_1'dv_2'$ as a patch of area on the $(3k - 1)$-dimensional surface Z. Thus we can write

$$(3.30) \quad dS(y')dv_1'dv_2' = J'dS(y)dv_1dv_2.$$

and (3.29) becomes

$$R = dt\, dx\, dv_1 \int_2 \int_\Delta |w'| f_1' f_2' J'.$$

It follows that

$$R - PQ = \mathscr{C} f\, dt\, dx\, dv_1$$

is, during the interval $(t, t + dt)$, the net gain in probability that a molecule occupies the box $[x, dx; v, dv]$ in state space T. In other words

$$(3.31) \quad \frac{R - PQ}{dx\, dv_1\, dt} = \mathscr{C} f$$

represents the time rate of growth of probability density at $(x, v_1) \in T$.

This can be calculated another way. If molecule 1 moves on the trajectory $(x(t), v_1(t)) \subset T$, then

$$(3.32) \quad \frac{d}{dt} f(t, x(t), v_1(t)) = f_t + \frac{dx}{dt} \cdot \nabla_x f + \frac{dv_1}{dt} \cdot \nabla_v f$$

represents the time rate of growth of probability density due to the motion of this molecule. Since molecule 1 is typical, the quantities calculated in (3.31) and (3.32) are the same, that is,

$$\mathscr{D} f_1 = \mathscr{C} f,$$

where we have assumed that $dx/dt = v$ and $dv/dt = q/m$.

This completes the motivation for (3.21). Notice especially the arguments in connection with (3.30). These are the reasons which make it seem natural to include the factor J' in our definition (3.17) for $\mathscr{E} f$.

The motivation for (3.22) is much shorter, but very similar. Let $dS \subset \partial D$ be a patch of area around $x \in \partial D$. If a molecule is to reach dS in the time interval $(t, t + dt)$, then (i) it must be headed toward dS, that is, $n(x) \cdot v > 0$, and (ii) at time t it must lie in a cylinder with base dS and height $(n(x) \cdot v)dt$. Let $[v, dv] \subset R^k$ represent a box around v with volume dv. Then the probability P^* that a molecule with velocity in $[v, dv]$ will reach dS during the time $(t, t + dt)$ is

$$(3.33) \quad P^* = f \cdot (n(x) \cdot v)dt\, dS\, dv, \ n(x) \cdot v > 0.$$

Similarly the probability Q^* that a molecule in $[v^*, dv^*] = A(x, [v, dv])$ will leave dS in the time $(t, t + dt)$ is

$$Q^* = f^* \cdot (-n(x) \cdot v^*)dt\, dS\, dv^*$$
$$= f^* \cdot (-n(x) \cdot v^*)J^*\, dt\, dS\, dv.$$

Since the molecules striking dS are the same molecules which leave it, P^* and Q^* are probabilities of the same event. The equation $P^* = Q^*$ is equivalent to (3.22).

Notice the similarity between the motivations for (3.21) and (3.22). The justification for (3.33) is conceptually identical to that for (3.25).

4. Criteria for a coherent theory. We now have before us, in axiomatic form, models 1, $1\frac{1}{2}$, and 2 for a gas composed of identical point molecules. Consequently we are in a position to investigate these models in the light of criteria (1.1)–(1.3) cited in § 1. Let us begin with (1.1).

For model $1\frac{1}{2}$, existence and uniqueness pose no problem. By hypothesis (2.7), the trajectory map Ψ is known for all time. Consequently (2.13) is the solution to (2.11)–(2.12) for all time. However, for model 1, the criterion (1.1) is harder. The difficulty hinges on the solvability of the modified system of ordinary differential equations (2.4)–(2.6). Known theorems on solutions to

conventional systems, at least for a finite time, make it seem plausible that the trajectory map Ψ can sometimes be found. Once Ψ is known, then, as in model $1\frac{1}{2}$, (2.13) is the solution for F.

Criterion (1.1) poses a still deeper problem for model 2 than it did for model 1. The difficulty now relates not to systems of ordinary differential equations, but to a boundary value problem for a non-linear integro-differential equation. Even for unconfined gases in R^3, with scattering laws which conserve energy and momentum, the questions of existence and uniqueness in general remain unsolved. However, as a check for the new boundary condition, we would like to know that (3.21)–(3.23) is well-posed in a few of the simplest cases. This matter is taken up again in § 7. We also indicate there where some of the difficulties for criterion (1.1) might lie, both in models 1 and 2.

In order to investigate criteria (1.2)–(1.3), we need

THEOREM 4.1. *Let $g(t, x, v) : R^1 \times \bar{D} \times R^k \to R^1$. Then in model 2, if $x \in D$,*

$$(4.1) \qquad \int_1 g_1 \mathscr{C} f = \frac{1}{4} \int_1 \int_2 \int_\Delta (g_1 + g_2 - g_1' - g_2') \mathscr{E} f.$$

Furthermore, in models 1 and 2, if $x \in \partial D$.

$$(4.2) \qquad \int gf = \int_+ \left[g - g^* \frac{n \cdot v}{n \cdot v^*} \right] f.$$

Proof. Let $z = (y, v_1, v_2) \in Z$ and let $z' = Bz$. Since $B^2 = I$, it follows that

$$(4.3) \qquad J'(z')J'(z) = 1.$$

Notice that

$$\int_1 g_1 \mathscr{C} f = \int_1 \int_2 \int_\Delta g_1 \mathscr{E} f(t, x, y, v_1, v_2)$$

$$= \int_Z g_1 \mathscr{E} f(t, x, z) dz$$

$$= \int_Z g_1' \mathscr{E} f(t, x, z') J'(z) dz$$

$$= \int_Z g_1' [|w| f_1 f_2 J'(z') - |w'| g_1' f_2'] J'(z) dz,$$

since $(v_i')' = v_i$, $i = 1$ or 2, and $(z')' = z$. Thus from (4.3),

$$(4.4) \qquad \int_1 g_1 \mathscr{C} f = \int_1 \int_2 \int_\Delta g_1 \mathscr{E} f = - \int_1 \int_2 \int_\Delta g_1' \mathscr{E} f.$$

Let B_e be the exchange operator defined in connection with (3.2), and notice that

$$\left| \frac{\partial B_e(z)}{\partial z} \right| = 1.$$

Furthermore, by (3.18), $\mathscr{E}f(t, x, z) = \mathscr{E}f(t, x, B_e z)$. Thus

$$\int_1 g_1 \mathscr{C}f = \int_z g_1 \mathscr{E}f dz = \int_z g_2 \mathscr{E}f dz,$$

upon transforming z to $B_e z$, since v_1 is then transformed to v_2. Therefore,

$$(4.5) \qquad \int_1 g_1 \mathscr{C}f = \int_1 \int_2 \int_\Delta g_2 \mathscr{E}f = -\int_1 \int_2 \int_\Delta g_2' \mathscr{E}f,$$

where the second equality holds in (4.5) for the same reasons that led to the second equality in (4.4). Combining (4.4) and (4.5) gives (4.1).

Equation (4.2) is proved in [**6**], but, for completeness, we include the proof here. We use the fact that (3.22) holds for both models 1 and 2. Thus, for $x \in \partial D$,

$$\int_- gf = \int_+ g^* f^* J^* = -\int_+ g^* \frac{n \cdot v}{n \cdot v^*} f,$$

where the first step involves a change of variable and the second uses (3.22). It follows that

$$\int gf = \int_- gf + \int_+ gf = \int_+ \left[g - g^* \frac{n \cdot v}{n \cdot v^*} \right] f.$$

This proves (4.2) and completes the proof of Theorem 4.1.

A straightforward (and typical) application of Theorem 4.1 is

THEOREM 4.2. *In both models* 1 *and* 2, *if* $f(t, \cdot)$ *is continuous on* T *for each* t, *then*

$$(4.6) \qquad n(x) \cdot \rho s = 0, x \in \partial D;$$

and, if f *is differentiable in all variables, then*

$$(4.7) \qquad \partial_t \rho + \nabla_x \cdot (\rho s) = 0, x \in D.$$

Proof. To prove (4.6), let $x \in \partial D$ and let $g = n(x) \cdot v$ in (4.2). Then

$$(4.8) \qquad n \cdot \rho s = \int n \cdot vf = \int_+ \left[n \cdot v - n \cdot v^* \frac{n \cdot v}{n \cdot v^*} \right] f = 0.$$

Equation (4.7) is proved for model 1 in [**6**]. To prove it for model 2, let $g = 1$ in (4.1) and observe that

$$(4.9) \qquad \int_1 \mathscr{D}f_1 = \int_1 \mathscr{C}f = \int_1 \int_2 \int_\Delta [1 + 1 - 1 - 1] \mathscr{E}f = 0,$$

that is,

$$(4.10) \qquad \int_1 \partial_t f + \int_1 \nabla_x \cdot (vf) + \frac{1}{m} \int_1 \nabla_v \cdot (gf) = 0.$$

But

$$(4.11) \quad \int_1 \nabla_v \cdot (qf) = \lim_{\delta \to +\infty} \int_{\partial S\delta} n(v) \cdot qf = 0,$$

where ∂S_δ is the surface of the sphere $S_\delta \subset R^k$ with radius δ and $n(v)$ is the outward unit normal vector at $v \in \partial S_\delta$. The limit in (4.11) is zero because we assume that f tends to zero fast enough as $|v| \to +\infty$. Equation (4.7) now follows from (4.10)–(4.11). This completes the proof of Theorem 4.2.

Using Theorem 4.2, we can now prove

THEOREM 4.3. *In models* 1 *and* $1\frac{1}{2}$,

$$(4.12) \quad \textit{if } F_0 \geqq 0 \textit{ and } \int_S F_0 d\rho = 1, \textit{ then } F \geqq 0 \textit{ and } \int_S F d\rho = 1;$$

and in model 2,

$$(4.13) \quad \textit{if } \int_T f_0 d\eta = 1, \textit{ then } \int_T f d\eta = 1.$$

Proof. The assertion about $\int_s F \, d\rho$ in (4.12) is an immediate consequence of (2.11)–(2.12), since $\Psi(t, S) = S$ for every t. Positivity in (4.12) follows from (2.13). To prove (4.13), we use (4.6)–(4.7). Performing $\int_D \ldots dx$ in (4.7) gives

$$(4.14) \quad \int_D \int \partial_t f + \int \int_D \nabla_x \cdot (vf) = 0.$$

However,

$$\int \int_D \nabla_x \cdot (vf) = \int \int_{\partial D} n \cdot vf = \int_{\partial D} n \cdot \rho s = 0$$

by (4.6). Thus (4.14) shows that

$$\frac{d}{dt} \int_T f = 0.$$

This proves (4.13) and completes the proof of Theorem 4.3.

We now have enough information to begin comment on the criteria (1.2) and (1.3) cited in § 1. Notice that Theorem 4.3 establishes (1.2) for models 1 and $1\frac{1}{2}$, as well as part of (1.2) for model 2. As stated in § 1, the positivity requirement (1.2) for model 2 is not discussed here. However, some work on this problem can be found in [**1**]. Theorem 4.2 is a first step toward establishing criterion (1.3) for all models. Equations (4.6) and (4.7) tell us that at least the first two macroscopic properties of the gas, ρ and s, are consistent with their interpretation as the density and velocity of a mass flow. Thus (4.6) says that no mass crosses the boundary of the confining domain, and (4.7) say

that mass is conserved by the flow in the interior of the domain. (4.6) and (4.7) are the most fundamental boundary condition and differential equation. They relate only to the notion that what we are finally dealing with is matter, and it is conserved.

However, in general we cannot say more without further information. In model 2, for example, if B is not constructed to conserve momentum during molecular interactions, we cannot expect momentum to be conserved macroscopically in the gas. Or, in either model, if A is not constructed so that individual molecules exert a tangential force on the boundary, we cannot expect to find a macroscopic tangential stress on the boundary. In summary, each model by its own nature implies that we are dealing with the flow of material. But the explicit rules by which that material flows remain to be fed in. (In model 1, the boundary behavior remains to be specified by the choice of a reflection law. The interior behavior *a priori* conforms to Newton's laws. In model 2, both boundary and interior behavior remain to be specified by choices for reflection and collision laws.)

Theorem 4.2 illustrates a general process by which macroscopic behavior can be deduced from molecular behavior. Equation (4.8) is the critical step in proving (4.6); the function $g = n(x) \cdot v$ has the property that $\int g f = 0$ at $x \in \partial D$. Similarly, (4.9) is the critical step in proving (4.7); the function $g = 1$ has the property that

$$\int_1 g_1 \mathscr{C} f = 0.$$

The basic tool in each procedure is Theorem 4.1. We can make this process completely formal and general with the

Definition. Let $\phi(v) : R^k \to R^1$. Let A be a reflection law and B be a collision law. Then the pair (A, ϕ) is called *reflection invariant* at $x \in \partial D$ if

(4.15) $n(x) \cdot v^* \phi = n(x) \cdot v \phi^*$ when $n(x) \cdot v > 0$.

Also the pair (B, ϕ) is called *collision invariant* if

(4.16) $\phi_1 + \phi_2 = \phi_1' + \phi_2'$ when $(y, v_1, v_2) \in Z$.

In connection with this definition, let

(4.17) $\bar{\phi}(t, x) = M \int \hat{\phi} f, \phi(t, x) = M \int v \phi f, \tilde{\phi}(t, x) = M \int (\nabla_v \phi) f$.

Then we can prove

THEOREM 4.4. *In models 1 and 2 if $f(t, \cdot)$ is continuous on T and (A, ϕ) is reflection invariant at $x \in \partial D$, then*

(4.18) $\bar{\phi}(t, x) = 0$.

Furthermore, in model 2, if f is differentiable on $R^1 \times T$ and (B, ϕ) is collision invariant, then

(4.19) $\partial_t \bar{\phi} + \nabla_x \cdot \hat{\phi} - \dfrac{1}{m} q \cdot \tilde{\phi} = 0$.

Proof. Equation (4.18) follows at once from (4.15) and (4.2). Similarly from (4.16) and (4.1), we see that

$$\int_1 \phi_1 \mathscr{D} f_1 = \int_1 \phi_1 \mathscr{C} f = 0.$$

Thus

$$0 = M \int \phi \partial_t f + M \int \phi \nabla_x \cdot (vf) + \frac{M}{m} \int \phi \nabla_v \cdot (qf)$$

$$= M \int \partial_t (\phi f) + M \int \nabla_x \cdot (v \phi f) + \frac{M}{m} \int \nabla_v \cdot (q \phi f)$$

$$- \frac{M}{m} \int (\nabla_v \phi) \cdot qf$$

$$= \partial_t \bar{\phi} + \nabla_x \cdot \hat{\phi} - \frac{1}{m} q \cdot \check{\phi},$$

since $\int \nabla_v (q \phi f) = 0$ for reasons already discussed in connection with (4.11). This proves (4.19) and completes the proof of Theorem 4.4.

If (A, ϕ) is reflection invariant, we call (4.18) a *corresponding boundary condition* for A. Similarly if (B, ϕ) is collision invariant, we call (4.19) a *corresponding differential equation* for B. Such boundary conditions and differential equations have this important feature: they are valid for *any* initial probability distribution f_0. Thus criterion (1.3) in general hinges on the existence of invariant pairs (A, ϕ) and (B, ϕ). In Theorem 4.2, we found that $(A, n(x) \cdot v)$ and $(B, 1)$ are invariant for any A and B. But beyond these examples, invariant pairs depend on special properties of A and B.

To illustrate this fact, consider the case of a *reverse gas*, which we define to be a model 2 gas in which

$$(4.20) \quad A(x, v) = -v, B(y, v_1, v_2) = (y, -v_1, -v_2), \quad q = 0, r = \begin{cases} +\infty, k \geqq 2 \\ 0 \quad , k = 1. \end{cases}$$

For such a gas, molecules reverse their motion along straight-line trajectories whenever they encounter each other or the boundary. (See also the discussion in connection with (3.6).) For a reverse gas, the set of corresponding boundary conditions and differential equations is

$$(4.21) \quad \bar{\phi} = 0, x \in \partial D, \text{ if } \phi(-v) = -\phi(v);$$

$$(4.22) \quad \partial_t \bar{\phi} + \nabla_x \cdot \check{\phi} - \frac{1}{m} q \cdot \check{\phi} = 0, x \in D, \text{ if } \phi(-v) = \phi(v).$$

Notice that (4.21)–(4.22) are an infinite set of requirements on macroscopic properties of the flow – for example, a boundary condition for every odd polynomial in the components of v and a differential equation for every even polynomial in the components of v.

We close this section with a short comment. We have consistently assumed that f has enough smoothness to justify the conclusions of Theorems 4.1–4.4. In fact, this smoothness may sometimes be impossible to achieve (as is often the case in initial boundary-value problems for partial differential equations). If so, it may be possible to resort to weak forms of the Maxwell-Boltzmann equation (3.21) and the moment equation (4.19). For model 1, weak moment equations are developed in [**6**].

5. Special properties of A and B. Reflection laws and collision laws are, after all, just functions with certain basic, physically motivated properties. However, as suggested in § 4, if we want to find invariant pairs (A, ϕ) and (B, ϕ) other than those leading to Theorem 4.2, we need more information about A and B. For example, this information might consist of an explicit knowledge of A and B, as in the case of a reverse gas. However, more generally, we can study additional physically reasonable properties of A and B to see how they influence the behavior of the gas. Our study is motivated by two concerns: first to increase our knowledge of invariant pairs and thus to elaborate criterion (1.3) for models 1 and 2, and second to see precisely how our definition for B in model 2 extends the special cases usually discussed in the literature.

The special properties of reflection and scattering laws which interest us here are listed in the following definitions. It is understood throughout this section that a statement about A refers to model 1 or 2, but a statement about B refers only to model 2.

Let $\mathscr{O}$ be the group of all rigid rotations of R^k about the origin. Let $\mathscr{O}_u$ be the subgroup of $\mathscr{O}$ which leaves fixed a given vector u. If $\Omega \in \mathscr{O}$ and $(y, v_1, v_2) \in Z$, let $\Omega(y, v_1, v_2) = (\Omega y, \Omega v_1, \Omega v_2)$, and note that $\Omega : Z \to Z$.

Let A be a reflection law. We say that A is *isotropic* if $\Omega \circ A(x, \cdot) = A(x, \cdot) \circ \Omega$ for every $\Omega \in \mathscr{O}_{n(x)}$ and every $x \in \partial D$. Also A is *planar* if v^* always lies in the 2-plane spanned by $n(x)$ and v. Let B be a collision law. Then B is *isotropic* if $B \circ \Omega = \Omega \circ B$ for every $\Omega \in \mathscr{O}$. Also B is *planar* if w' always lies in the 2-plane spanned by w and y and if w' is a function of w and y. We say that B *conserves momentum* if

$$v_1' + v_2' = v_1 + v_2 \text{ for every } (y, v_1, v_2) \in Z.$$

Similarly B *conserves energy* if

$$|v_1'|^2 + |v_2'|^2 = |v_1|^2 + |v_2|^2 \text{ for every } (y, v_1, v_2) \in Z.$$

Finally, B is *conservative* if B conserves both energy and momentum.

Each of these requirements on A and B makes a certain physical sense. For example, if the wall can be approximated by a tangent plane at $x \in \partial D$, then A should presumably be isotropic. That is, rotating the incident velocity about $n(x)$ should correspondingly rotate the reflected velocity. Furthermore, unless we suppose that the wall can add new components of tangential momentum to

molecules during reflection, A will be planar. To say that B is isotropic is, essentially, to say that the molecules are spherically symmetric as judged by their effect on each other. That is, rotating both the incident velocities and the impact parameter for a collision results in a corresponding rotation of the scattered velocities. Furthermore, if B is determined from a central force law acting between any two molecules, then a standard theorem occurring in classical mechanics implies that B should be planar. Finally, if B is derived from Newtonian mechanics, it should be conservative.

An example of the significance of further restrictions on A for the important criterion (1.3) is given in

THEOREM 5.1. *Let $k = 3$. Let A be a planar, isotropic scattering law. Then (A, ϕ) is reflection invariant for some polynomial ϕ of degree 2 or less in the components of v if and only if*

(5.1) $A(x, v) = -\lambda(x, v)v, x \in \partial D$, or

(5.2) $A(x, v) = v - [1 + \lambda(x, v)][n(x) \cdot v]n(x), x \in \partial D$,

where $\lambda : \partial D \times R^k \to R^1$ with $\lambda > 0$ when $n(x) \cdot v > 0$. The corresponding boundary conditions for (5.1) and (5.2) are, respectively,

(5.3) $\rho s = 0, x \in \partial D$, and

(5.4) $n(x) \cdot \rho s = 0, [n(x) \cdot \sigma \cdot n(x)]n(x) = \sigma \cdot n(x), x \in \partial D$.

This theorem is proved in [6]. Notice that with $\lambda = 1$ (5.1) is the reflection law for a reverse gas given in (4.20). Also, when $\lambda = 1$, (5.2) is specular reflection, that is, reflection in which molecules retain their tangential velocity and reverse their normal velocity. The resulting boundary conditions (5.3) and (5.4) say that the gas either sticks to the wall or slides without resistance along it. Extensive discussion of these and other boundary conditions may be found in [6].

Let $v = (v^1, \ldots, v^k)$. Then an elementary example of the significance of further restrictions on B is given in

THEOREM 5.2. *Let B be a collision law. Then B conserves momentum if and only if (B, v^i) is collision invariant for each $i = 1, \ldots, k$. The corresponding differential equations are*

(5.5) $\rho \partial_t s + \rho(s \cdot \nabla_x)s + \nabla_x \cdot \sigma - \dfrac{\rho q}{m} = 0$.

Also, B conserves energy if and only if $(B, |v|^2)$ is collision invariant, in which case the corresponding differential equation is

(5.6) $\rho \partial_t \epsilon + \rho s \cdot \nabla_x \epsilon + \nabla_x \cdot \tau + \sigma \cdot (\nabla_x s)$

$$+ s \cdot \left(\rho \partial_t s + \rho(s \cdot \nabla_x)s + \nabla_x \cdot \sigma - \frac{\rho q}{m} \right) = 0.$$

Proof. By the definition of invariance, conservation of momentum and energy are equivalent to the invariance (B, v^i) and $(B, |v|^2)$, respectively. Equations (5.5) and (5.6) result from straightforward applications of (4.17) and (4.19), using the definitions (2.19)–(2.21). It is also necessary in (5.5) and (5.6) to use the mass conservation equation (4.7). This proves Theorem 5.2.

Theorem 5.2 shows, of course, that conservation of momentum and energy at the molecular level leads to macroscopic conservation of these properties of the flow. However, to obtain the usual energy equation from (5.6), we must also use (5.5); that is, we must assume that B conserves *both* momentum and energy.

We continue our investigation of conservative scattering laws in a slightly different direction. We want to show next how our definition of a collision law fits naturally into the context of conservative laws. To make this clear, we begin with a few definitions. A function $b : Z \to R^{2k}$ is called a *pre-collision law*. We write

$$(v_1{}', v_2{}') = b(y, v_1, v_2), \; (y, v_1, v_2) \in Z.$$

Notice that we can interpret b as a definite rule for determining scattered velocities $(v_1{}', v_2{}')$ from incident velocities (v_1, v_2) and an impact parameter y. However, b does not specify an impact parameter y' by which $(v_1{}', v_2{}')$ can be returned to (v_1, v_2). We say that b is *differentiable* if $b \circ \gamma$ is differentiable for every differentiable curve γ on Z. Also we call b *isotropic* if

$$(\Omega v_1{}', \Omega v_2{}') = b(\Omega y, \Omega v_1, \Omega v_2)$$

for every $\Omega \in \mathcal{O}$. Similarly we can define *planar* and *conservative* for b in analogy with the definitions for B. Finally we say that b *can be extended to a collision law* B if there exists a $y' : Z \to R^k$ such that

$$B(y, v_1, v_2) = (y'(y, v_1, v_2), b(y, v_1, v_2))$$

is a collision law.

If a pre-collision law can be extended to a collision law, the extension may not be unique. There may be many possible choices for y', that is, many circumstances by which the scattered velocities $(v_1{}', v_2{}')$ can be re-scattered back to (v_1, v_2). However, we have

THEOREM 5.3. *Suppose that a pre-collision law can be extended to two different collision laws B and $\bar{B}$. Then, for given values of the remaining input parameters in model 2, B and $\bar{B}$ pose the same initial value problem (3.21)–(3.23) for a function $f : R^1 \times D \times R^k \to R^1$.*

Proof. Let $\mathscr{C}f$ and $\overline{\mathscr{C}f}$ be the collision integrals for B and $\bar{B}$, respectively. Since the collision law enters (3.21)–(3.23) only in the definition of $\mathscr{C}$, we

need only show that

(5.7) $\mathscr{C}f = \overline{\mathscr{C}}f$

for any given f. Because B and $\bar{B}$ both extend b, we can write

$$B(y, v_1, v_2) = (y', v_1', v_2'), \bar{B}(y, v_1, v_2) = (\bar{y}', v_1', v_2').$$

Consequently, since $B^2 = I$,

$$\bar{B} \circ B(y', v_1', v_2') = \bar{B}(y, v_1, v_2) = (\bar{y}', v_1', v_2').$$

Thus the map $C = \bar{B} \circ B$ is a bijection on Z which alters only the value of y, not v_1 or v_2. We write

$$C(y, v_1, v_2) = (\bar{y}, v_1, v_2).$$

Then $B = \bar{B}^{-1} \circ C = \bar{B} \circ C$, so that

(5.8) $J'(y, v_1, v_2) = \bar{J}'(\bar{y}, v_1, v_2)J_c(y, v_1, v_2),$

where J', $\bar{J}'$, and J_c are respectively the Jacobians of B, $\bar{B}$, and C.

Notice that C induces a natural bijection from $\Delta(r, v_1, v_2)$ onto itself whose Jacobian is also J_c. If we transform $\int_\Delta$ in the definition of $\overline{\mathscr{C}}f$ by means of this map, we obtain

$$\overline{\mathscr{C}}f = \int_2 \int_\Delta [|w'|f_1'f_2'J' - |w|f_1f_2]J_c$$

$$= \int_2 \int_\Delta [|w'|f_1'f_2'J' - |w|f_1f_2J_c],$$

where we have used (5.8). Since $|w|f_1f_2$ is independent of $y \in \Delta$, we have, when $r < +\infty$,

$$\int_\Delta |w|f_1f_2 = \int_\Delta |w|f_1f_2J_c = |w|f_1f_2 \cdot (area\ of\ \Delta).$$

Thus, for $r < +\infty$,

$$\overline{\mathscr{C}}f = \int_2 \int_\Delta [|w'|f_1'f_2'J' - |w|f_1f_2] = \mathscr{C}f.$$

This proves (5.7) when $r < +\infty$. A limiting argument in which Δ is approximated by large discs also proves (5.7) when $r = +\infty$. This proves Theorem 5.3.

Because of Theorem 5.3, we will call two collision laws *equivalent* if they are extensions of the same pre-collision law. Not every pre-collision law can be extended to a collision law. For example, $b(y, v_1, v_2) = (\frac{1}{2}v_1, \frac{1}{2}v_2)$ cannot. Neither can $b(y, v_1, v_2) = (v_1, -v_2)$. However, we have

THEOREM 5.4. *Let $k = 3$, and let b be a differentiable, isotropic, planar, conservative pre-collision law. Then b can be extended to a collision law B which is*

also isotropic, planar, and conservative, and for which

(5.9) $|w'| = |w|$, *and*

(5.10) $J' = 1$.

Proof. Since b conserves momentum,

(5.11) $|v_1' + v_2'|^2 = |v_1 + v_2|^2$,

and since b conserves energy,

(5.12) $|v_1'|^2 + |v_2'|^2 = |v_1'|^2 + |v_2|^2$.

It follows that

(5.13) $|v_2' - v_1'|^2 = |v_2 - v_1|^2$,

since, by (5.12), (5.11) and (5.13) are both equivalent to $v_1' \cdot v_2' = v_1 \cdot v_2$. This proves (5.8) for b, and consequently also for B, if B exists.

Next notice that

(5.14) $\begin{aligned} v_1' &= \tfrac{1}{2}(v_1 + v_2) - \tfrac{1}{2}w' \\ v_2' &= \tfrac{1}{2}(v_1 + v_2) + \tfrac{1}{2}w' \end{aligned}$

since $\tfrac{1}{2}(v_1 + v_2) = \tfrac{1}{2}(v_1' + v_2')$ by conservation of momentum. Thus $b(y, v_1, v_2)$ is completely determined by a knowledge of

(5.15) $w' = w'(y, w)$,

where the explicit form of the function in (5.15) is guaranteed by the hypothesis that b is planar. (So we need not write $w' = w'(y, v_1, v_2)$.) We also know in (5.15) that w', y, and w are coplanar.

In (5.15) the vectors w and y are perpendicular since $(y, v_1, v_2) \in Z$. Let $\bar{y}$ and $\bar{w}$ be any other pair of perpendicular vectors with $|y| = |\bar{y}|$ and $|w| = |\bar{w}|$. Then there is a rotation $\overline{\Omega}$ which brings y to $\bar{y}$ and w to $\bar{w}$. Furthermore, by isotropy,

$$w'(\bar{y}, \bar{w}) = \overline{\Omega} w'(y, w),\ and$$

$$\frac{w'(y, w) \cdot w}{|w^2|} = \frac{\overline{\Omega} w'(y, w) \cdot \overline{\Omega} w}{|\overline{\Omega}w|^2} = \frac{w'(\bar{y}, \bar{w}) \cdot \bar{w}}{|\bar{w}|^2}\ .$$

It follows that $w' \cdot w/|w|^2$ is a function of $|y|$ and $|w|$ only. Thus we can define uniquely the angle $\theta = \theta(|y|, |w|)$ between w and w' by

$$\cos \theta = \frac{w' \cdot w}{|w|^2},\quad 0 \leqq \theta \leqq \pi.$$

Since $|w| = |w'|$, the function (5.15) is simply a rotation of w through the angle $\theta(|y|, |w|)$ in the plane of y and w. This rotation may be either "clockwise" or "counterclockwise" when one faces in the direction of $y \times w$. But isotropy shows that the "sense" of the rotation is always the same for fixed $|y|$ and $|w|$.

(The reader can convince himself with a few simple pictures that "counter-clockwise" corresponds to a repulsive force between molecules, and "clockwise" to an attractive force.) Let $\Omega(y \times w, \theta)$ denote the rotation around $y \times w$ through the angle θ in the prescribed sense. Then (5.15) becomes

$$(5.16) \quad w' = \Omega(y \times w, \theta)w = \Omega(y \times w, \theta)(v_2 - v_1).$$

Now define

$$(5.17) \quad y' = -\Omega(y \times w, \theta)y,$$

and notice from (5.14) and (5.16) that

$$(5.18) \quad v_1' = \tfrac{1}{2}[I + \Omega(y \times w, \theta)]v_1 + \tfrac{1}{2}[I - \Omega(y \times w, \theta)]v_2$$

$$(5.19) \quad v_2' = \tfrac{1}{2}[I - \Omega(y \times w, \theta)]v_1 + \tfrac{1}{2}[I + \Omega(y \times w, \theta)]v_2,$$

where I is the identity operator on R^k. We have proved that b is given explicitly by (5.18)–(5.19). We define B by means of (5.17)–(5.19). Then B is an extension of b, and it remains only to show that B has all the desired proporties.

To begin, notice that (5.18)–(5.19) imply (5.16), as we would expect. It follows from (5.16)–(5.17) that $y \cdot w = 0$ implies $y' \cdot w' = 0$. Thus $B : Z \to Z$. Next replace y by $-y$ and exchange v_1 and v_2 in (5.17)–(5.19). This, in effect, changes w to $-w$, so that $(-y) \times (-w) = y \times w$ is unchanged. Also $\theta(|y|, |w|)$ is unchanged. Consequently Ω is unchanged. Thus we can see by direct substitution in (5.17)–(5.19) that

$$B(-y, v_2, v_1) = (-y', v_2', v_1').$$

This proves (3.2) for B.

We must next calculate $B(y', v_1', v_2')$. To do so, make the following observations from (5.16)–(5.19): $|y| = |y'|$, $|w| = |w'|$, $\theta(|y'|, |w'|) = \theta(|y|, |w|)$, (y, w, y', w') are coplanar, and $y' \times w' = -y \times w$. From these observations, it follows that

$$(5.20) \quad \Omega(y' \times w', \theta(|y'|, |w'|)) = \Omega^{-1}(y \times w, \theta(|y|, |w|)).$$

Using (5.20), we see that

$$(y')' = -\Omega^{-1}(-\Omega y) = y,$$
$$(v_1')' = \tfrac{1}{2}(I + \Omega^{-1})[\tfrac{1}{2}(I + \tfrac{1}{2}(I + \Omega)v_1 - \Omega)v_2]$$
$$+ \tfrac{1}{2}(I - \Omega^{-1})[\tfrac{1}{2}(I - \Omega)v_1 + \tfrac{1}{2}(I + \Omega)v_2$$
$$= v_1,$$

and, similarly, $(v_2')' = v_2$. This proves (3.1) for B.

We can deduce from the corresponding properties for b, or directly from (5.17)–(5.19), that B is isotropic, planar, and conservative. Thus we need only show that $J' = 1$ to complete the proof of the theorem. Let $z^* = (y^*, v_1^*, v_2^*) \in Z$

with $w^* = v_2{}^* - v_1{}^*$ and define, for $\delta \geqq 0$,

$$Z_\delta{}^* = \{(y, v_1, v_2) \in Z : |y^*| \leqq |y| \leqq |y^*| + \delta,$$
$$|w^*| \leqq |v_2 - v_1| \leqq |w^*| + \delta\}.$$

Notice that $B : Z_\delta{}^* \to Z_\delta{}^*$ for every $\delta \leqq 0$. Let dS^* be a small "cylindrical" volume around z^* in $Z_\epsilon{}^*$, for some $\epsilon > 0$, whose "base" lies in $Z_0{}^*$. It follows from (5.17)–(5.19) that B preserves both the area of the base of dS^* and its height. Thus B is locally volume-preserving. This proves (5.10), and completes the proof of Theorem 5.4.

A consequence of Theorems 5.3 and 5.4 is that we can express the Maxwell-Boltzmann equation in its usual form for classical collision laws. This is done in

COROLLARY 5.5. *Let* $k = 3$ *and let* B *be an isotropic, planar, conservative collision law. Then* $|w| = |w'|$ *and we can assume without loss of generality that* $J' = 1$ *and*

$$(5.21) \quad \mathscr{C}f = \int_2 \int_\Delta |w|(f_1'f_2' - f_1 f_2).$$

Proof. We can use B to define a pre-scattering law b which satisfies the hypotheses of Theorem 5.4. Then we can extend b to a scattering law $\bar{B}$ for which $J' = 1$. (Note, by the arguments (5.11)–(5.13), that $|w'| = |w|$ is automatic for both B and $\bar{B}$). Since B is equivalent to $\bar{B}$, by Theorem 5.3 these two collision laws pose the same problem for f. Thus, without loss of generality, we can replace B by $\bar{B}$, for which $\mathscr{C}f$ has the form (5.21). This proves Corollary 5.5.

6. Entropy. We come at last to the concept of entropy. The theorem which we are about to state could have appeared immediately after Theorem 4.1. However, as indicated in § 1, it has been necessary first to formulate a rigorous version of model 2, to demonstrate that it is coherent in certain ways, and to place it in the historical context of earlier versions of the Maxwell-Boltzmann equation.

Boltzmann's definition for the total entropy of the gas at time t is

$$\eta(t) = -\int_D \int f \log f,$$

where $\int_D = \int_D \ldots dx$. Motivation for this definition is given in [**8**]. Our basic result for the entropy is

THEOREM 6.1. *In model* 2,

$$(6.1) \quad \frac{d\eta}{dt}(t) = \tfrac{1}{4} \int_D \int_1 \int_2 \int_\Delta |w|\left[\left(\frac{|w'|}{|w|}\,J'\right)f_1'f_2' - f_1 f_2\right]\log\left(\frac{f_1'f_2'}{f_1 f_2}\right)$$
$$+ \int_{\partial D} \int_+ (n \cdot v)f \log\left(\frac{|n \cdot v^*|}{n \cdot v}\,J^*\right).$$

Proof. Since $\mathscr{D}$ is a first order, homogeneous, linear differential operator,

$$\mathscr{D}(f_1 \log f_1) = \log f_1 \, \mathscr{D} f_1 + \mathscr{D} f_1$$
$$= (1 + \log f_1) \mathscr{C} f.$$

Therefore,

$$(6.2) \qquad \int_D \int_1 \mathscr{D}(f_1 \log f_1) = \int_D \int_1 (\log f_1) \mathscr{C} f,$$

since $\int_1 \mathscr{C} f = 0$ by (4.1) with $g = 1$. Furthermore, letting $g = \log f$ in (4.1), we obtain

$$\int_D \int_1 (\log f_1) \mathscr{C} f = - \tfrac{1}{4} \int_D \int_1 \int_2 \int_\Delta \log \left(\frac{f_1' f_2'}{f_1 f_2} \right) \mathscr{E} f,$$

that is,

$$(6.3) \qquad \int_D \int_1 (\log f_1) \mathscr{C} f = - \tfrac{1}{4} \int_D \int_1 \int_2 \int_\Delta |w| \left[\left(\frac{w'}{w} J' \right) f_1' f_2' - f_1 f_2 \right]$$
$$\log \left(\frac{f_1' f_2'}{f_1 f_2} \right).$$

Also, notice that

$$(6.4) \qquad \int_D \int \nabla_v \cdot \left(\frac{q}{m} f \log f \right) = 0,$$

for reasons similar to those accompanying (4.11), and

$$\int \int_D \nabla_v \cdot (vf \log f) = \int \int_{\partial D} (n \cdot v) f \log f$$
$$= \int_{\partial D} \int_+ \left[(n \cdot v) \log f - (n \cdot v^*)(\log f^*) \frac{n \cdot v}{n \cdot v^*} \right] f,$$

where we have applied (4.2) with $g = (n \cdot v) \log f$. Thus

$$\int_D \int \nabla_v \cdot (vf \log f) = \int_{\partial D} \int_+ (n \cdot v) \left(\log \frac{f}{f^*} \right) f.$$

Since

$$\frac{f}{f^*} = \frac{|n \cdot v^*|}{n \cdot v} J^*$$

by (3.22),

$$(6.5) \qquad \int_D \int \nabla_x \cdot (vf \log f) = \int_{\partial D} \int_+ (n \cdot v) f \log \left(\frac{|n \cdot v^{*1}|}{n \cdot v} J^* \right).$$

Moreover,

$$(6.6) \qquad \int_D \int \partial_t (f \log f) = - \frac{d\eta}{dt}.$$

Combining (6.4)–(6.6), we see that

$$(6.7) \qquad \int_D \int_1 \mathscr{D}(f_1 \log f_1) = -\frac{d\eta}{dt} + \int_{\partial D} \int_+ (n \cdot v)f \log \left(\frac{n \cdot v^*}{n \cdot v} J^* \right).$$

Finally, combining (6.2), (6.3), and (6.7) gives (6.1). This proves Theorem 6.1. (Notice that, as usual, Theorem 4.1 is the principal tool in the proof.)

Equation (6.1) gives the time rate of entropy change as a sum of two terms, the first representing the effect of molecular collisions and the second representing reflections. It is this second term

$$(6.8) \qquad W = \int_{\partial D} \int_+ (n \cdot v)f \log \left(\frac{n \cdot v^*}{n \cdot v} J^* \right)$$

which is called the "wall term" in § 1. Earlier authors (for example [4] and [8]) invariably arrive at this term in the form

$$(6.9) \qquad W = \int_{\partial D} \int (n \cdot v)f \log f;$$

indeed so do we during the proof of Theorem 6.1. If we insist on entropy *growth*, then we must require $W \geqq 0$. But the implications of this condition for the gas are not clear from (6.9), in general. All authors agree that, if the wall reflects molecules specularly, then $W = 0$ in (6.9). But this requirement certainly is not acceptable generally, since specular reflection is *inconsistent* with the very common no-slip boundary condition for a gas. (See Theorem 5.1, as well as [6].) A more general approach is taken by Grad [4], who simply says from (6.9) that $W = 0$ if there is no flux of the vector field

$$H = \int vf \log f$$

across the boundary of D. That is true, of course, but it sheds no light on general physical mechanisms which might prevent the flow of H across ∂D.

The difficulty with the expression (6.9) for W is that it contains the factor $\log f$. It appears that the sign of W depends on f, that is, on the local state of the gas. For this reason authors have always been compelled to impose *ad hoc* hypotheses to arrange that $W \geqq 0$. But in (6.8), it is clear that the sign of W depends *only* on

$$\log \left(\frac{|n \cdot v^*|}{|n \cdot v|} J^* \right),$$

that is, on the reflection law alone. We have seen in §§ 2–5 that the hypothesis of reflection, together with the associated boundary condition on f, gives us a coherent kinetic theory. And now we also find that this hypothesis is precisely what is needed to make a definite statement about wall mechanisms which contribute to increasing entropy. We exploit this fact in the remainder of the paper. First, we have

COROLLARY 6.2. *In model 2, if*

(6.10) $|w'|J' = |w|, (y, v_1, v_2) \in Z$, *and*

(6.11) $|n(x) \cdot v^*|J^* \geqq n(x) \cdot v, x \in \partial D, n(x) \cdot v > 0$, *then*

(6.12) $\dfrac{d\eta}{dt} \geqq 0$ *for all t.*

Proof. Notice that $f_1'f_2' - f_1f_2$ and $\log (f_1'f_2'/f_1f_2)$ always have the same sign. Thus, with the condition (6.10), the first term on the right hand side of (6.1) is non-negative. Similarly, with the condition (6.11), the second term is also non-negative. This proves (6.12) and completes the proof of the corollary.

We can also state a result still closer to the classical entropy theorem, namely

COROLLARY 6.3. *In model 2, if $k = 3$ and B is isotropic, planar, and conservative, and if (6.11) holds or if A is specular, then $d\eta/dt \geqq 0$ for all t.*

Proof. The conditions on B imply that B is equivalent to a collision law for which (6.10) holds. Furthermore, if A is specular, $|n \cdot v^*| = |n \cdot v|$ and $J^* = 1$, so (6.11) holds. This proves the corollary.

Notice that (6.1) is an equality. Thus if either of the conditions (6.10) or (6.11) fails, there is a chance that $d\eta/dt \leqq 0$. One very simple device which we might use to study the failure of (6.11) is

COROLLARY 6.4. *In model 2 if $\mathscr{C}f = 0$, then*

(6.13) $\dfrac{d\eta}{dt} = \displaystyle\int_{\partial D} \int_{+} (n \cdot v) f \log \left(\dfrac{|n \cdot v^*|}{n \cdot v} J^* \right)$.

Proof. (6.13) follows at once from (6.1) and (6.3).

We can also cite one very concrete example:

COROLLARY 6.5. *In a reverse gas, $d\eta/dt \geqq 0$.*

Proof. The conditions (4.20) imply (6.10)–(6.11).

7. Counterexamples: a one-dimensional gas.
The simplest of all gases is one in which the motion of the molecules is confined to a line. Just as the vibrating string provides an elementary and instructive example for the study of the wave equation, so the one-dimensional gas is a natural setting in which to study model 2 (and also model $1\frac{1}{2}$, as we shall see). In some cases the initial boundary value problem for such a gas can be solved explicitly. However, solutions may not be unique, or they may even violate criterion (1.2). Furthermore, in cases when both criteria (1.1) and (1.2) are satisfied, the entropy may decrease. From such examples we can gain physical insight into the properties of a reflection law which lead to decreasing entropy.

A one-dimensional gas is, of course, a gas for which $k = 1$ in the input data. To standardize our choices for the remaining data, we define a *standard one-dimensional gas* to be a model 2 gas in which (1) $k = 1$, (2) $m > 0$, (3) $D = [-L, L]$, $L > 0$, (4) $q = 0$, (5) A is given at both $x = -L$ and $x = L$ by the same differentiable odd function $A : R^1 \to R^1$ with $dA/dv = A'(v) < 0$ for $v \neq 0$, (6) $r = 0$ since $k = 1$, and (7) $B : R^2 \to R^2$ is differentiable with $B^2 = I$ and $B \circ B_e = B_e \circ B$.

It is natural to make some restrictions on the initial data f_0 for such a gas. With this in mind, we define a function class $\mathscr{A}$ as follows. For given A, we say that $f_0 \in \mathscr{A}$ if

(7.1) $f_0 \in C^1([-L, L] \times R^1)$,

(7.2) $f_0(\pm L, A(v)) = \dfrac{v}{A(v)A'(v)} f_0(\pm L, v)$, $\pm v > 0$,

(7.3) $\partial_x f_0(-L, v) = \partial_x f_0(L, v) = 0$,

(7.4) $f_0 \geq 0$ and $\displaystyle\int_{-L}^{L} \int_{-\infty}^{\infty} f_0(x, v) dv\, dx = 1$.

Notice that the two equations (7.2) are compatibility requirements between the initial condition (3.23) and the boundary condition (3.22) for f. The reason for condition (7.3) is made clear later, in the proof of Theorem 7.2.

It is also possible to describe a one-dimensional gas by means of model $1\frac{1}{2}$. To see this, consider a system of N molecules moving on $[-L, L]$ according to the following five rules. (i) Molecules move with constant velocity except at moments (a) when one or more occupy the points $x = \pm L$ or (b) when two or more occupy the same point in $(-L, L)$. (ii) In case (a), each molecule instantly has its incident velocity converted to a reflected velocity prescribed by a reflection law A. (iii) In case (b), if exactly two molecules meet, their incident velocities are instantly converted to scattered velocities prescribed by a collision law B. (iv) In case (b), if three or more molecules meet, their velocities are unaltered. (v) After reflection and collision, the motion continues as in (i). These five rules are enough to allow us to determine explicitly trajectories of the form (2.3), where, by convention, every point on a trajectory represents the condition of molecules after collision and reflection. Thus we can actually compute the trajectory map Ψ. Furthermore the function Ψ can be seen to satisfy (2.8)–(2.10). (The property (3.2) for B is used in proving (2.10).)

Given a standard one-dimensional gas with reflection and scattering laws A and B, we now define a *corresponding model $1\frac{1}{2}$ gas* to be one in which (1) $k = 1$, (2) $N \geq 1$, (3) $m > 0$, (4) $D = [-L, L]$, and (5) Ψ is computed from A and B by rules (i)–(v) above. Notice, incidentally, that no definition for a "corresponding model 1 gas" is possible since, in general, no forces q_i give rise to rule (iii) for Ψ.

For each standard gas, there are many possible corresponding model $1\frac{1}{2}$ gases, depending on the choice of $N \geqq 1$. One particular choice is $N = 1$. In this case rules (iii) and (iv) never enter the computation for Ψ, because two molecules cannot meet if there is only one. In effect, the "molecules" ignore each other. Such a gas is called a *Knudsen gas*. We call its trajectory map Ψ_1.

We can ask, is the behavior of the corresponding model $1\frac{1}{2}$ gas somehow the same as the behavior of the standard gas? In general, the answer is surely no. For example, a one-dimensional reverse gas (which is standard) can be shown to behave differently from its corresponding Knudsen gas. However, a theorem is still possible. We begin with a definition. If $f(t, x, v)$ and $F(t, x_1, \ldots, x_N, v_1, \ldots, v_N)$ are solutions to initial value problems for a standard one-dimensional gas and its corresponding model $1\frac{1}{2}$ gas, respectively, then the solutions are said to be *compatible at time t* if (2.17) holds for f and F, that is, if

$$f(t, x_1, v_1) = \int_{[-L,L]^{N-1} \times R^{N-1}} F(t, x_1, \ldots, x_N, v_1, \ldots, v_N)$$

$$\times \, dx_2 \ldots dx_N \, dv_2 \ldots dv_N.$$

We can now state

THEOREM 7.1. *Suppose that a standard one-dimensional gas has a conservative collision law B and that a corresponding model $1\frac{1}{2}$ gas has indistinguishable molecules. Let f and F be solutions to initial value problems for the standard and corresponding gases, respectively, or the time interval $[0, t_0]$. Then, if f and F are initially compatible, they remain compatible for all $t \in [0, t_0]$. Furthermore*

$$(7.5) \quad f(t, x, v) = f_0 \circ \Psi_1(-t, x, v) \left| \frac{\partial \Psi_1}{\partial (x, v)} \, (-t, x, v) \right| , \, t \in [0, t_0]$$

where f_0 is initial data for f.

Proof. Since B is conservative,

$$(7.6) \quad v_1 + v_2 = v_1' + v_2', \, |v_1 - v_2| = |v_1' - v_2'|,$$

as shown in the proof of Theorem 5.5. Since $k = 1$, it follows from (7.6) that B is one of the two laws

$$B_i(v_1, v_2) = (v_1, v_2) \text{ or } B_e(v_1, v_2) = (v_2, v_1).$$

Thus molecules either ignore each other or exchange velocities. In each case, it follows that $\mathscr{C}f = 0$, so that the initial value problem for the standard gas is

$$(7.7) \quad \partial_t f + v \partial_x f = 0, \, -L \leqq x \leqq L, \, t \geqq 0,$$

$$(7.8) \quad vf(t, \pm L, v) = A(v)A'(v)f(t, \pm L, A(v)), \, \pm v \leqq 0, \, t \geqq 0,$$

$$(7.9) \quad f(0, x, v) = f_0(x, v), \, x \in [-L, L].$$

Suppose first that $N = 1$ in the corresponding gas. Then the trajectory map

for this case in Ψ_1 regardless of the choice for B, and by (2.13)

$$(7.10) \quad F(t, x, v) = F_0 \circ \Psi_1^{-1}(t, x, v) \left| \frac{\partial \Psi_1^{-1}}{\partial(x, v)}(t, x, v) \right|,$$

where F_0 is initial data for F. Furthermore since F and f are initially compatible and $N = 1$,

$$(7.11) \quad F_0(x, v) = f_0(x, v).$$

We can show that the problem (7.7)–(7.9) for f and (7.10)–(7.11) for F have the same solution. In Theorem 2.2, p. 1190, of [6] the Jacobian $|\partial \Psi_1/\partial(x, v)|$ is computed and found to be constant on trajectories of a molecule at $x \in (-L, L)$ but to jump by a factor $(A(v)A'(v))/v$ at $x = \pm L$. Equations (7.7)–(7.8) are equivalent to these same two requirements for f. Since F and f have the same initial data, they must remain always the same, namely the function given by (7.10), that is, (7.5). This proves the theorem when $N = 1$ in the corresponding gas and also proves (7.5) for the standard gas.

Next suppose that $N > 1$ and $B = B_i$. Let Ψ_N be the trajectory map for the corresponding gas. Then

$$(7.12) \quad \Psi_N(t, x_1, \ldots, x_N, v_1, \ldots, v_N) = (\Psi_1(t, x_1, v_1), \ldots, \Psi_1(t, x_N, v_N)),$$

since trajectories of individual molecules are independent of collisions with other molecules. Also

$$(7.13) \quad F = F_0 \circ \Psi_N^{-1} \left| \frac{\partial \Psi_N^{-1}}{\partial \zeta} \right|$$

from (2.13). Integrating (7.13) with respect to $(x_2, \ldots, x_N, v_2, \ldots, v_N)$ and taking account of (7.12) gives (7.5), where f is related to F by (2.17). This proves the theorem when $B = B_i$ for any $N > 1$.

Finally suppose $B = B_e$. Then, according to the rules for Ψ, at each collision two molecules trade location in state space and then continue as if nothing had happened. Consequently, after any number of collisions the system has evolved as it would if $B = B_i$, except that certain molecules have traded places. Thus

$$(7.14) \quad \Psi = P(t)\Psi_N$$

where Ψ and Ψ_N are the trajectory maps for the N-molecule corresponding gas with $B = B_e$ and $B = B_i$, respectively, and $P(t)$ is some permutation in Γ_N for each time t. It follows from (7.14) and (2.13) that

$$(7.15) \quad F = F_0 \circ (P(t)\Psi_N^{-1}) \left| \frac{\partial(P(t)\Psi_N^{-1})}{\partial \zeta} \right|.$$

But $F_0(P\zeta) = F_0(\zeta)$ by indistinguishability, and $|\partial P/\partial \zeta| = 1$. Thus (7.15) implies (7.13). As in the previous paragraph, the theorem now follows when $B = B_e$ for any $N > 1$. This proves Theorem 7.1.

In the preceding theorem we have supposed that solutions to the initial value problem for a standard gas exist. They may not, in fact. But we can state a simple condition for their existence. If A is the reflection law for a standard gas, let A^{-1} be the inverse of the (monotone) function A. Define inductively

$$A_0(v) = v, \ A_n(v) = -A^{-1} \circ A_{n-1}(v), \ n \geqq 1.$$

It follows that, since A is odd, $v/A_n(v) > 0$ for $n \geqq 0$ and $v \neq 0$. Using this definition, we can state

THEOREM 7.2. *Let A be the reflection law for a standard one-dimensional gas with a conservative collision law. Then the initial value problem (3.21)–(3.23) for this gas has a unique differentiable solution for every $f_0 \in \mathscr{A}$ for all time $t \in [0, +\infty)$ if and only if*

$$(7.16) \quad \sum_{k=1}^{\infty} \frac{v}{A_k(v)} = +\infty \ \text{for all } v > 0.$$

Proof. Equations (3.21)–(3.23) for this gas take the form (7.7)–(7.9). From (7.7)

$$(7.17) \quad f(t, x, v) = g(x - vt, v), \ t \geqq 0,$$

for some function $g(x, v)$. In terms of g equations (7.8) and (7.9) take the form

$$(7.18) \quad g\left[\frac{A(v)}{v}(x \mp L) \pm L, A(v)\right] = \frac{v}{A(v)A'(v)} g(x, v), \ \pm v \geqq 0,$$

$$(7.19) \quad g(x, v) = f_0(x, v), \ -L \leqq x \leqq L.$$

Thus equations (7.17)–(7.19) are equivalent to the problem (3.21)–(3.23) for the gas.

We can use (7.18) and (7.19) to determine g from the initial data for f by a method of reflection. To do this, define

$$P_0 = \{(x, v) \in R^2 : -L \leqq x \leqq L, v \geqq 0\},$$

$$P_n = \left\{(x, v) \in R^2 : -L - 2L \sum_{k=1}^{n} \frac{v}{A_k(v)}\right.$$

$$\left. \leqq x \leqq -L - 2L \sum_{k=1}^{n-1} \frac{v}{A_k(v)}, v > 0\right\}, \ n \geqq 1,$$

$$Q_n = \{(x, v) \in R^2 : (-x, -v) \in P_n\}, \ n \geqq 0,$$

where $\sum_1^0 = 0$. Notice that (7.19) determines g on the set $P_0 \cup Q_0$. Furthermore,

$$(x, v) \in Q_n$$

$$\Leftrightarrow (-x, -v) \in P_n$$

$$\Leftrightarrow L - 2L \sum_{k=0}^{n} \frac{v}{A_k(v)} \leqq -x \leqq L - 2L \sum_{k=0}^{n-1} \frac{v}{A_k(v)}, v < 0$$

$$\Leftrightarrow -2L \left(-\frac{v}{A(v)} \right) \sum_{k=1}^{n+1} \frac{A(v)}{-A_{k-1}(v)}$$

$$\leqq -(x + L) \leqq -2L \left(-\frac{v}{A(v)} \right) \sum_{k=1}^{n} \frac{A(v)}{-A_{k-1}(v)}, v < 0$$

$$\Leftrightarrow -L - 2L \sum_{k=1}^{n+1} \frac{A(v)}{A_k(A(v))}$$

$$\leqq \frac{A(v)}{v} (x + L) - L \leqq -L - 2L \sum_{k=1}^{n} \frac{A(v)}{A_k(A(v))}, A(v) > 0$$

$$\Leftrightarrow \left[\frac{A(v)}{v} (x + L) - L, A(v) \right] \in P_{n+1}$$

for $n \geqq 1$. A slightly modified proof holds when $n = 0$. Thus (7.18), with the lower sign, can be used to determine g in P_{n+1} from its values in Q_n. Similarly (7.18), with the upper sign, gives g in Q_{n+1} from its values in P_n. Thus (7.18) and (7.19) determine g uniquely on the set

$$Q_* = \bigcup_{n=0}^{\infty} (P_n \cup Q_n)$$

$$= \Big\{ (x, v) \in R^2 : -L \leqq x \leqq L, \text{ or } -L - 2L \sum_{k=1}^{\infty} \frac{v}{A_k(v)}$$

$$< x \leqq -L \text{ and } v > 0, \text{ or } L \leqq x \leqq L + 2L \sum_{k=1}^{\infty} \frac{v}{A_k(v)} \text{ and } v < 0 \Big\}.$$

Recall that f is determined by g from (7.17). To know f for all $x \in [-L, L]$, $t \geqq 0$, and $v \in R^1$ is equivalent to knowing g on the set

$$P_* = \{ (x, v) \in R^2 : -L \leqq x \leqq L, \text{ or } x \leqq -L \text{ and }$$
$$v > 0, \text{ or } x \geqq L \text{ and } v < 0 \}.$$

Notice that $Q_* \subseteq P_*$. If $Q_* = P_*$, then f is determined uniquely by (7.17)–(7.19), that is, by (3.21)–(3.23). On the other hand, if $Q_* \neq P_*$, then g can be assigned *any* value consistent with (7.18) on the set $P_* - Q_*$. The initial condition (7.19) has no effect on the values of g in $P_* - Q_*$. Thus f is *not* determined uniquely in this case. In short, unique solution to (3.21)–(3.23) for a standard one-dimensional gas is equivalent to the condition $P_* = Q_*$.

But this condition is equivalent to (7.16), as can be seen from the definitions of P_* and Q_*.

If (7.16) holds, the solution found by the method described above is differentiable. To prove this, we need only show that g is differentiable on the set $P_* = Q_*$. In the method of reflection the only possible non-differentiable points for g are points on the boundaries of P_n and Q_n. However, the conditions (7.2) on $f_0 \in \mathscr{A}$ and (7.18) on g assure us (by induction on n) that the method at least gives a continuous g. Furthermore, derivatives of g in the tangential direction to the boundaries of P_n and Q_n are continuous at these boundaries. Finally (7.17) shows that the values of g on the line $v = v_0$ in P_n (or Q_n) determine g on the line $v = A(v_0)$ in Q_{n+1} (or P_{n+1}). By induction from (7.3), it follows that $\partial x\, g = 0$ on the boundaries of P_n and Q_n for all n. It is for this step that we require (7.3) for $f_0 \in \mathscr{A}$. Thus at each boundary point of P_n and Q_n, g has continuous directional derivatives in two independent directions. (The tangential direction is independent of the direction along $v = $ constant because $A'(v) < 0$ for $v \neq 0$.) It follows that g is differentiable. This proves Theorem 7.2.

What is the physical significance of the condition (7.16) on the reflection law A? One way to assess this is to consider what happens when A is *linear*. In this case we have

THEOREM 7.3. *Exactly one of three alternatives holds for the initial value problem for a standard one-dimensional gas with A linear and B conservative. These alternatives are:*

(1) *The solution to the problem is not unique for any $f_0 \in \mathscr{A}$ on any time interval* $[0, t_1)$, $t_1 > 0$; *however, for each $f_0 \in \mathscr{A}$ there is exactly one solution f which satisfies criterion* (1.2) *and exists for all time $t \geqq 0$.*

(2) *The problem has a unique solution for every $f_0 \in \mathscr{A}$ and all $t \geqq 0$; however, for each f_0 there is a time $t_1 > 0$ when*

$$(7.20) \quad \int_{-L}^{L} \int_{-\infty}^{\infty} f(t_1, x, v) dv\, dx < 1.$$

(3) *The problem has a unique solution for every $f_0 \in \mathscr{A}$ and all $t \geqq 0$; furthermore, each solution satisfies criterion* (1.2) *and the entropy is constant:*

$$(7.21) \quad \eta(t) = \eta(0), t \geqq 0.$$

Before proceeding to the proof of this theorem, notice that alternatives (1) and (2) seem to contradict Theorem 4.3. According to that theorem, criterion (1.2) holds for solutions to both models $1\frac{1}{2}$ and 2. However, in (1) and (2), hypotheses of Theorem 4.3 are violated. We have assumed in model $1\frac{1}{2}$ that $\Psi^{-1}(t, \cdot)$ exists with $\Psi^{-1}(t, S) = S$ and in model 2 that $\int vf$ exists. Neither of these hypotheses is valid in (1) or (2) for all $t > 0$ and all solutions f. These difficulties will be clarified in the proof of the theorem and the comments which follow it.

Proof of Theorem 7.3. Since A is linear,

$$(7.22) \quad A(v) = -av$$

for some constant $a > 0$. We will show that $0 < a < 1$ implies (1), $a > 1$ implies (2), and $a = 1$ implies (3). This will prove the theorem.

For the reflection law (7.22), it is a straightforward matter to find the set $P_* - Q_*$ defined in the proof of theorem 7.2. Notice that

$$A^{-1}(v) = -\frac{1}{a}v, \; A_n(v) = \frac{v}{a_n}, \; \frac{v}{A_n(v)} = a^n, \text{ and}$$

$$P_* - Q_* = \begin{cases} \left\{ (x, v) : L + \frac{2L}{1-a} \leqq |x|, \, xv < 0 \right\}, \; a < 1, \\ E, \; a \geqq 1, \end{cases}$$

where E is the empty set.

If $0 < a < 1$, g can be prescribed arbitrarily on a vertical strip in $P_* - Q_*$. Furthermore, for any $t > 0$ and $x \in [-L, L]$, there is a v large enough (positive or negative) so that the point $(x - vt, v)$ lies in this strip. Since $f(t, x, v) = g(x - vt, v)$, it follows that f is not determined uniquely for any $t > 0$ or any $f_0 \in \mathscr{A}$.

Let $\bar{g}$ be the particular g which vanishes in $P_* - Q_*$. With this choice we can show that the moments $\rho(t, x)$ and $\rho s(t, x)$ are defined and differentiable so that Theorem 4.3 holds. It follows that criterion (1.2) applies to the solution $\bar{f}$ determined from $\bar{g}$. Any other f comes from a g not always zero in $P_* - Q_*$. If $g < 0$ somewhere, then (1.2) fails. On the other hand, if $g \geqq 0$, then

$$\int_{-L}^{L} \int f > 1$$

for some $t > 0$ because supp $g \supsetneqq$ supp $\bar{g}$. Again (1.2) fails. This proves (1) when $0 < a < 1$.

If $a > 1$, then $P_* = Q_*$, and the problem has a unique global solution for each $f_0 \in \mathscr{A}$, as shown in Theorem 7.2. However, in computing the trajectory map Ψ_1 for this case, we find that a molecule starting at (x, v) with $x \in [-L, L]$ and $v \neq 0$ reaches infinite speed by the time

$$t = -\frac{x}{v} + \frac{L}{|v|} + \frac{2L}{|v|} \sum_{k=1}^{\infty} \frac{1}{a^k} = -\frac{x}{v} + \frac{L}{|v|} \frac{a+1}{a-1},$$

because at each reflection the molecule's speed is increased by the factor $a > 1$. Using this fact, we can show that

$$(7.23) \quad \Psi_1^{-1}(t, T) = T(t), \; t > 0,$$

where $T = [-L, L] \times R^1$ and

$$T(t) = \left\{ (x, v) : -L \leqq x \leqq L, \left| v + \frac{x}{t} \right| < \frac{L}{t} \frac{a+1}{a-1} \right\}.$$

By (7.23) and conservation of probability for model $1\frac{1}{2}$,

$$(7.24) \quad \int_T f(t, x, v)dx\,dv = \int_{T(t)} f_0(x, v)dx\,dv.$$

As $t \to +\infty$, $T(t) \to [-L, L] \times \{0\}$. Thus for some $t_1 > 0$, $T(t_1)$ is smaller that the support of f_0. With this t_1, the left hand side of (7.24) is less than 1. This proves (2), in particular (7.20), when $a < 1$.

When $a = 1$, again $P_* = Q_*$ and global solutions always exist. Furthermore, molecules are not speeded up by reflection and $\Psi_1^{-1}(t, T) = T$. From this, criterion (1.2) follows. Also, $d\eta/dt = 0$ by (6.73), since

$$\log\left(\frac{n \cdot v^*}{n \cdot v} J^*\right) = \log 1 = 0$$

when $a = 1$. This proves (3), in particular (7.21), when $a = 1$, and completes the proof of Theorem 7.3.

Using Theorem 7.1, we can describe the physical significance of each of the alternatives in Theorem 7.3. According to (7.5), the value of f at time t is obtained by referring backward along trajectories of a single molecule. Let A be the linear law, $A(v) = -av$. If $0 < a < 1$, then the molecule is slowed down every time it reflects. However, following a trajectory *backward*, we find that a molecule is *sped up* by reflection. In fact, the speed-up effect is geometric; at each backward reflection the molecule's speed is increased by the factor $1/a$. Thus the molecule always reaches infinite speed in finite time along a backward trajectory with $v \neq 0$. Precisely this fact is detected by the failure of (7.16) when $a < 1$. It follows that $\Psi_1(-t, x, v)$ is not defined for any fixed $t > 0$ when $|v|$ is large enough. This difficulty leads to alternative (1) in Theorem 7.3.

On the other hand, if $a > 1$, the molecule is sped up on forward trajectories but only slowed down on backward trajectories. Thus $\Psi_1(-t, x, v)$ exists for all $t > 0$ and (7.5) gives a solution $f(t, x, v)$ for $t > 0$. However, there is a a serious difficulty with this solution. Although backward trajectories exist for all time, forward trajectories do not; the molecule always reaches infinite speed in finite time unless $v = 0$. A molecule with infinite speed is, in effect, lost from state space. Thus mass is not conserved and criterion (1.2) is violated. This leads to alternative (2) of Theorem 7.3.

Alternative (2) poses a much more serious difficulty than (1). In (1), although f is not determined uniquely by the axioms of model 2, there is a unique f satisfying both these axioms and criterion (1.2). This f is defined to be zero whenever $\Psi_1(-t, x, v)$ does not exist and is otherwise given by (7.5). However, in alternative (2) the failure of criterion (1.2) cannot be avoided.

According to Theorem 7.3, either criterion (1.1) fails, or (1.2) fails, or the entropy is constant. It seems that the model "wants" a constant entropy. However, this is the case only for linear reflection laws as we see in

THEOREM 7.4. *It is possible to choose the input data for model* 2 *and the initial distribution* f_0 *in such a way that the following three conditions hold:*

(1) *the initial value problem is uniquely solvable for all time and criterion* (1.2) *holds;*

(2) *the macroscopic gas satisfies the no-slip boundary condition,* $\rho s = 0$ *on* ∂D; *and*

(3) *the entropy* η *is strictly decreasing for all time* $t \geqq 0$.

Proof. Choose the data for a standard one-dimensional gas with $A(v) = -v^3$ and B conservative. Let

$$(7.25) \quad f_0(x, v) = \left(1 + \sin\frac{\pi x}{2L}\right)\phi(v) + \left(1 - \sin\frac{\pi x}{2L}\right)\phi(-v), \text{ where}$$

$$(7.26) \quad \phi \in C^1(R^1),$$

$$(7.27) \quad \phi(v) > 0 \text{ when } 0 < v < \alpha, \phi(v) = 0 \text{ when } v \geqq \alpha, \alpha \in (0, \tfrac{1}{2})$$

$$(7.28) \quad \phi(-v^3) = \frac{1}{3v^4}\phi(v), v > 0, \text{ and}$$

$$(7.29) \quad \int_{-\infty}^{\infty} \phi(v)dv = \frac{1}{4L}.$$

The function f_0 so defined lies in $\mathscr{A}$, since the statements (7.25)–(7.29) imply (7.1)–(7.4).

Notice that

$$A^{-1}(v) = -v^{1/3}, A_n(v) = v^{3^{-n}}, \text{ and } \frac{v}{A_n(v)} = v^{1-3^{-n}} = \left(v^{3^{-n}}\right)^{3^n-1}.$$

This is positive for $v \neq 0$ since $3^n - 1$ is even. Furthermore,

$$\sum_{k=1}^{\infty} \frac{v}{A_k(v)} = \sum_{k=1}^{\infty} v^{1-3^{-n}} = +\infty, v \neq 0.$$

Thus the condition (7.16) applies to this gas; the initial value problem has a unique solution f for all $t \geqq 0$ and any $f_0 \in \mathscr{A}$, in particular (7.25). As in the proof of Theorem 7.2, we can write

$$f(t, x, v) = g(x - vt, v), t \geqq 0,$$

where g is found from f_0 by a method of reflection.

We next prove by induction that

$$(7.30) \quad g(x, v) = 0 \text{ if } (x, v) \in P_n \cup Q_n \text{ and } |v| \geqq \alpha^{3^n}.$$

By definition of f_0, in particular (7.27), it follows that (7.30) is true for $n = 0$ since $g = f_0$ in $P_0 \cup Q_0$. Furthermore the values of g on the line $v = v_0$ in $P_n \cup Q_n$ are used to define g on the line $v = A(v_0)$ in $P_{n+1} \cup Q_{n+1}$. Thus, if $g = 0$ for $|v| \geqq \alpha^{3^n}$ in $P_n \cup Q_n$, then $g = 0$ for $|v| \geqq (\alpha^{3^n})^3 = \alpha^{3^{n+1}}$

in $P_{n+1} \cup Q_{n+1}$. This proves (7.30). Figure 1 illustrates the support for g in the (x, v)-plane and the regions P_n and Q_n which enter into the construction of g. Notice that there is a band along the x-axis, increasingly narrow as x tends to $\pm\infty$, in which g is non-zero.
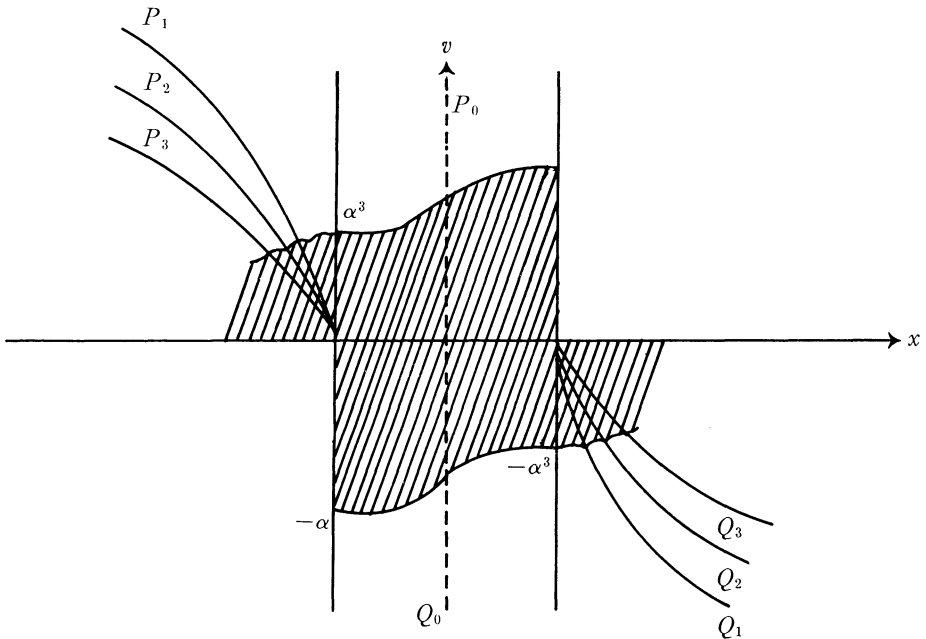

FIGURE 1.   The support for g (shaded) in Theorem 7.4. The vertical scale is distorted.

For $x \in [-L, L]$ and $t \geqq 0$, notice that $\rho(t, x)$, $\rho s(t, x)$,and $\eta(t)$ are integrals which reference the values of g on the lines

$$l_{x,t} = \{(y, v) : y = x - vt, v \in R^1\}$$

in P_*. Since g is differentiable with compact support on each $l_{x,t}$ (see Figure 1), it follows that these moments exist and are differentiable. The hypotheses leading to (4.13) are satisfied, and, since $g \geqq 0$ by construction, criterion (1.2) holds. This proves (1). Also, notice from (5.1) and (5.3) that the reflection law $A(v) = -v^3 = -|v|^2 v$ implies the boundary condition $\rho s = 0$. This proves (2).

To prove (3), notice that by (6.13)

$$(7.31) \quad \frac{d\eta}{dt} = \int_{-\infty}^{0} (-v)g(-L - vt, v) \log (3v^4)dv$$

$$+ \int_{0}^{\infty} vg(L - vt, v) \log (3v^4)dv.$$

These integrals reference values of g along the lines $l_{\pm L, t}$ for fixed $t \geqq 0$. Any such line crosses the support of g, so the integrals are not zero. However, $g = 0$ for $v \geqq \frac{1}{2} > \alpha \geqq \alpha^{3^n}$. Consequently, if $g(v) \neq 0$, then $3v^4 < 3(\frac{1}{2})^4 < 1$; that is, if $g > 0$, then $\log (3v^4) < 0$. Using this fact in (7.31), we find $d\eta/dt < 0$ for $t \geqq 0$. This completes the proof of Theorem 7.4.

To understand the physical significance of Theorem 7.4, notice that f_0 is chosen to admit only slow molecules with speeds less than $\frac{1}{2}$. Since $A(v) = -v^3$, such molecules never attain a speed greater than 1, either on backward or forward trajectories. Consequently, trajectories for these molecules are defined for all positive and negative time, and there is no difficulty with criteria (1.1) and (1.2).

On forward trajectories these slow molecules are slowed still further by reflection. This is precisely the significance of the shrinking support for g as $x \to \pm\infty$ in figure 7. Thus the state of the gas moves from a comparatively wide distribution of speeds to an increasingly narrow distribution. This is a change from more "chaos" to less. In effect, the boundary feeds information into the system: it says, "Slow down". As a result, we can have more accurate information later than earlier. After a long time we can say with near certainty that the molecules have almost stopped.

The reader may be tempted to think that the only examples of decreasing entropy are those in which the gas is brought to a stop. This is not true, however. Another entropy-reducing reflection law is shown in figure 2, along with the important ratio

$$\frac{A(v)A'(v)}{v}$$

which appears in (6.13). In this case molecules with speeds in the interval (v_1, v_2) are slowed toward the speed v_1 by reflection but, beyond that, are slowed no further. Beginning with a probability distribution which admits only speeds in this range, we find that the band of available speeds shrinks, as time passes, toward v_1. And, since $(A(v)A'(v))/v < 1$ on (v_1, v_2), we can use (6.13) to show that $d\eta/dt < 0$.

The important feature of entropy-reducing reflection laws seems to be "entrainment", the tendency to entrain the molecules into a narrow band of possible speeds. A reflection law which "entrains" supplies information to the gas. The entropy detects this increasing information as a concentration of the probability distribution f over a shrinking support in velocity-space.

The rigorous examples of this section have all been one-dimensional to keep the analysis simple. But the physical and mathematical phenomena which they suggest can be extended to higher dimensions. For example, versions of Theorems 7.3 and 7.4 certainly exist for a Knudsen gas confined to a sphere. In such a gas, a molecule never travels farther than the sphere diameter between reflections. Thus, when $A(x, v) = -av$ on the surface of the sphere,
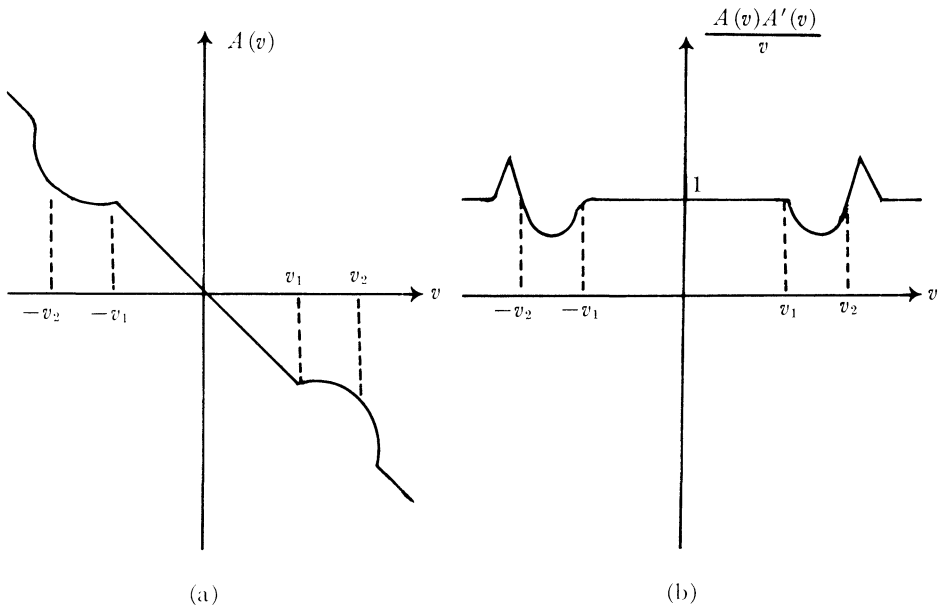
FIGURE 2.   Another entropy-reducing reflection law.

with $a > 0$ and $a \neq 1$, molecules are sped up geometrically by reflection on either forward or backward trajectories. Because of this, the difficulties (1) and (2) of theorem 7.3 carry over to a sphere. Similarly, if $A(x, v) = -|v|^2 v$ on the surface of the sphere, slow molecules are slowed further by reflection along forward trajectories. If we choose f_0 to admit only slow speeds, then we can exhibit a Knudsen gas flow in the sphere which satisfies the no-slip boundary condition as well as $d\eta/dt < 0$ for $t \geqq 0$.

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