

KINETIC THEORY AND BOUNDARY CONDITIONS FOR FLUIDS

JON SCHNUTE AND MARVIN SHINBROT

Summary. A rigorous derivation of the molecular theory of a confined, deterministic gas is given. Then, a molecular reflection law is presented with the property that the corresponding fluid does not slip at the boundary. It is also shown that, within a certain reasonable class of reflection laws, the one we give is the only one that leads to no-slip. Finally, and again within the framework of certain reasonable hypotheses, it is shown that no-slip is the only non-paradoxical boundary condition a fluid can be expected to satisfy

1. Introduction. It is not known what the molecules of a gas do when they encounter the walls of a container. The simplest hypothesis would seem to be that they reflect specularly, but Maxwell pointed out nearly a century ago [6] that a gas with specularly reflecting molecules can exert no tangential stresses on its boundary and, therefore, that specular reflection is impossible for ordinary fluids. In place of specular reflection, Maxwell suggested diffuse reflection, which is a stochastic law in which the reflected velocity is not uniquely determined by its incident velocity.

As he makes clear in the paper [6], Maxwell was led to this idea by viewing a wall as a large number of essentially stationary molecules that interact with any gas molecule that gets close enough. However, it is a formidable problem to integrate the equations of motion and determine the exact effect on a mobile gas molecule of a large number of fixed molecules. As Maxwell points out, and his criticism applies even if the wall consists of hard, immovable spheres, “. . . there is considerable difficulty in calculating the effect when the direction of rebound from the first impact is such as to lead to a second or third impact . . .”. It was in part difficulties such as these that led Maxwell to treat interaction with a wall as a stochastic process.

What this means is that diffuse reflection is an approximation and, in a sense, it is as much a description of our ignorance as it is of the behavior of molecules. The question remains open of whether there is a deterministic treatment of reflections that describes the behavior of a gas as well as Maxwell's stochastic law. In this paper, instead of proposing an approximate, stochastic solution of the difficult mechanical problem of reflection, we approximate the problem itself by a simpler one that has an exact, deterministic solution, and we explore the consequences of this approximation.

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The approximation consists in replacing the wall by a smooth surface and assuming that when a particle encounters the wall, it “reflects”—that is, its velocity instantaneously changes from its incident value to another “reflected” value, this one being such as to take the particle back into the domain of the gas. We call any such transformation of incident velocities to reflected ones a *reflection law*, and we study the possible reflection laws.

We began originally by asking how one might “reasonably” restrict reflection laws and what consequences such restrictions would have for the motion. For example, we took as a “reasonable” restriction the conditions that the law be isotropic. Surprisingly, once this and other simple restrictions were imposed, there turned out to be only two “reasonable” laws and, of these, one had the same consequence as specular reflection: zero tangential stress on the boundary. This left essentially one reflection law, which we called “reverse reflection”.

A reverse reflection law is one in which the direction of the velocity is reversed upon contact with the boundary. Although a mechanism for such a law seems a little hard to imagine, we carried our analysis a little further and found that a gas consisting of reversely reflecting molecules sticks to any bounding surface: the macroscopic velocity of such a gas at a rigid boundary is zero.

Now, it is an experimental fact that to a very high degree of approximation real gases under ordinary circumstances have the property just defined: they do not slip at bounding surfaces. The fact that we were able to show that the only “reasonable” reflection law—the criteria of “reasonableness” being on the microscopic level of molecules—leads to the experimentally verified macroscopic boundary condition of no-slip seemed to us remarkable enough to warrant publishing.

On the other hand, when we tried to write up in a rigorous way the results of which we were by then convinced, we found the task quite impossible without revamping the entire theory of confined systems of particles. This led to the material of §§ 2-4, where we discuss the statistical mechanics of systems of particles in the presence of reflection laws.

All the work of §§ 2-4 is based directly on the fundamental hypothesis of conservation of probability (the Liouville description), rather than the more usual Boltzmann equation. There is certainly no harm in this, for the Boltzmann equation can be derived (formally) from conservation of probability [3; 12] and anything true for Liouville systems is (presumably), *a fortiori*, true for Boltzmann systems. (We should like to thank the referee for pointing out the interesting reference [12] to us.) On the other hand, the Liouville formulation is more fundamental and, in addition, has the tremendous advantage to us of separating the mechanics of the molecules from their statistics.

Sections 5 and 6 contain a discussion of certain specific reflection laws. In § 5, we consider reverse reflection and show that it implies no-slip. In addition, we prove in § 5 that reverse reflection is essentially the *only* law that

implies no-slip. Then, in § 6, we present the results that we actually began with, listing all “reasonable” reflection laws and deriving the boundary conditions associated with each. The results of § 6 can be interpreted as meaning that no-slip is the only “reasonable” boundary condition a fluid can satisfy.

This conclusion is a little anomalous for, although it is known that no-slip is usually a very good approximation, it is also known that the approximation is not perfect, and all real fluids slip a little. What this means, of course, is that the approximation of the interaction of a molecule with a wall by a reflection law is not perfect either and that when a fluid slips appreciably the interaction cannot be so approximated. On the other hand, our success in predicting no-slip may indicate that, under conditions that produce no-slip, the idea of a reflection law is an adequate approximation to the real situation. What is more, our results show that, in this case, the correct reflection law is reverse.

In § 7, the evidence for the slippage of real fluids is discussed, and we speculate on how our model might be changed to predict the actual slippage of such fluids. The discussion of § 7 also serves to provide some small insight into the physics of reverse reflection and perhaps helps to rationalize some of the features of that reflection law. Finally, we also discuss in § 7 some of the more obvious difficulties that stand in the way of easy experimental verification of reverse reflection.

2. Confined systems. It is usual in discussions of kinetic theory to assume that the molecules under consideration are, at least in principle, free to occupy any position in space. (See, e.g., [3; 8].) If the matter is discussed at all, the confinement of a gas to a domain is achieved by supposing—not that the molecules are restricted to this domain—but that the probability of their leaving it is zero. In our view, a mixture such as this of mechanics and statistics is untenable and can only lead to trouble. Our first task, therefore, is to construct a model of a gas in which the molecules are explicitly constrained to remain in a domain $V \subset R^3$. We call such a system *confined*.

Before going on, we note that in all that follows, molecules are supposed to be point masses, with no internal structure.

In a system confined to a domain V , a particle must somehow be reflected back into V whenever it reaches the boundary (∂V) of V . Actual molecular reflections probably occur because the molecules of ∂V exert a repulsive force on gas molecules that get close enough to ∂V . This “wall force” prevents escape of gas molecules from V . To obtain a simple model of a confined fluid, however, in this paper we assume the molecules to be entirely unaffected by the boundary until one of them actually strikes it. At such a time, the incident velocity of the molecule is changed to a reflected velocity that returns the particle to V , and the motion then proceeds according to Newton’s laws.

To state just how the motion proceeds, we need a little more precision in the definition of a reflection law. Let q be any point on ∂V , and let $n = n(q)$

be the inward normal to V at q . A map $A: \partial V \times R^3 \rightarrow R^3$ is called a *reflection law* if, for every $q \in \partial V$, $n(q) \cdot \xi < 0$ implies $n(q) \cdot A(q, \xi) > 0$. What this means, of course, is that reflection laws map *incident velocities* ($n(q) \cdot \xi < 0$) into *reflected velocities* ($n(q) \cdot A(q, \xi) > 0$). More conditions are imposed on reflection laws farther on. (It is important to notice that these conditions are all valid if the reflection law is obtained as a limit of the wall forces mentioned above as their ranges goes to zero.) For now, we simply remark that, when the context makes the meaning clear, we often suppress the dependence of A on q , writing $A(\xi)$ instead of $A(q, \xi)$.

Now suppose we have N identical particles of mass m . Whenever they all lie in V , Newton's equations are satisfied:

$$(2.1) \quad m\dot{q}^i = Q^i(q^1, \dots, q^N), \quad i = 1, \dots, N.$$

Here, Q^i denotes the force on the i th particle. It includes, not only intermolecular forces, but any external forces that may be present. It should be noted that Q^i is assumed not to depend on the velocities of the particles. This hypothesis is used to simplify our analysis, but it is not hard to take account of velocity dependent forces in any situation where they may occur.

In all that follows, we denote the velocity of the i th particle by ξ^i , so that (2.1) can be written as the first order system

$$(2.2) \quad \dot{q}^i = \xi^i,$$

$$(2.3) \quad \xi^i = \frac{1}{m} Q^i.$$

The behavior of a confined system is described by combining these equations with a reflection law. To make this clear, we first define a *trajectory* of the system of particles as a function

$$\zeta: t \rightarrow \zeta(t) = (q^1(t), \dots, q^N(t), \xi^1(t), \dots, \xi^N(t))$$

for which the following conditions hold:

- (i) ζ is defined and piecewise continuous on an interval $(t_1, t_2) \subset R^1$ and takes values in the set $S = \bar{V}^N \times R^{3N}$;
- (ii) ζ is continuous from the right, so that

$$(2.4) \quad \zeta(t_0) = \lim_{t \rightarrow t_0+0} \zeta(t);$$

- (iii) if $q^i(t_0) \in V$, then $q^i(t)$ and $\xi^i(t)$ are differentiable at $t = t_0$ and satisfy (2.2-3) there;

- (iv) if $q^i(t) \in \partial V$, then $q^i(t)$ is continuous at $t = t_0$, but the velocity $\xi^i(t)$ jumps from its *incident* value

$$(2.5) \quad \xi^i(t_0^-) = \lim_{t \rightarrow t_0-0} \xi^i(t)$$

to its *reflected* value

$$(2.6) \quad \xi^i(t_0) = A(\xi^i(t_0^-)).$$

We refer to points of S as *states* of the system. It follows from the above definition that trajectories actually take values in the smaller set

$$(2.7) \quad S^+ = \{\zeta \in S: n \cdot \xi^i \geq 0 \text{ whenever } q^i \in \partial V\},$$

the set of *reflected states*. Clearly there is an element of choice in this matter: we could instead have defined trajectories to be continuous from the left, in which case they would take values in the set

$$(2.8) \quad S^- = \{\zeta \in S: n \cdot \xi^i \leq 0 \text{ whenever } q^i \in \partial V\}$$

of *incident states*. This element of choice has important consequences later on.

Let $\zeta_0 \in S^+$. We call the problem of finding a trajectory $\zeta: t \rightarrow \zeta(t)$ such that $\zeta(0) = \zeta_0$ the *initial value problem*. As things now stand, it is natural to think of solving the initial value problem for $t \geq 0$. However, if the reflection law $A(q, \cdot)$ is one-to-one and maps $R^3_-(q) = \{\xi \in R^3: n(q) \cdot \xi \leq 0\}$ homeomorphically onto $R^3_+(q) = \{\xi \in R^3: n(q) \cdot \xi \geq 0\}$, it is also possible to solve the initial value problem for $t < 0$. In all that follows, we assume A satisfies this hypothesis.

We say the initial value problem has a *global solution* if it has a solution for all $t \in (-\infty, \infty)$. It is usual in kinetic theory (when the system is unconfined) to assume the initial value problem has a global solution for all initial states. However, such a circumstance is not possible in general for confined systems, principally because of the possibility that a particle can arrive at the boundary of V with zero normal velocity. Because of this difficulty, we replace the assumption that a global solution always exists by the following. Let $\mathbf{q}_0 = (q_0^1, \dots, q_0^N) \in \bar{V}^N$. Let $E(\mathbf{q}_0)$ be the set of all points $\xi_0 = (\xi_0^1, \dots, \xi_0^N) \in R^{3N}$ with the following properties:

- (a) $\zeta_0 = (q_0^1, \dots, q_0^N, \xi_0^1, \dots, \xi_0^N) \in S^+$;
- (b) the initial value problem associated with ζ_0 does *not* have a global solution.†

Then, we always assume that *for each \mathbf{q}_0 and each $i = 1, \dots, N$, the (three dimensional) measure of*

$$\{\xi_0^i: \xi_0 \in E(\mathbf{q}_0)\}$$

is zero.

Physically this means that for a given set of initial positions of the particles, the system has a global trajectory for almost all initial velocities of each individual particle. We denote the set of all states for which a global solution exists by S_0^+ . Our hypotheses imply that both the $3N$ -dimensional measure of $E(\mathbf{q}_0)$ and the $6N$ -dimensional measure of $S^+ - S_0^+$ are zero.

Next, we define the *trajectory map* $\psi(t; \cdot): S_0^+ \rightarrow S_0^+$ by the formula

$$(2.9) \quad \psi(t; \zeta(0)) = \zeta(t)$$

†In certain cases, the sets $E(\mathbf{q}_0)$ are empty, at least for $\mathbf{q}_0 \in V^N$. An example is a Knudsen gas in a smooth convex domain V .

where $\zeta: t \rightarrow \zeta(t)$ is any trajectory. In other words, $\psi(t; \cdot)$ is the map taking the initial state of a trajectory into the state of the trajectory at time t . Clearly, the trajectory map has the group property

$$\psi(t_1; \psi(t_2; \zeta)) = \psi(t_1 + t_2; \zeta),$$

and, therefore, the inverse map $\psi^{-1}(t; \cdot)$ exists and is given by

$$\psi^{-1}(t; \zeta) = \psi(-t; \zeta).$$

It follows that $\psi(t; \cdot)$ is a bijection between S_0^+ and S_0^+ . We always assume that $\psi(t; \cdot)$ is measurable on S_0^+ for each t and takes sets of measure zero to sets of measure zero. Substituting $-t$ for t shows that these same statements apply to $\psi^{-1}(t; \cdot)$.

Our first task is to find a formula for the Jacobian $\partial\psi/\partial\zeta$ of the trajectory map. For this purpose, we need a number of smoothness hypotheses. We state them here and note that they are made everywhere in the sequel without further mention. The hypotheses are that three objects are C^1 : the forces† Q^i occurring in (2.1), the boundary of V , and the reflection law A .

For brevity, we often write (2.2-3) in the compact form

$$(2.10) \quad \dot{\zeta} = Z(\zeta),$$

where $\zeta = (q^1, \dots, q^N, \xi^1, \dots, \xi^N)$ and $Z = (\xi^1, \dots, \xi^N, (1/m)Q^1, \dots, (1/m)Q^N)$. With this notation, we have

LEMMA 2.1. *Let $H \subset S^+$ be a C^1 hypersurface of dimension $6N - 1$, and let*

$$\Delta = \{\psi(t; \zeta) : \zeta \in H, 0 < t < T\}.$$

Let $|H|$ be the $(6N - 1)$ dimensional volume of H , δ the diameter of H , and $u(\zeta)$ the unit normal to H at the point ζ of H . If no reflections occur for $0 < t < T$, then the volume of Δ is given by

$$(2.11) \quad |\Delta| = |u(\zeta_0) \cdot Z(\zeta_0)| \cdot |H| T + o(|H| T) \text{ as } \delta + T \rightarrow 0.$$

Here, ζ_0 is any point of H that remains in H as δ goes to zero.

Proof. Notice that Δ is defined for all $\zeta \in H$ when δ and T are small enough since $\psi(t; \zeta)$ is determined by Newton's equations (2.10) alone.

Introduce a coordinate system with origin at ζ_0 in which the normal to H at ζ_0 has the representation $u(\zeta_0) = (1, 0, \dots, 0)$. Then, in a neighborhood of ζ_0 , H can be described by an equation of the form

$$\zeta^1 = f(\zeta^2, \dots, \zeta^{6N}),$$

where all first derivatives of f vanish when $\zeta^2 = \dots = \zeta^{6N} = 0$.

†Obviously, this eliminates such things as inverse power laws, but such laws can be taken account of by truncation. With reference to this hypothesis, one should also consider Brush's remarks [1] on the choice of force laws.

Define a transformation $z = \Phi_1(\zeta)$ by

$$z^1 = \zeta^1 - f(\zeta^2, \dots, \zeta^{6N}); \quad z^k = \zeta^k, \quad k = 2, \dots, 6N.$$

Let $z_0 = \Phi_1(\zeta_0)$ and $H_1 = \Phi_1(H) \subset \{z: z^1 = 0\}$. This transformation is invertible near $z = z_0$ and the Jacobian $\partial\Phi_1^{-1}(z)/\partial z$ is easily calculated:

$$(2.12) \quad \frac{\partial\zeta}{\partial z} = 1.$$

Furthermore, $|H| = |H_1| + o(|H|)$ as $\delta \rightarrow 0$. This fact can be verified by a computation using the integral

$$|H| = \int_{H_1} (1 + |\nabla f|^2)^{\frac{1}{2}} d\zeta^2 \dots d\zeta^{6N}.$$

If $\zeta(t)$ satisfies (2.10), then $z(t) = \Phi_1(\zeta(t))$ satisfies an equation

$$(2.13) \quad \dot{z} = \tilde{Z}(z),$$

where

$$\begin{aligned} \tilde{Z}^1 &= Z^1 - \sum_{k=2}^{6N} \frac{\partial f}{\partial \zeta^k} Z^k, \\ \tilde{Z}^k &= Z^k, \quad k = 2, \dots, 6N. \end{aligned}$$

Integrating (2.13), we find that

$$(2.14) \quad z(t) = z(0) + \int_0^t \tilde{Z}(z(\tau)) d\tau.$$

Notice that $\Phi_1(\Delta)$ is just the set of all points traced out by solutions of (2.13) in $(0, T)$, with initial data in H_1 .

Next, we define a second transformation $z = \Phi_2(w)$ with $w = (w^1, \dots, w^{6N})$. Given a suitable w , let $t = w^1$ and $z(0) = (0, w^2, \dots, w^{6N})$. Use t and $z(0)$ as data in (2.14) to find $z(t)$ and define $\Phi_2(w) = z(t)$. Notice that $H_2 = \Phi_2^{-1}(H_1)$ is just H_1 with coordinates relabelled w^i rather than z^i . Thus

$$(2.15) \quad |H_2| = |H_1| = |H| + o(|H|) \text{ as } \delta \rightarrow 0.$$

For convenience, let $H_2^* = \{(w^2, \dots, w^{6N}): w = (w^1, w^2, \dots, w^{6N}) \in H_2\}$. A typical point $\zeta \in \Delta$ can now be thought of as

$$\zeta = \Phi_1^{-1}(\Phi_2(w)), \quad w \in (0, T) \times H_2^*.$$

Let $w_0 = \Phi_2^{-1}(z_0) = \Phi_2^{-1}(\Phi_1(\zeta_0))$. We can calculate the Jacobian $(\partial z / \partial w)_{w=w_0}$ directly from (2.14). The result is

$$\left(\frac{\partial z}{\partial w} \right)_{w=w_0} = \tilde{Z}_1(z_0) = Z_1(\zeta_0) = u(\zeta_0) \cdot Z(\zeta_0),$$

where we have used the fact that the derivatives of f vanish at $\zeta = \zeta_0$. Thus,

from (2.12), we find

$$(2.16) \quad \left(\frac{\partial \zeta}{\partial w} \right)_{w=w_0} = \left(\frac{\partial \zeta}{\partial z} \right)_{z=z_0} \left(\frac{\partial z}{\partial w} \right)_{w=w_0} = u(\zeta_0) \cdot Z(\zeta_0).$$

But, since the Jacobian is an approximate ratio of volumes near a point,

$$|\Delta| = \left| \left(\frac{\partial \zeta}{\partial w} \right)_{w=w_0} \right| |H_2|T + o(|H_2|T) \text{ as } \delta + T \rightarrow 0.$$

This implies (2.11) by (2.15-16).

With t fixed, we denote the Jacobian of the trajectory map $\zeta \rightarrow \psi(t; \zeta)$ by $(\partial\psi/\partial\zeta)(t; \zeta)$. We also denote the Jacobian of the map $\xi \rightarrow A(q, \xi)$ (with q fixed) by $(\partial A/\partial\xi)(q, \xi)$. As before, when the meaning is clear, we suppress the dependence on q , writing

$$\left(\frac{\partial A}{\partial \xi} \right)(q, \xi) = \left(\frac{\partial A}{\partial \xi} \right)(\xi) = A'(\xi).$$

With this notation, we have

THEOREM 2.2. *For each fixed t , the Jacobian $(\partial\psi/\partial\zeta)(t; \zeta)$ exists for almost all ζ in S_0^+ . At every point of the Lebesgue set of the map $\zeta \rightarrow (\partial\psi/\partial\zeta)(t; \zeta)$, the following conclusions hold.*

- (i) $(\partial\psi/\partial\zeta)(0; \zeta) = 1$.
- (ii) $(\partial\psi/\partial\zeta)(t; \zeta)$ is constant in any time interval in which $\psi(t; \zeta)$ lies in the interior of S^+ .
- (iii) If $\psi(t_0; \zeta)$ lies on the boundary of S^+ , let

$$\psi(t_0^-; \zeta) = \lim_{t \rightarrow t_0-0} \psi(t; \zeta) = (q_0^1, \dots, q_0^N, \xi_0^1, \dots, \xi_0^N),$$

where $q_0^i \in \partial V$ for $i \in I$, while $q_0^i \in V$ for $i \notin I$. Then, wherever the formula makes sense,

$$(2.17) \quad \left| \left(\frac{\partial \psi}{\partial \zeta} \right)(t_0; \zeta) \right| = \left| \left(\frac{\partial \psi}{\partial \zeta} \right)(t_0^-; \zeta) \right| \cdot \left| \prod_{i \in I} \left(\frac{\partial A}{\partial \xi} \right)(q_0^i, \xi_0^i) \frac{n(q_0^i) \cdot A(q_0^i, \xi_0^i)}{n(q_0^i) \cdot \xi_0^i} \right|.$$

Proof. The existence of $\partial\psi/\partial\zeta$ almost everywhere follows from our hypotheses that the map $\psi(t; \cdot)$ is measurable and that $\psi^{-1}(t; \cdot)$ takes sets of measure zero into sets of measure zero. Thus, it remains to prove that, where it exists, $\partial\psi/\partial\zeta$ satisfies (i)-(iii).

(i) is immediate, since $\psi(0; \zeta) \equiv \zeta$. Also, (ii) follows from the fact that, as long as $\psi(t; \zeta) \in V$, the trajectory is determined entirely as a solution of the differential equations (2.10). However, the solutions of such differential equations always have constant Jacobian as long as the forces Q^i do not depend on the velocities [8]. This is just a simple theorem from the theory of ordinary differential equations. Thus, it remains to prove (iii).

Take $T > 0$. Then, $\psi(t_0; \zeta)$ is determined from $\psi(t_0 - T; \zeta)$ (and the reflection law A). Moreover, if we call J the Jacobian of the map

$$\psi(t_0 - T; \zeta) \rightarrow \psi(t_0; \zeta),$$

the assertion (2.17) is that when J exists, it is given by

$$(2.18) \quad |J| = \left| \prod_{i \in I} A'(\xi^i) \frac{n \cdot A(\xi^i)}{n \cdot \xi^i} \right|, \text{ almost everywhere}$$

if T is small enough. (We use (ii) in this argument.)

Since $\psi(t_0; \zeta) = \psi(0, \psi(t_0; \zeta))$, while $\psi(t_0 - T; \zeta) = \psi(-T; \psi(t_0; \zeta))$, it suffices to prove (2.18) assuming $t_0 = 0$. Thus, we may assume

$$\lim_{t \rightarrow t_0 - 0} \psi(t; \zeta) = (q_0^1, \dots, q_0^N, \xi_0^1, \dots, \xi_0^N) = \zeta_0,$$

where $q_0^i \in \partial V$ when $i \in I$, $q_0^i \in V$ when $i \notin I$, and I is not empty.

Suppose first that $q_0^1 \in \partial V$ while $q_0^i \in V$, $i \neq 1$. In this case, let $q_0^1 \in P$, a patch of area on ∂V , and suppose that $n(q_0^1) \cdot \xi_0^1 \neq 0$. For some sufficiently small $\sigma > 0$, let

$$P_1 = \{(q, \xi) : q \in P, n(q) \cdot \xi < 0, |\xi - \xi_0^1| < \sigma\}.$$

Note that P_1 is a five-dimensional surface. Let $(q_0^2, \dots, q_0^N) \in C_1$, a cube of dimension $3N - 3$ contained in V^{N-1} , and let $(\xi_0^2, \dots, \xi_0^N) \in C_2$, a cube in R^{3N-3} . Define $H = P_1 \times C_1 \times C_2$, and let $A(H) = A(P) \times C_1 \times C_2$. We consider two sets: the set V^- consisting of all states swept out in an interval $-T < t < 0$ by trajectories that arrive at H at $t = 0$, and the set V^+ consisting of all states swept out in an interval $0 < t < T$ by trajectories that leave $A(H)$ at $t = 0$. In symbols,

$$\begin{aligned} V^- &= \{\psi(-t; \zeta) : 0 < t < T, \zeta \in A(H)\}, \\ V^+ &= \{\psi(t; \zeta) : 0 < t < T, \zeta \in A(H)\}. \end{aligned}$$

We have

$$\begin{aligned} \psi(T; V^-) &= \{\psi(T; \psi(-t; \zeta)) : 0 < t < T, \zeta \in A(H)\} \\ &= \{\psi(T - t; \zeta) : 0 < t < T, \zeta \in A(H)\} \\ &= \{\psi(t; \zeta) : 0 < t < T, \zeta \in A(H)\} \\ &= V^+. \end{aligned}$$

It follows from this and from known properties of Jacobians that if ζ_0 lies in the Lebesgue set of $(\partial\psi/\partial\zeta)(t; \cdot)$, then

$$(2.19) \quad |V^+| = |J| \cdot |V^-| + o(V^-)$$

as the diameter of the set $V^- \cup \{\zeta_0\}$ goes to zero.

The volumes $|V^+|$ and $|V^-|$ can be computed with the aid of Lemma 2.1.

The results are

$$\begin{aligned} |V^-| &= |n \cdot \xi_0^1| \cdot |H| T, \\ |V^+| &= |n \cdot A(\xi_0^1)| \cdot |A(H)| T \\ &= |n \cdot A(\xi_0^1)| \cdot |A'(\xi_0^1)| \cdot |H| T, \end{aligned}$$

to terms of lowest order. Using these estimates in (2.19), and letting $\delta + T$ go to zero, we find

$$|J| = \left| A'(\xi_0^1) \frac{n \cdot A(\xi_0^1)}{n \cdot \xi_0^1} \right|,$$

and this is (2.18) when $I = \{1\}$. It is clear that this proof is quite general and shows that (2.18) is valid whenever the set I consists of a single element.

When I contains more than one element, the proof is similar. In the definition of H , the patch P is replaced by a set consisting of k patches, where k is the number of elements in I . There is a corresponding change in the definitions of P_1 and $A(H)$. Then, when Lemma 2.1 is applied to find the volumes $|V^-|$ and $|V^+|$, the results are

$$\begin{aligned} |V^-| &= \prod_{i \in I} |n \cdot \xi_0^i| \cdot |H| T, \\ |V^+| &= \prod_{i \in I} |n \cdot A(\xi_0^i)| \cdot |A'(\xi_0^i)| \cdot |H| T, \end{aligned}$$

to terms of lowest order. These observations lead to an expression for $|J|$ as a product, and the desired conclusion (2.18) follows.

In the remainder of this paper, we *define* $|\partial\psi/\partial\zeta|$ everywhere on $R^1 \times S_0^+$ by (i), (ii), and (iii). Notice that this is necessary. For fixed t , $|(\partial\psi/\partial\zeta)(t; \cdot)|$ exists almost everywhere in S_0^+ . On the other hand, (i), (ii), and (iii) define a function everywhere in S_0^+ . The only way $|(\partial\psi/\partial\zeta)(t; \cdot)|$ can be defined on all of S_0^+ in such a way that it agrees with the function defined by (i), (ii), and (iii) wherever $\partial\psi/\partial\zeta$ exists is by defining $|\partial\psi/\partial\zeta|$ by (i), (ii), and (iii) everywhere.

3. Kinetic theory of confined systems. It is usual in statistical mechanics to suppose that the state of a system is not known precisely but is determined by a probability distribution $F(t; \cdot)$. The interpretation of $F(t; \cdot)$ is this: if D is a domain in R^{6N} , then

$$\int_D F(t; \zeta) d\zeta$$

is the probability that the state of the system lies in D at time t .

One of the fundamental problems of kinetic theory is the determination of $F(t; \cdot)$ from $F(0; \cdot)$: given an initial distribution of the particles in a system, to find their distribution at a later time. The solution depends on what is assumed, of course, but the most basic hypothesis that can be made is *conservation of probability*. This hypothesis can be stated as follows. Let

D be any ($6N$ -dimensional) domain in S^+ , and let $\psi(t; \cdot)$ be the trajectory map. Then, conservation of probability is the hypothesis that the probability of the state of the system lying in $\psi(t; D)$ at time t is independent of t . In symbols

$$(3.1) \quad \int_{\psi(t; D)} F(t; \xi) d\xi = \int_D F(0; \xi) d\xi \text{ for every domain } D \subset S^+.$$

This equation asserts that the distribution of states at time t is exactly what one should expect from the initial distribution of states. Conservation of probability says, in short, that no demons unexpectedly tamper with the affairs of systems of particles.

Notice that (3.1) does not make sense unless $D \subset S_0^+$, for otherwise $\psi(t; D)$ is not defined. However, by our hypotheses concerning S_0^+ , the ($6N$ -dimensional) measure of $D - (D \cup S_0^+)$ is zero for any $D \subset S$. Thus if we replace D with $D \cap S_0^+$ in (3.1), the right-hand side is unchanged, and the left-hand side becomes meaningful. Whenever necessary, we always interpret (3.1) in this way.

Of course we assume

$$(3.2) \quad \int_S F(0; \xi) d\xi = 1,$$

since we want the system to be confined. Since the trajectory map takes S onto itself (ignoring a set of measure zero), it then follows from (3.1) and (3.2) that

$$(3.3) \quad \int_S F(t; \xi) d\xi = 1$$

for all t .

In the usual analyses (of unconfined systems), it is proved that $F(t; \cdot)$ exists and, if $F(0; \cdot)$ is differentiable, so is $F(t; \cdot)$, and $F(t; \cdot)$ satisfies Liouville's equation [3; 8]. For confined systems, however, it is not always true that $F(t; \cdot)$ is differentiable, no matter how smooth $F(0; \cdot)$ may be. On the other hand, it is not much harder to write down a formula for $F(t; \cdot)$ when the system is confined than when it is not. Indeed, we have

THEOREM 3.1. *Let $F_0(\cdot)$ be a probability distribution supported in S^+ . Then, there is a probability distribution $F(t; \cdot)$ that equals $F_0(\cdot)$ when $t = 0$ and satisfies conservation of probability. This distribution is unique up to sets of ($6N$ -dimensional) measure zero and is given by the formula*

$$(3.4) \quad F(t; \psi(t; \xi)) \left| \left(\frac{\partial \psi}{\partial \xi} \right) (t; \xi) \right| = F_0(\xi).$$

Proof. It is best to prove uniqueness first, for this shows the origin of the formula (3.4). Suppose, then, that we have a function $F(t; \cdot)$ satisfying the

conditions of the theorem. Changing variables in the integration, we have

$$\int_{\psi(t;D)} F(t; \zeta) d\zeta = \int_D F(t; \psi(t; \zeta)) \left| \left(\frac{\partial \psi}{\partial \zeta} \right) (t; \zeta) \right| d\zeta.$$

On the other hand, if probability is conserved, this equals

$$\int_D F_0(\zeta) d\zeta.$$

Therefore,

$$\int_D \left[F(t; \psi(t; \zeta)) \left| \left(\frac{\partial \psi}{\partial \zeta} \right) (t; \zeta) \right| - F_0(\zeta) \right] d\zeta = 0,$$

and this must be true for every domain $D \subset S$. It follows that (3.4) holds almost everywhere, as required.

To prove existence, we show that the function defined by (3.4) satisfies the conditions of the theorem. First, set $t = 0$ in (3.4). Then, (2.9) and Theorem 2.2(i) show that $F(0; \zeta) = F_0(\zeta)$. Also, the hypotheses imply (3.2), so that (3.3) is satisfied. Finally, if $F(t; \cdot)$ is defined by (3.4), then, given any $D \subset S$,

$$\begin{aligned} \int_D F_0(\zeta) d\zeta &= \int_D F(t; \psi(t; \zeta)) \left| \left(\frac{\partial \psi}{\partial \zeta} \right) (t; \zeta) \right| d\zeta \\ &= \int_{\psi(t;D)} F(t; \zeta) d\zeta. \end{aligned}$$

This is conservation of probability.

For each t , (3.4) defines $F(t; \zeta)$ for almost all $\zeta \in S_0^+$. However, we need the definition on a larger set. A natural extension of F is achieved in two steps. First, notice that the right side of (3.4) is independent of t . Therefore, it is natural to suppose that the left side is a continuous function of t for each fixed ζ . With this hypothesis, we conclude immediately that (3.4) holds on *all* of $R^1 \times S_0^+$.

Second, recall that in defining a trajectory we emphasized a certain element of choice. Trajectories might have been taken to be continuous from the left instead of the right. Had this been our choice, the argument that led to (3.4) would have given, instead,

$$F(t; \psi^*(t; \zeta)) \left| \left(\frac{\partial \psi^*}{\partial \zeta} \right) (t; \zeta) \right| = F_0(\zeta),$$

where $\psi^*(t; \cdot)$ is the trajectory map associated with left-continuity. Now, it is easy to see that $\psi^*(t; \zeta) = \psi(t^-; \zeta)$, so that left-continuous trajectories, conservation of probability, and continuity in time imply, instead of (3.4),

$$(3.5) \quad F(t; \psi(t^-; \zeta)) \left| \left(\frac{\partial \psi}{\partial \zeta} \right) (t^-; \zeta) \right| = F_0(\zeta)$$

for all ζ in the set

$$S_0^- = \{\psi(t^-; \zeta) : \zeta \in S_0^+\}.$$

Notice that when $\psi(t; \zeta)$ is in the interior of S , $\psi(t; \zeta) = \psi(t^-; \zeta)$, so that (3.4) and (3.5) agree in this case. Also, (3.4) and (3.5) define F everywhere on $R^1 \times S_0$, where

$$S_0 = S_0^- \cup S_0^+.$$

We summarize these results in

THEOREM 3.2. *Let $F(t; \cdot)$ and $F_0(\cdot)$ be probability distributions on S_0 and S_0^+ respectively. Suppose that the following two hypotheses are true whether trajectories are defined to be continuous from the left or continuous from the right.*

(i) $F(t; \cdot)$ satisfies conservation of probability.

(ii) For each fixed ζ , $F(t; \psi(t; \zeta)) |(\partial\psi/\partial\zeta)(t; \zeta)|$ is a continuous function of t . Then $F(t; \zeta)$ is given by (3.4-5) on $R^1 \times S_0$ with $F(0; \zeta) = F_0(\zeta)$ for $\zeta \in S_0^+$. Furthermore, if F is defined by (3.4-5), then (i) and (ii) hold for either definition of trajectory.

All assertions of this theorem have been proved except the last. But it is a straightforward process to verify that (i) and (ii) hold for an F given by (3.4-5).

The one-particle probability distribution obtained by averaging out all the particles but one is of interest. If the molecules are indistinguishable, it does not matter which molecule we do not average out, and we select the first for this purpose. Write q for q^1 , ξ for ξ^1 , and ζ^* for $(q^2, \dots, q^N, \xi^2, \dots, \xi^N)$. In the obvious notation, we also write $F(t; q, \xi, \zeta^*)$ instead of $F(t; \zeta)$. Then, we define

$$(3.6) \quad f(t; q, \xi) = \int_{V^{N-1} \times R^{3N-3}} F(t; q, \xi, \zeta^*) d\zeta^*.$$

We have

LEMMA 3.3. *Let $q \in \partial V$. Then,*

$$(3.7) \quad f(t; q, A(\xi)) = \left| \frac{n \cdot \xi}{n \cdot A(\xi)} \right| \frac{f(t; q, \xi)}{|A'(\xi)|}$$

for almost all $\xi \in R^3$.

Proof. According to the definitions (3.4) and (3.5),

$$\begin{aligned} \frac{F(t; \psi(t^-; \zeta))}{F(t; \psi(t; \zeta))} &= \left| \frac{(\partial\psi/\partial\zeta)(t; \zeta)}{(\partial\psi/\partial\zeta)(t^-; \zeta)} \right| \\ &= \left| \prod_{i \in I} A'(\xi^i) \frac{n \cdot A(\xi^i)}{n \cdot \xi^i} \right| \end{aligned}$$

if $\psi(t; \zeta) \in \partial S^+$, by Theorem 2.2(iii). Let $\psi(t^-; \zeta) = (q, \xi, \psi^*)$, where

$\psi^* \in \bar{V}^{N-1} \times R^{3N-3}$. If $q \in \partial V$ while $\psi^* \in V^{N-1} \times R^{3N-3}$, then we have $\psi(t; \xi) = (q, A(\xi), \psi^*)$, and

$$\frac{F(t; q, \xi, \psi^*)}{F(t; q, A(\xi), \psi^*)} = \left| A'(\xi) \cdot \frac{n \cdot A(\xi)}{n \cdot \xi} \right|.$$

Now, we have

$$\begin{aligned} f(t; q, \xi) &= \int_{V^{N-1} \times R^{3N-3}} F(t; q, \xi, \psi^*) d\psi^* \\ &= \left| A'(\xi) \cdot \frac{n \cdot A(\xi)}{n \cdot \xi} \right| \int_{V^{N-1} \times R^{3N-3}} F(t; q, A(\xi), \psi^*) d\psi^* \\ &= \left| A'(\xi) \cdot \frac{n \cdot A(\xi)}{n \cdot \xi} \right| f(t; q, A(\xi)). \end{aligned}$$

This is equivalent to (3.7).

Using Lemma 3.3, it is easy to prove the very useful

LEMMA 3.4. *Let $\varphi: \xi \rightarrow \varphi(\xi)$ be a measurable function such that $\varphi(\cdot)f(t; q, \cdot)$ is integrable. Then,*

$$(3.8) \quad \int_{R^3} \varphi(\xi)f(t; q, \xi)d\xi = \int_{R^3_-} \left[\varphi(\xi) - \varphi(A(\xi)) \frac{n \cdot \xi}{n \cdot A(\xi)} \right] f(t; q, \xi)d\xi$$

whenever $q \in \partial V$.

Proof. Making the transformation $\xi \rightarrow A(\xi)$, we see that

$$\begin{aligned} \int_{R^3_+} \varphi(\xi)f(t; q, \xi)d\xi &= \int_{R^3_-} \varphi(A(\xi))f(t; q, A(\xi))|A'(\xi)|d\xi \\ (3.9) \quad &= \int_{R^3_-} \varphi(A(\xi)) \left| \frac{n \cdot \xi}{n \cdot A(\xi)} \right| f(t; q, \xi)d\xi, \end{aligned}$$

by (3.7). Since A is a reflection law, $(n \cdot \xi)/(n \cdot A(\xi)) < 0$. (3.8) follows from this and (3.9).

4. The conservation equations. Throughout this section, we assume that the initial distribution F_0 has compact support in S^+ . This hypothesis is stronger than we actually need, but it is convenient, and it will be clear how it can be weakened.

Of primary interest in fluid mechanics are the first few moments of f . Write

$$(4.1) \quad \rho(t; q) = mN \int_{R^3} f(t; q, \xi)d\xi,$$

and

$$(4.2) \quad \rho(t; q)s(t; q) = mN \int_{R^3} \xi f(t; q, \xi)d\xi.$$

The functions ρ and s so defined are called the (mass) *density* and the *velocity* of the system, respectively. We call the quantity ρs the *momentum density* of the system. As before, m is the mass of a single molecule, and N is the number of molecules in the system.

With these two definitions, we can prove the following result which shows that on the level of the entire system (the *fluid* level), we have been successful in achieving confinement.

THEOREM 4.1. *Define ρ and s by (4.1) and (4.2), and let n be the normal to ∂V . Then,*

$$(4.3) \quad n \cdot (\rho s) = 0$$

for all $q \in \partial V$.

(4.3) says that at every point of ∂V , either $\rho = 0$ or $n \cdot s = 0$. The equation $\rho = 0$ can be interpreted to mean that there is no “fluid” at the point, while $n \cdot s = 0$ means that the normal component of the “fluid” velocity is zero at the point. In either case, “fluid” cannot escape from V at the point. Notice that Theorem 4.1 is valid whatever the reflection law A may be.

The proof of Theorem 4.1 is a simple exercise in the use of Lemma 3.4. By (4.2) and (3.8), we have

$$n \cdot (\rho s) = mN \int_{R^3_-} n \cdot \left[\xi - A(\xi) \frac{n \cdot \xi}{n \cdot A(\xi)} \right] f(t; q, \xi) d\xi = 0.$$

This proves the theorem.

In the usual analyses of unconfined fluids, it is shown that ρ and s are connected by the *continuity equation*.

$$(4.4) \quad \rho_t + \nabla \cdot (\rho s) = 0,$$

where ∇ denotes the gradient with respect to q , while $\rho_t = \partial\rho/\partial t$. In our situation, however, it is not possible to derive (4.4) because F (and, therefore, f , and ρ and s) are not differentiable. Consequently, we make do by showing that ρ and s are *weak* solutions of (4.4).

We begin with F . Again, it is usual to show that F is a solution of *Liouville's equation*

$$(4.5) \quad F_t + \mathbf{D} \cdot FZ + 0,$$

where \mathbf{D} is the gradient in R^{6N} and we use the notation introduced in (2.10). In the present context F may not have enough smoothness to satisfy (4.5) (cf. Theorem 2.2.). Therefore we begin by showing that F is a weak solution of (4.5).

To do that, we need a definition. Let $\zeta = (q^1, \dots, q^N, \xi^1, \dots, \xi^N) \in S^-$. We define $A(\zeta)$ to be that element of S^+ obtained from ζ by reflecting any velocities corresponding to points lying on ∂V . Thus, for example, if $q^1 \in \partial V$,

while $q^2, \dots, q^N \in V$, we set $A(\zeta) = (q^1, q^2, \dots, q^N, A(\xi^1), \xi^2, \dots, \xi^N)$. We denote by \mathcal{T} the set of all real-valued functions $\Phi: (t; \zeta) \rightarrow \Phi(t; \zeta)$ in $C^1([0, \infty) \times S)$ satisfying the two conditions

$$(4.6) \quad \Phi(t; \zeta) = \Phi(t; A(\zeta)) \quad \text{for } \zeta \in \partial S^-$$

and

$$(4.7) \quad \nabla_{q^i} \Phi = 0, \quad \nabla_{\xi^i} \Phi \text{ independent of } \xi^i, \text{ whenever } q^i \in \partial V.$$

Note that the space \mathcal{T} of test functions contains the space C_0^∞ of infinitely differentiable functions with compact support in $[0, \infty) \times \text{int } S$. What we really need for our test functions is that they be differentiable functions of t on trajectories. For this, C_0^∞ is sufficient, but so is \mathcal{T} , and use of \mathcal{T} allows us to prove more than we could prove if we chose C_0^∞ for our test space. At any rate, it is to achieve smoothness on trajectories that we assume (4.6) and (4.7).

We can now prove

THEOREM 4.2. *Let F_0 have compact support in S^+ , and define F by (3.4) and (3.5). Then, if $\Phi \in \mathcal{T}$, the integral*

$$\int_{S^+} \Phi(t; \zeta) F(t; \zeta) d\zeta$$

is in $C^1[0, \infty)$. Moreover,

$$(4.8) \quad \frac{d}{dt} \int_{S^+} \Phi(t; \zeta) F(t; \zeta) d\zeta = \int_{S^+} (\Phi_t + Z \cdot \mathbf{D}\Phi)(t; \zeta) F(t; \zeta) d\zeta, \quad t \geq 0,$$

for all $\Phi \in \mathcal{T}$.

We call a function F satisfying (4.8) for all $\Phi \in \mathcal{T}$ a *weak solution* of the Liouville equation (4.5.) Notice that if F is smooth and satisfies (4.8), then it satisfies (4.5).

To prove the theorem, we remark that for ζ fixed, $\Phi(t; \psi(t; \zeta)) \in C^1[0, \infty)$. To see this, notice first that $\psi(t; \zeta)$ is smooth for all t such that $\psi(t; \zeta)$ lies in the interior of S^+ . Thus, the only problem occurs on the boundary of S^+ . However, when $\psi(t; \zeta) \in \partial S^+$, $A(\psi(t^-; \zeta)) = \psi(t; \zeta)$. Therefore, at such a value of t ,

$$\begin{aligned} \lim_{\tau \rightarrow t_0+0} \Phi(\tau; \psi(\tau; \zeta)) &= \Phi(t; \psi(t; \zeta)) \\ &= \Phi(t; A(\psi(t^-; \zeta))) \\ &= \Phi(t; \psi(t^-; \zeta)), \end{aligned}$$

by (4.6). It follows from this that $\Phi(t; \psi(t; \zeta))$ is continuous. Second, in the interior of S^+ ,

$$\frac{d}{dt} \Phi(t; \psi(t; \zeta)) = (\Phi_t + Z \cdot \mathbf{D}\Phi)(t; \psi(t; \zeta)).$$

In view of (4.7) and (4.6),

$$\begin{aligned} \lim_{\tau \rightarrow t_0+0} \frac{d}{d\tau} \Phi(\tau; \psi(\tau; \zeta)) &= \Phi_t(t; \psi(t; \zeta)) \\ &= \Phi_t(t; A(\psi(t^-; \zeta))) \\ &= \Phi_t(t; \psi(t^-; \zeta)) \\ &= \lim_{\tau \rightarrow t_0-0} \frac{d}{d\tau} \Phi(\tau; \psi(\tau; \zeta)). \end{aligned}$$

Thus, $\Phi(t; \psi(t; \zeta))$ also has a continuous derivative.

Now, consider

$$\begin{aligned} \int_{S^+} \Phi(t; \zeta) F(t; \zeta) d\zeta &= \int_{S^+} \Phi(t; \zeta) \frac{F_0(\psi^{-1}(t; \zeta))}{|(\partial\psi/\partial\zeta)(t; \psi^{-1}(t; \zeta))|} d\zeta \\ &= \int_{S^+} \Phi(t; \psi(t; \zeta)) F_0(\zeta) d\zeta. \end{aligned}$$

This is differentiable since $\Phi(t; \psi(t; \zeta))$ is and F_0 has compact support.

To prove (4.8), let $\Phi \in \mathcal{F}$, and observe that

$$\begin{aligned} \frac{d}{dt} \int_{S^+} \Phi(t; \zeta) F(t; \zeta) d\zeta &= \frac{d}{dt} \int_{S^+} \Phi(t; \psi(t; \zeta)) F_0(\zeta) d\zeta \\ &= \int_{S^+} (\Phi_t + Z \cdot \mathbf{D}\Phi)(t; \psi(t; \zeta)) F_0(\zeta) d\zeta \\ &= \int_{S^+} (\Phi_t + Z \cdot \mathbf{D}\Phi)(t; \zeta) \frac{F_0(\psi^{-1}(t; \zeta))}{|(\partial\psi/\partial\zeta)(t; \psi^{-1}(t; \zeta))|} d\zeta \\ &= \int_{S^+} (\Phi_t + Z \cdot \mathbf{D}\Phi)(t; \zeta) F(t; \zeta) d\zeta \end{aligned}$$

by (3.4). This completes the proof of Theorem 4.2.

To obtain a weak form of the continuity equation (4.4), we restrict our attention to functions $\Phi \in \mathcal{F}$ of the form

$$(4.9) \quad \Phi(t; \zeta) = \varphi(t; q),$$

where $\zeta = (q, \xi, \zeta^*)$ and $\zeta^* \in \bar{V}^{N-1} \times R^{3N-3}$. It is easily checked that a function Φ of this form lies in \mathcal{F} if and only if $\varphi \in C^1([0, \infty) \times \bar{V})$ and

$$(4.10) \quad \nabla\varphi(t; q) = \mathbf{0} \quad \text{for } q \in \partial V.$$

We now prove

THEOREM 4.3. *The functions ρ and s defined by (4.1) and (4.2) satisfy the equation*

$$(4.11) \quad \frac{d}{dt} \int_V \varphi(t; q) \rho(t; q) dq = \int_V (\varphi_t + s \cdot \nabla\varphi)(t; q) \rho(t; q) dq$$

for all $\varphi \in C^1([0, \infty) \times \bar{V})$ satisfying (4.10). If ρ and s are continuously differentiable in $[0, \infty) \times \bar{V}$, then they satisfy the continuity equation (4.4).

Proof. Substitute a function $\Phi \in \mathcal{F}$ of the form (4.9) into (4.8). Using the definition (3.6) of f , we find

$$\frac{d}{dt} \int_{V \times R^3} \varphi(t; q) f(t; q, \xi) d\xi dq = \int_{V \times R^3} (\varphi_t + \xi \cdot \nabla \varphi)(t; q) f(t; q, \xi) d\xi dq.$$

This implies (4.11) because of the definitions of ρ and s .

To prove the last sentence of the theorem, let ρ and s be smooth. Differentiating under the integral sign, we find, from (4.11),

$$(4.12) \quad \int_V \varphi \rho_t dq = \int_V \rho s \cdot \nabla \varphi dq.$$

The divergence theorem and (4.3) now give

$$(4.13) \quad \int_V \varphi [\rho_t + \nabla \cdot (\rho s)] dq = 0.$$

Since φ is arbitrary in V , this shows that ρ and s are connected by (4.4).

It was to be able to derive (4.13) from (4.12) in the way that we did that the test functions were taken to lie in \mathcal{F} instead of in C_0^∞ . (4.13) follows from (4.12) for $\Phi \in C_0^\infty$ also, but, in this case, it is because everything that happens on ∂V is wiped out, and not because of Theorem 4.1. It was to display the computational coincidence (if that is what it is) that (4.13) follows from (4.12) via Theorem 4.1 that we defined the test functions in the way that we did.

We say that ρ and s are *weak solutions* of the continuity equation (4.4) if they satisfy (4.11) for all φ in the class defined in the theorem.

The process by which we proved that ρ and s are weak solutions of the continuity equation is quite general and can be used to show that the appropriate moments of f are weak solutions of any of higher order conservation equations also.

Let $P: \xi \rightarrow P(\xi)$ be any form in the components of ξ . Associated with every such form we define another by means of the formula

$$(4.14) \quad P_1(\xi) = \xi P(\xi)$$

as well as a function \bar{P} defined by the equation

$$\bar{P}(t; q) = mN \int_{R^3} P(\xi) f(t; q, \xi) d\xi.$$

The functions \bar{P} are called the *moments* of f . It is well-known in the unconfined case that the moments \bar{P} and \bar{P}_1 are related [3; 8]. The equations expressing this relation are called *conservation equations*. The simplest conservation equation is the continuity equation (4.4); (4.4) is a conservation

equation since the density ρ is the moment associated with the form $P^0(\xi) \equiv 1$. Of course, in this case, $\rho = \tilde{P}^0$, while $\rho s = \tilde{P}^0_1$.

We can obtain weak conservation equations of a general type from the weak Liouville equation (4.8) by considering test functions $\Phi \in \mathcal{F}$ of the form

$$(4.15) \quad \Phi(t; \zeta) = P(\xi)\varphi(t; q),$$

where we use the notation of (4.9). It turns out that, when $P(\xi)$ is not identically constant, a function of the form (4.15) lies in \mathcal{F} if and only if $\varphi \in C^*1$, where

$$C^*1 = \{\varphi \in C^1([0, \infty) \times \bar{V}): \varphi(t; q) = \nabla\varphi(t; q) = 0, \quad q \in \partial V\}.$$

When $P(\xi)$ is constant, say $P(\xi) = P^0(\xi) \equiv 1$, then, as we saw earlier, $\varphi(t; q)$ need not be zero on ∂V .

Before deriving general weak conservation equations, we need one more definition. Recall that $Q^1(q^1, \dots, q^N) = Q^1(q, q^2, \dots, q^N)$ is the force on the first particle. (Cf. (2.1).) An object featured in the conservation equations is a kind of average force on the particle, defined by

$$\bar{Q}(t; q, \xi) = mN \int_{V^{N-1} \times R^{3N-1}} Q^1(q, q^2, \dots, q^N) F(t; q, \xi, \zeta^*) d\zeta^*.$$

With this notation we can state

THEOREM 4.4. *Let $P: \xi \rightarrow P(\xi)$ be a form in the components of ξ . Define P_1 by (4.13). Then the moments \tilde{P} and \tilde{P}_1 are related by the following weak conservation equation:*

$$(4.16) \quad \frac{d}{dt} \int_V \varphi \tilde{P} dq = \int_V (\varphi_t \tilde{P} + \nabla\varphi \cdot \tilde{P}_1) dq + \frac{1}{m} \int_V \varphi \int_{R^3} \nabla_\xi P \cdot \bar{Q} d\xi dq,$$

valid when $t \geq 0$ for every $\varphi \in C^*1$. If $P(\xi) \equiv 1$, then (4.16) is satisfied even if $\varphi(t; q)$ is not zero on ∂V .

Proof. Substitute a test function $\Phi \in \mathcal{F}$ of the form (4.15) into (4.8). The result is easily simplified to produce (4.16). Of course, the last sentence of Theorem 4.5 is just the first part of Theorem 4.4.

Corresponding to the weak conservation equation (4.16), there is, of course, a classical equation. If we assume that $\tilde{P}(t, q)$ and $\tilde{P}_1(t, q)$ are smooth, then (4.15) can be written

$$\int_V \varphi \left(\frac{\partial \tilde{P}}{\partial t} + \nabla \cdot \tilde{P}_1 \right) dq = \frac{1}{m} \int_V \varphi \int_{R^3} \nabla_\xi P \cdot \bar{Q} d\xi dq$$

for $\varphi \in C^*1$. A consequence is that

$$(4.17) \quad \frac{\partial \tilde{P}}{\partial t} + \nabla \cdot \tilde{P}_1 = \frac{1}{m} \int_{R^3} \nabla_\xi P \cdot \bar{Q} d\xi,$$

valid in the interior of V . Because of this fact, we may call the functions \bar{P} and \bar{P}_1 *weak solutions* of the conservation equation (4.17) if they satisfy (4.16) for all $\varphi \in C^*_1$.

Besides (4.4), the most interesting conservation equations for fluid mechanics are those associated with the forms $P^1(\xi) = \xi$ and $P^2(\xi) = |\xi|^2$. To cast these equations in a more usual notation, introduce a coordinate system in R^3 , and let $s = (s^1, s^2, s^3)$ (cf. (4.2)) and $\xi = (\xi^1, \xi^2, \xi^3)$ in that coordinate system. Define

$$(4.18) \quad \tau^{ij} = mN \int_{R^3} (\xi^i - s^i)(\xi^j - s^j)f(t; q, \xi)d\xi,$$

$$p = \frac{1}{3} \sum \tau^{ii},$$

and

$$\sigma = \tau - pI,$$

where I is the identity matrix. The matrices τ and σ are called the *stress tensor* and the *reduced stress tensor* of the system, respectively. p is called the *pressure*. At a point on ∂V at which n is the normal vector, the vector τn is called the *stress*.

If $q = (q^1, q^2, q^3)$, we define the *deformation tensor* to be the matrix whose ij th component is

$$D^{ij} = \frac{1}{2} \left(\frac{\partial s^i}{\partial q^j} + \frac{\partial s^j}{\partial q^i} \right).$$

The *Stokes hypothesis* is that σ is a function of D . A system of particles that satisfies the Stokes hypothesis is called a *fluid* [7; 8].

In terms of the quantities just defined, the conservation equation associated with $P^1(\xi) = \xi$ can be written in the form

$$(4.19) \quad \frac{\partial}{\partial t} (\rho s^i) + \sum_j \frac{\partial}{\partial q^j} (\rho s^i s^j + \tau^{ij}) = G^i,$$

where

$$G = (G^1, G^2, G^3) = \frac{1}{m} \int \nabla_{\xi} \xi \cdot \bar{Q} d\xi$$

is called the *external force* on the system. An equivalent form for (4.19) is

$$\frac{\partial}{\partial t} (\rho s^i) + \sum_j \frac{\partial}{\partial q^j} (s^i s^j + \sigma^{ij}) = - \frac{\partial p}{\partial q^i} + G^i.$$

(4.19) represents conservation of momentum.

Another equation can be derived by taking $P(\xi) = P^2(\xi) = |\xi|^2$ in (4.17). The resulting equation represents conservation of energy. For this, see [3].

5. Reverse reflection. Our results up to this point in no way depend on which reflection law A is operating. In this section, we consider a particular

class of reflection laws and explore some of their consequences. Let

$$\lambda: (q, \xi) \rightarrow \lambda(q, \xi)$$

be a real-valued function with $\lambda(q, \xi) > 0$ for $(q, \xi) \in \partial V \times \text{int } R^3_-$. We call any function A of the form

$$(5.1) \quad A(q, \xi) = -\lambda(q, \xi)\xi$$

reverse reflection if it satisfies the other conditions required for it to be a reflection law. We note that this definition is not vacuous, since the function A corresponding to $\lambda(q, \xi) \equiv 1$ is a reflection law.

We do not specify the function λ more definitely than we have for two reasons. First, as we show below, whatever the function λ may be, the boundary conditions satisfied by the system remain the same. Second, this freedom in the choice of λ may allow it to be picked in such a way that A has other desirable properties. For example, λ might be chosen so that a certain proportion of a particle's energy is lost each time it undergoes a reflection.

We begin by showing that any system of particles reflecting reversely does not slip at the boundary of the domain.

THEOREM 5.1. *Consider a system of particles moving as in § 2, with the reflection law being reverse. Then the momentum density ρs vanishes on ∂V . If $\rho \neq 0$, then s vanishes on ∂V , and the system does not slip.*

Proof. With the machinery we have built up, the proof is trivial. (4.2) and Lemma 3.4 give

$$(5.2) \quad (\rho s)(t; q) = mN \int_{R^3_-} \left[\xi - \frac{n \cdot \xi}{n \cdot A(\xi)} A(\xi) \right] f(t; q, \xi) d\xi.$$

Using (5.1), the theorem follows.

With Theorem 5.1, we have completed a coherent kinetic theory, based on conservation of probability—that most fundamental hypothesis of statistical mechanics—and including a molecular reflection law that implies the experimentally observed phenomenon of no-slip. We believe this is the first time such a theory has been presented.

On the other hand, reverse reflection has the strange feature that a molecule on impact with the boundary reverses itself, leaving the boundary in exactly the opposite direction from that which it arrived. It is perhaps hard to imagine how such an interaction between a molecule and the boundary of V might take place, at least if one persists in thinking of molecules as little rubber balls and ∂V as a hard, immovable wall.

We return to this matter in § 7. Meanwhile, we note that no-slip *is* observed in real fluids. Is it possible, then, that there are reflection laws other than (5.1) that imply no-slip? To answer this question, we must first address the problem of what it means for a reflection law to imply no-slip or, for that matter, any boundary condition. In general, a *boundary condition* for the system consists of a statement that a certain linear combination of moments vanishes

on the boundary. A linear combination of moments is, of course, an integral. Using Lemma 3.4, we can always reduce the range of integration to R^3_- . We say that a *boundary condition is implied in the standard way* if, once this reduction is completed, the integrand defining the boundary condition vanishes. As an example, we have Theorem 5.1, in which it is proved not only that reverse reflection implies no-slip, but that it implies it in the standard way. Another example is furnished by Theorem 4.1. There it is proved in the standard way that the boundary condition $n \cdot \rho s = 0$ is valid for any reflection law.

Shortly, we prove that the only reflection law that implies no-slip in the standard way is reverse reflection. There are two remarks we should like to make about this result. First, we note that we know of no other way to obtain a boundary condition besides the standard way. According to the definition, a boundary condition is an equation of the form

$$(5.3) \quad \int_{R^3_-} \left[\varphi(\xi) - \varphi(A(\xi)) \frac{n \cdot \xi}{n \cdot A(\xi)} \right] f(t; q, \xi) d\xi = 0, \quad q \in \partial V,$$

where φ is a polynomial. This boundary condition is implied in the standard way if

$$(5.4) \quad \varphi(\xi) - \varphi(A(\xi)) \frac{n \cdot \xi}{n \cdot A(\xi)} = 0.$$

To say that we know of no other way to obtain a boundary condition except the standard way is to say that our mathematical technology, so to speak, is not advanced enough for us to be able to answer the question: given φ and f , for what reflection laws A is (5.3) valid? It is certainly possible that, for a given φ and f , there is a reflection law A for which (5.3) is true, yet (5.4) is false.

On the other hand, notice that (5.3) actually *implies* (5.4) when (5.3) is true for all f in a wide enough class. Now, we *would* like any boundary condition to be valid whatever f may be, for f is determined, via (3.6) and (3.4-5), by F_0 , and a fluid should satisfy whatever boundary conditions it does satisfy regardless of the initial distribution of its molecules. However, it is presumably false that every initial distribution makes a system of particles into a fluid. But since it is not even known that there are *any* initial distributions that rigorously imply the Stokes hypothesis† [8], to assume a boundary condition is implied in the standard way is certainly not to go farther into the realm of speculation than it is to assume the Stokes hypothesis itself.

With all this said, let A be a reflection law that implies no-slip in the standard way. Then, we have (5.4) with $\varphi(\xi) = \xi$. Writing

$$-\frac{n(q) \cdot A(q, \xi)}{n(q) \cdot \xi} = \lambda(q, \xi),$$

†Rigorously. For a formal derivation, see [3].

we see from (5.4) that

$$A(q, \xi) = -\lambda(q, \xi)\xi.$$

The definition of a reflection law shows that $\lambda(q, \xi) > 0$ for $\xi \in \text{int } R^3_-$. Therefore, we have

THEOREM 5.2. *The only reflection law that implies no-slip in the standard way is reverse reflection (5.1).*

6. Other reflection laws. In view of the seemingly strange behavior of molecules experiencing reverse reflection, as well as the fact that all real fluids slip a little, it is interesting to ask for the class of *all* reflection laws that imply boundary conditions in the standard way. In fact, this was the question we originally set and which led to all the results reported herein.

We ask this question because of the difficulty in imagining a mechanism short of a demon that produces reverse reflection. The most reasonable reflection law seems, on its face, to be specular reflection, but specular reflection is to be discarded because of the paradox of zero drag—a paradox on the fluid level. While reverse reflection seems to lead to no paradox on this level, and while a molecule reversing itself on ∂V is not precisely a paradox, reverse reflection still seems difficult to accept on first exposure. Therefore, we broaden our attitude and ask if there are any reflection laws that, while being more acceptable than reverse reflection on the molecular level, also lead to no apparent paradoxes on the fluid level. The answer, we show below, is no.

Of course, the question as posed is too broad. To expect to find an answer, one has to narrow the class of reflection laws in a reasonable way. One extremely natural restriction is this: the reflection law implies boundary conditions. If a real fluid satisfies enough boundary conditions to determine the flow, and if kinetic theory provides an adequate model for the fluid, then kinetic theory must also imply those conditions. For the reasons discussed in § 5, when we assume a reflection law implies boundary conditions, we also assume they are implied in the standard way.

All reflection laws automatically imply the condition $n \cdot \rho s = 0$ on ∂V (cf. Theorem 4.1). Therefore, in the following, we study reflection laws that imply boundary conditions in addition to $n \cdot \rho s = 0$.

Let \tilde{P} be any moment of f . We call the order of the corresponding form P the *order of the moment* \tilde{P} . We call the *order of a boundary condition* the order of the highest moment appearing in the condition. No-slip, of course, is a first order condition. Specular reflection, as Maxwell pointed out, implies the tangential stresses are zero. Thus this boundary condition is second order, as the definition (4.18) of the stress tensor shows. Many boundary conditions have been proposed in one context or another [4; 7], but to our knowledge, no one has as yet suggested a condition of higher than second order, at least

for incompressible fluid flow. In this context, note that at least two boundary conditions besides $n \cdot \rho s = 0$ are required to determine the flow.

In addition to insisting that the reflection law implies boundary conditions, we may impose certain simple physical restrictions on it. As before, let n be the inward normal to V . We say that the reflection law A is *planar* if the reflected velocity $A(\xi)$ always lies in the plane spanned by n and the incident velocity ξ . We say that A is *isotropic* if the result of rotating ξ through an angle is to rotate $A(\xi)$ through the same angle. Precisely, if Ω is any rotation about the normal vector n , then A is isotropic if

$$(6.1) \quad A(\Omega\xi) = \Omega A(\xi)$$

for every such rotation Ω .

We now prove

THEOREM 6.1. *There are only two planar, isotropic reflection laws that imply in the standard way a second order (or less) boundary condition besides (4.3). One is reverse reflection, and the other is the law*

$$(6.2) \quad A(q, \xi) = \xi - [1 + \lambda(q, \xi)](n \cdot \xi)n$$

where $\lambda(q, \xi) > 0$ for all $(q, \xi) \in \partial V \times \text{int } R^3_-$.

Proof. The calculation which follows leaves the point $q \in \partial V$ fixed, and, as usual, we suppress the dependence of functions on q . Introduce cylindrical coordinates in R^3 with the z -axis in the direction of n . Then any vector can be written in the form

$$(6.3) \quad \xi = (r \cos \theta, r \sin \theta, z).$$

Since A is a homeomorphism between R^3_- and R^3_+ , A takes ∂R^3_- into ∂R^3_+ , that is, $n \cdot A(\xi) = 0$ when $n \cdot \xi = 0$. Furthermore, A is C^1 . Therefore, A has the form

$$A(\xi) = (R \cos \theta, R \sin \theta, -\lambda z),$$

where R , θ , and λ are real valued, C^1 functions of r , θ , and z . By the definition of a reflection law, $\lambda > 0$ when $z > 0$.

An easy calculation shows that if A is isotropic, then R and λ are functions of r and z alone, while

$$(6.4) \quad \theta(r, \theta, z) = \theta + \varphi(r, z) \pmod{2\pi}.$$

Furthermore,

$$(6.5) \quad R(r, z)|_{r=0} = 0$$

for any $z \leq 0$, since if $\xi = (0, 0, z)$ then $\xi = \Omega\xi$ and then isotropy gives $A(\xi) = \Omega A(\xi)$ for any rotation Ω about n . Also, if A is planar, then φ in

(6.4) can take only the values 0 and π , Therefore, incorporating a sign into R (if that is necessary), $A(\xi)$ takes the form

$$(6.6) \quad A(\xi) = (R \cos \theta, R \sin \theta, -z)$$

where R and λ are functions of r and z .

In this same coordinate system, let $s = (s^1, s^2, s^3)$, and let $\tau = ((\tau^{ij}))_{i,j=1}^3$ be the stress tensor. Suppose that A implies in the standard way the boundary condition

$$(6.7) \quad \alpha \rho + \sum_{i=1}^2 \beta_i \rho s^i + \sum_{i,j=1}^3 \gamma_{ij} (\tau^{ij} + \rho s^i s^j) = 0.$$

There is no term ρs^3 here because $\rho s^3 = n \cdot \rho s$, and this is zero by (4.3). The coefficients in (6.7) are constants, and, because τ is symmetric, we may assume $\gamma_{ij} = \gamma_{ji}$.

Notice that $(n \cdot \xi)/(n \cdot A(\xi)) = -1/\lambda(\xi)$. Therefore, if $\xi = (\xi^1, \xi^2, \xi^3)$ and $A(\xi) = (A^1, A^2, A^3)$, then by (5.4),

$$\alpha(1 + 1/\lambda) + \sum_{i=1}^2 \beta_i (\xi^i + \frac{1}{\lambda} A^i) + \sum_{i,j=1}^3 \gamma_{ij} (\xi^i \xi^j + \frac{1}{\lambda} A^i A^j) = 0.$$

Using (6.3) and (6.6) to supply expressions for the quantities ξ^i and A^i , we find, upon simplification,

$$[\alpha(1 + 1/\lambda) + \frac{1}{2}(\gamma_{11} + \gamma_{22})(r^2 + R^2/\lambda) + \gamma_{33}(1 + \lambda)z^2] + [\beta_1(r + R/\lambda) + 2\gamma_{13}z(r - R)] \cos \theta + [\beta_2(r + R/\lambda) + 2\gamma_{23}z(r - R)] \sin \theta + \frac{1}{2}(\gamma_{11} - \gamma_{22})(r^2 + R^2/\lambda) \cos 2\theta + \gamma_{12}(r^2 + R^2/\lambda) \sin 2\theta = 0.$$

Since λ , r , and R are independent of θ , this equation implies

$$(6.8) \quad \alpha(1 + 1/\lambda) + \frac{1}{2}(\gamma_{11} + \gamma_{22})(r^2 + R^2/\lambda) + \gamma_{33}(1 + \lambda)z^2 = 0,$$

$$(6.9) \quad \beta_1(r + R/\lambda) + 2\gamma_{13}z(r - R) = 0,$$

$$(6.10) \quad \beta_2(r + R/\lambda) + 2\gamma_{23}z(r - R) = 0,$$

$$(6.11) \quad \gamma_{11} = \gamma_{22},$$

$$(6.12) \quad \gamma_{12} = 0.$$

Now let $r = 0$ in (6.8). By (6.5), we obtain

$$(6.13) \quad [\alpha(1 + 1/\lambda) + \gamma_{33}(1 + \lambda)z^2]_{r=0} = 0.$$

Letting $z \rightarrow 0$ in (6.13), we conclude that $\alpha = 0$ (even if $\lambda(r, z) = 0$ when $r = z = 0$). Then (6.13) implies $\gamma_{33} = 0$, and, by (6.9), $\gamma_{11} + \gamma_{22} = 0$. Thus, from (6.11), $\gamma_{11} = \gamma_{22} = 0$.

The remaining equations (6.9-10) can be written more compactly if we define the complex quantities $\beta = \beta_1 + i\beta_2$ and $\gamma = 2\gamma_{13} + 2i\gamma_{23}$. Then (6.9-10) are equivalent to

$$(6.14) \quad \beta(r + R/\lambda) + \gamma z(r - R) = 0.$$

If (6.7) is a non-trivial boundary condition, then either β or γ must be non-zero. Thus if $\beta = 0$, (6.14) implies that

$$(6.15) \quad R \equiv r.$$

Similarly if $\gamma = 0$,

$$(6.16) \quad R \equiv -\lambda r.$$

The only remaining possibility is that both β and γ are non-zero. We show that this case is impossible. There are a number of proofs possible, but the neatest seems to be the following. If β is not zero,

$$(\gamma/\beta)z(R - r) = (r + R/\lambda),$$

and, since (6.15) and (6.16) cannot both be true (λ being positive), we conclude that γ/β is real. Furthermore, from (6.14),

$$(6.17) \quad R\left(\frac{\gamma}{\beta} + \frac{1}{n \cdot A(\xi)}\right) = r\left(\frac{\gamma}{\beta} + \frac{1}{n \cdot \xi}\right).$$

If γ is different from zero, γ/β is either positive or negative. If $\gamma/\beta > 0$, then (6.17) shows that A maps the plane

$$\Pi_1 = \{\xi: n \cdot \xi = -\beta/\gamma\}$$

into the line $R = 0$. This is not possible since the restriction of A to Π_1 is a homeomorphism, and no homeomorphism exists mapping a plane into a line. On the other hand, if $\gamma/\beta < 0$, then A^{-1} maps the plane

$$\Pi_2 = \{A\xi: n \cdot A(\xi) = -\beta/\gamma\}$$

into the line where $r = 0$. Again this is impossible.

It follows that (6.15) or (6.16) must be true. This proves Theorem 6.1, since an easy computation using (6.6) shows that (6.15) implies (6.2), while (6.16) implies (5.1).

When the function λ appearing in (6.2) is identically equal to unity, (6.2) is what is usually called specular reflection. Therefore, we refer to (6.2) as (*generalized*) *specular reflection*, dropping the adjective when there seems no chance for confusion.

The next result describes the boundary conditions implied by the two possible isotropic, planar reflection laws.

THEOREM 6.2. *At any point on ∂V where A is reverse, the momentum density vanishes. At any point on ∂V where A is generalized specular, the tangential stress vanishes.*

Proof. The first sentence of the result is just Theorem 5.1, of course. We restate that theorem here so that the boundary conditions for all planar, isotropic laws are gathered in one place.

To prove the second part of the theorem, note that specular reflection corresponds to the case $R \equiv r$ (cf. (6.15)). When $R \equiv r$, however, equations (6.8-12) imply nothing at all about γ_{13} and γ_{23} , while, just as before, all the other coefficients are zero. Therefore, the boundary condition (6.7) takes the form

$$\gamma_{13}\tau^{13} + \gamma_{23}\tau^{23} = 0.$$

Since γ_{13} and γ_{23} are arbitrary, it follows that τ^{13} and τ^{23} are zero, and these two numbers are the tangential components of the stress. This proves the second sentence of the theorem.

The conclusion to be drawn from the last part of Theorem 6.2 is that specular reflection—even generalized specular reflection—is impossible for ordinary fluids. It might seem possible, however, that the applicable reflection law is reverse on part of ∂V and specular on other parts—say, reverse on the wetted portion of a body and (generalized) specular in the wake, shading off smoothly from one to the other. The point of our next result is that this is not possible.

THEOREM 6.3. *Let A satisfy the hypothesis of Theorem 6.1. Then, if A is reverse at a single point of a connected component of ∂V , it is reverse everywhere on that component. If A is generalized specular at a point of a connected component of ∂V , it is generalized specular everywhere on that component.*

Proof. At any point where A is reverse, it has the form

$$(6.18) \quad A(q, \xi) = -\lambda_1(q, \xi)\xi,$$

while at any point where it is specular, it has the form

$$A(q, \xi) = \xi - [1 + \lambda_2(q, \xi)](n \cdot \xi)n.$$

Since A (by definition) is a continuous function of $q \in \partial V$, if A were to go from one form to the other on the same component of V , there would be a value of q for which

$$-\lambda_1(q, \xi)\xi = \xi - [1 + \lambda_2(q, \xi)](n \cdot \xi)n$$

for all $\xi \in R^3_-$. Taking the dot product of both sides with a vector e orthogonal to n , we find

$$-\lambda_1(q, \xi)(e \cdot \xi) = e \cdot \xi$$

for all $\xi \in R^3_-$. It follows from this that $\lambda_1 = -1$, and this is impossible, for if $\lambda_1 = -1$, (6.18) shows that

$$A(q, \xi) = \xi,$$

and A is not a reflection law. This proves Theorem 6.3.

The condition in Theorem 6.1 that A be planar is reasonable enough, but it can be eliminated. The result in this case is

THEOREM 6.4. *There are only four isotropic reflection laws that imply in the standard way a second order boundary condition besides (4.3). One is reverse reflection, and another is generalized specular reflection. A third is given by*

$$(6.19) \quad A(q, \xi) = \pm \sqrt{\lambda}(n \times \xi) - \lambda(n \cdot \xi)n,$$

where

$$(6.20) \quad \lambda = \lambda(q, \xi) > 0 \quad \text{on} \quad \partial V \times \text{int } R^3_-.$$

The fourth law has the form

$$(6.21) \quad A(q, \xi) = \eta\Omega(\varphi)\xi - (\eta + \lambda)(n \cdot \xi)n.$$

Here λ satisfies (6.20), and $\Omega(\varphi)$ is the rotation about n through the angle φ . The quantities $\eta(q, \xi) \geq 0$ and $\varphi(q, \xi) \in [0, 2\pi)$ are determined by the equation

$$(6.22) \quad \eta e^{i\varphi} = \lambda(q, \xi) \frac{n \cdot \xi \sigma(q) + 1}{\lambda(q, \xi)n \cdot \xi \sigma(q)},$$

where $\sigma: q \rightarrow \sigma(q)$ is a function from ∂V to the non-real complex numbers.

Proof. We use the notation of the proof of Theorem 6.1. According to (6.4), A has the form

$$(6.23) \quad A(\xi) = (R \cos(\theta + \varphi), R \sin(\theta + \varphi), -\lambda z)$$

where, as before, we suppress the dependence on q . Here, R , φ , and λ are functions of r and z , since A is isotropic. The argument in the proof of Theorem 6.1 shows that if A implies the boundary condition (6.7) in the standard way, then we have, in place of (6.8-12),

$$(6.24) \quad \alpha \left(1 + \frac{1}{\lambda}\right) + \frac{1}{2}(\gamma_{11} + \gamma_{22}) \left(r^2 + \frac{1}{\lambda} R^2\right) + \gamma_{33} z^2 (1 + \lambda) = 0,$$

$$(6.25) \quad \beta_1 \left(r + \frac{1}{\lambda} R \cos \varphi\right) + \beta_2 \left(\frac{1}{\lambda} R \sin \varphi\right) + 2\gamma_{13} z (r - R \cos \varphi) - 2\gamma_{23} z (R \sin \varphi) = 0,$$

$$(6.26) \quad -\beta_1 \left(\frac{1}{\lambda} R \sin \varphi\right) + \beta_2 \left(r + \frac{1}{\lambda} R \cos \varphi\right) + 2\gamma_{13} z (R \sin \varphi) + 2\gamma_{23} z (r - R \cos \varphi) = 0,$$

$$(6.27) \quad \frac{1}{2}(\gamma_{11} - \gamma_{22}) \left(r^2 + \frac{1}{\lambda} R^2 \cos 2\varphi\right) + \gamma_{12} \left(\frac{1}{\lambda} R^2 \sin 2\varphi\right) = 0,$$

$$(6.28) \quad -\frac{1}{2}(\gamma_{11} - \gamma_{22}) \left(\frac{1}{\lambda} R^2 \sin 2\varphi\right) + \gamma_{12} \left(r^2 + \frac{1}{\lambda} R^2 \cos 2\varphi\right) = 0.$$

As in Theorem 6.1, (6.24) (cf. (6.8)) implies that $\alpha = \gamma_{11} + \gamma_{22} = \gamma_{33} = 0$. If we let $\beta = \beta_1 + i\beta_2$, $\gamma = 2\gamma_{13} + 2i\gamma_{23}$, and $\delta = \frac{1}{2}(\gamma_{11} - \gamma_{22}) + i\gamma_{12} =$

$\gamma_{11} + i\gamma_{12}$, then the remaining four equations (6.25-28) are equivalent to

$$(6.29) \quad \beta(r + Re^{-i\varphi}/\lambda) + \gamma z(r - Re^{-i\varphi}) = 0,$$

$$(6.30) \quad \delta(r^2 + R^2e^{-2i\varphi}) = 0.$$

From (6.30), if $\delta \neq 0$, then $R^2e^{-2i\varphi} = -r^2$, and

$$(6.31) \quad R = \sqrt{\lambda}r, \quad \varphi = n\pi/2 \quad (n \text{ an odd integer}).$$

Using (6.31) in (6.23), we obtain the reflection law (6.19). Furthermore, substituting (6.31) into (6.29), we obtain after algebraic reduction

$$(6.32) \quad \beta \pm i\gamma\sqrt{\lambda}z = 0.$$

Letting $z = 0$ in (6.32), we find that $\beta = 0$, and then, in turn, $\gamma = 0$. It follows that if either β or γ is non-zero, then $\delta = 0$.

In case $\beta = 0$ and $\gamma \neq 0$, we must have $Re^{-i\varphi} - r \equiv 0$ by (6.29). This implies via (6.23) that A is generalized specular (cf. (6.15)). If $\beta \neq 0$ and $\gamma = 0$, then $r + Re^{-i\varphi}/\lambda \equiv 0$, and A is reverse. Hence Theorem 6.4 is proved in every case except possibly when $\delta = 0$, $\beta \neq 0$, and $\gamma \neq 0$. When this is true, (6.29) can be written in the form

$$Re^{-i\varphi} \left(\frac{\gamma}{\beta} + \frac{1}{n \cdot A(\xi)} \right) = r \left(\frac{\gamma}{\beta} + \frac{1}{n \cdot \xi} \right),$$

and the argument following (6.17) shows that γ/β is not real. But with γ/β complex, we find from (6.29) that

$$(6.33) \quad Re^{-i\varphi} = \lambda r \frac{(\gamma/\beta)z + 1}{\lambda(\gamma/\beta)z - 1},$$

since the denominator of (6.33) never vanishes. (6.33) implies (6.21-22) with $\eta = R/r$ and

$$(6.34) \quad \sigma = \bar{\gamma}/\bar{\beta}.$$

Notice that, while σ is independent of ξ , it may vary with $q \in \partial V$. This completes the proof of Theorem 6.4.

If a molecule reflects according to the law (6.19), its tangential velocity is rotated by 90° . For this reason we refer to (6.19) as *rotational reflection*. The law (6.20) implies a similar kind of rotation, except that in this case the angle of rotation depends on the vertical component of velocity, $n \cdot \xi$. Referring to (6.22), we see that $\varphi \approx \pi$ when $n \cdot \xi$ is small, and $\varphi \approx 0 \pmod{2\pi}$ when $n \cdot \xi$ is large. We call (6.20) *helical reflection*. Before discussing these laws further, we notice their significance to the fluid in

THEOREM 6.5. *At any point of V where A is rotational,*

$$e_1 \cdot (\rho\hat{s} + \tau) \cdot e_2 = 0.$$

Here (e_1, e_2) is any pair of vectors forming an orthonormal basis for the tangent plane to ∂V at the point under consideration, and \hat{s} is the matrix $((s^i s^j))_{i,j=1}^3$. At any point on ∂V where A is helical, the tangential component of

$$s + |\sigma| \Omega(-\arg \sigma) \tau n$$

is zero. In symbols,

$$(6.36) \quad e \cdot [s + |\sigma| \Omega(-\arg \sigma) \tau n] = 0,$$

for any vector e orthogonal to n . As before, $\Omega(\varphi)$ is the rotation about n through the angle φ .

Proof. In the proof of Theorem 6.4, we found that rotational reflection occurs only when $\delta = \gamma_{11} + i\gamma_{12} = -\gamma_{22} + i\gamma_{12}$ is free and the remaining coefficients in (6.7) vanish. But then (6.7) has the form

$$(6.37) \quad \gamma_{11}[\rho(s^1)^2 + \tau^{11} - \rho(s^2)^2 - \tau^{22}] + 2\gamma_{12}[\rho s^1 s^2 + \tau^{12}] = 0,$$

and it follows that the two expressions in brackets vanish. In particular, we have $\rho s^1 s^2 + \tau^{12} = 0$, and this is just (6.35) with $e_1 = (1, 0, 0)$, $e_2 = (0, 1, 0)$ in the coordinate system we chose in defining ρs and τ . However, this choice of coordinate system is arbitrary. Thus, (6.35) is true for any orthonormal basis for the tangent plane.

Notice, incidentally, that the other bracketed term in (6.37) is just the left side of (6.35) with $e_1 = (1, 1, 0)$ and $e_2 = (1, -1, 0)$.

To establish (6.36), notice that A is helical only when all coefficients in (6.7) vanish except possibly β_1 , β_2 , γ_{13} , and γ_{23} , and when $\sigma = \sigma_1 + i\sigma_2$, given by (6.34), is not real. In this case (6.7) has the form

$$\beta_1 s^1 + \beta_2 s^2 + (\sigma_1 \beta_1 + \sigma_2 \beta_2) \tau^{13} + (\sigma_1 \beta_2 - \sigma_2 \beta_1) \tau^{23} = 0.$$

Here β_1 and β_2 are free, so that

$$s^1 + \sigma_1 \tau^{13} - \sigma_2 \tau^{23} = s^2 + \sigma_2 \tau^{13} + \sigma_1 \tau^{23} = 0,$$

that is,

$$(6.38) \quad e_1 \cdot s + (\sigma_1 e_1 - \sigma_2 e_2) \cdot \tau n = e_2 \cdot s + (\sigma_2 e_1 + \sigma_1 e_2) \cdot \tau n = 0,$$

where $e_1 = (1, 0, 0)$ and $e_2 = (0, 1, 0)$ in the coordinate system we have chosen. The equations (6.38) give (6.36) in two independent cases whose linear combinations yield the full result (6.36). This completes the proof of Theorem 6.5.

There remains the question of whether rotational or helical reflection is in any way to be preferred to reverse reflection. We look first at rotational reflection. The boundary conditions (6.35) lead to no immediately apparent paradox, from which we conclude that rotational reflection is to be preferred at least to specular reflection. On the other hand, the conditions are much more difficult than no-slip, since they are non-linear. Thus it is hard to see why they would be preferred to no-slip unless it were shown that no-slip itself leads to a paradox.

On the molecular level, rotationally reflecting molecules must, upon arriving at the boundary, make a 90° turn to the right or left (depending on the sign in (6.19)). On our part, we find it far easier to believe that a molecule reverses itself than that it can consistently distinguish right from left.

Unlike rotational reflection, helical reflection has some features that make it seem attractive at first. If we let $|\sigma| \rightarrow 0$ in (6.22), then, for a fixed velocity ξ , $A(\xi) \rightarrow -\lambda\xi$, so that the reflection becomes reverse. Furthermore, as $|\sigma| \rightarrow 0$ in (6.36), the boundary condition tends to no-slip. Similarly letting $|\sigma| \rightarrow \infty$, we find that the reflection becomes specular and the boundary condition implies small tangential stress. Thus helical reflection seems to be an intermediate law, between reverse and specular. As such it seems to furnish a non-planar law for which the conclusion of Theorem 3.3 is false: one might now hope to find a reflection law which varies continuously from reverse to specular on a component of ∂V . In addition to all this, (6.36) is a boundary condition which allows a fluid to slip, the amount of slip depending on the size of $|\sigma|$.

Nevertheless, helical reflection has some very peculiar features. On the molecular level, on impact with the boundary, a helically reflecting molecule must consistently turn through the angle φ of (6.22). We find this circumstance no more conceivable than the right or left turns of rotationally reflecting molecules. The boundary condition (6.36) is strange for a similar reason. According to (6.36) the fluid can slip, but in order to do so its tangential velocity must be proportional to the tangential stress in another predetermined direction. Thus the fluid itself must somehow have a directional sense. In view of these difficulties, we remain as skeptical of helical as of rotational reflection.

7. Concluding remarks. The physically correct conditions satisfied at the boundary of a viscous fluid are not known, although consideration of the matter goes back at least to 1845 [9]. However, as we pointed out earlier, the no-slip boundary condition is the one most commonly proposed and studied. (Which is not to say, of course, it is the only one studied. See, e.g., [3; 6; 12].) No-slip was first suggested by Stokes, and he also supplied a plausible argument for the adoption of this hypothesis [9], an argument that has been quoted with approval by later writers [5; 7]. On the other hand, Stokes himself was not satisfied with his hypothesis or his argument for, immediately after advancing it, he points out that its consequences do “not at all agree with experiment” [9, p. 96].

The no-slip hypothesis has had this kind of checkered history throughout its life. Lamb [5, p. 546] seems doubtful of it, aerodynamic studies [11] show that it is violated badly at high altitudes, and recent, very delicate experiments seem to show that it is violated even under standard laboratory conditions [2]. The most serious view is taken by Truesdell who says, speaking of a program of future research in theoretical fluid dynamics, “Here there is

one great hindrance to future progress: *lack of proper boundary conditions . . .*" [10].

In spite of this, all works that we know of on existence of viscous fluid flows assume no-slip, as do most other works on fluids. There are, perhaps, three reasons for this. First, there is the mathematical convenience of the hypothesis. Second, there is the fact that it has as yet led to no gross paradoxes. Finally—and most important—no-slip is in extremely close agreement with observation under ordinary conditions. In [2], Elrick and Emrich had to measure fluid velocities *as close as two microns from the wall of the container* to detect (and then barely) a deviation from no-slip.

All this suggests that no-slip is an approximation to what actually happens at the boundary of a fluid, valid in the limit as some parameter goes to zero. The evidence is that the appropriate parameter is the mean free path. With this in mind, we should like to speculate on the possible position of this paper in the program of the determination of the physically correct boundary conditions satisfied by fluids.

First, we note that, since the hypothesis that a reflection law is the mechanism for interaction between gas molecules and a wall seems to lead inevitably to no-slip, some other mechanism of interaction must be operating when fluids do slip. A better approximation than that of a reflection law is probably obtained if the wall is treated as a scatterer acting on the particles that get close enough to it. Such scattering can be very complicated, varying with time as the molecules of the wall itself move, interacting with the gas molecules, and so on. But the fact that no-slip is so nearly correct when the mean free path is small, when taken along with the results of sections 5 and 6, suggests the following structure for the force exerted by the wall on gas molecules. As the mean free path goes to zero, the range of the force goes to zero also, and the scattering produced tends more and more to resemble reverse reflection, reversing the velocities of incident molecules and, perhaps, multiplying their magnitudes by a scalar.

It seems to us that this brief speculation provides enough structure to allow some mathematical experimentation into possible wall forces and scattering laws, generalizing the notion of a reflection law, the eventual aim being the explication of the interaction between gas molecules and those of a wall, as well as the resulting boundary conditions for a fluid.

Finally, a remark on the possible experimental verification of reverse reflection. A moment's thought yields several simple experiments involving reflection of tagged molecules. However, when the mean free path is long enough for these experiments to be performed easily, it is probably true that the fluid slips and, therefore, that the reflection is not reverse. If, on the other hand, matters are arranged so that the fluid does not slip, then, necessarily it seems, the mean free path is short, and measurement is accordingly difficult. We feel that an experiment designed to determine whether or not molecular reflection is approximately reverse in a situation where the corre-

sponding fluid does not slip would be of enormous interest, but such an experiment must take account of the sort of difficulty just mentioned.

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*University of British Columbia,
Vancouver, British Columbia;
University of Victoria,
Victoria, British Columbia*