Journal of Statistical Physics, Vol. 71, Nos. 5/6, 1993

Maximum Number of Collisions among Identical Hard Spheres

T. J. Murphy[1] **and E. G. D. Cohen**[2]

Received October 26, 1992

It is proved that the maximum number of collisions among three identical hard spheres in more than one dimension is four. It is conjectured that the maximum number of collisions among n hard spheres in d dimensions is independent of d, provided $d \geqslant n-1$.

KEY WORDS: Classical mechanics; collisions; maximum collision number; collision sequences; hard spheres; generalized Boltzmann equation; transport coefficients.

1. INTRODUCTION

The systematic generalization of the Boltzmann equation, which describes the nonequilibrium properties of dilute gases, to higher densities leads to a number of dynamical questions. This generalization is usually carried out using cluster expansions, which reduce the dynamical many-particle problem of the entire gas to that of isolated groups of 2, 3, 4,... particles.[1] In this way the very complicated collision sequences occurring in the many-particle problem are reduced to those of small subsets of particles, free from the influence of particles outside the subset. The classical work of Boltzmann dealt with the simplest possible case where only subsets of two particles undergoing a single binary collision were considered.[2] Extension of this treatment to include the effects of the correlation of successive collisions among particles in subsets of more than two requires a determination of the set of sequences of collisions which are dynamically possible among these particles. Then the dynamics of each particular sequence (in particular

[1] Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland 20742.
[2] The Rockefeller University, New York, New York 10021.

0022-4715/93/0600-1063$07.00/0

its time evolution) can be studied to determine its contribution to the various nonequilibrium properties of the entire gas, such as the transport coefficients.

The simplest subset of particles after the pair studied by Boltzmann is of course a set of three particles, and a particularly simple nontrivial dynamical case is that of three classical, Newtonian, perfectly elastic hard spheres of equal mass and diameter, which we will deal with in this paper. Although we use the term "spheres," we do not restrict ourselves to systems in three dimensions; thus our particles are more properly called "rods" in a one-dimensional system, "disks" in a two-dimensional system, and "hyperspheres" in a system of more than three dimensions. We will address ourselves to one of the simplest dynamical questions about this system: what is the maximum possible number of collisions among these three spheres?

It is expected that the study of this particular system will throw some light on more complex cases, particularly on those involving more than three particles. Results obtained for this system are, however, useful in their own right; Sengers *et al.*[3] have already used the results for this subsystem in their calculation of the density dependence of the transport coefficients of a moderately dense hard-sphere gas.

To enumerate the possible sequences of collisions, we need only make use of the simple Newtonian dynamics of identical hard elastic spheres: between collisions the particles move uniformly at constant velocity; upon colliding they simply exchange the components of their velocities along their line of centers. All the rest is geometry.

Although it has long been known that in one dimension a maximum of three collisions is possible (after the third collision, in the reference frame of the "middle" particle, the particles on either side are moving away; see Section 2 below, and also Appendix A), it was found by Thurston and Sandri,[4] and independently by Foch,[5] that initial conditions exist in two or more dimensions which can lead to a sequence of four collisions. Subsequently, Sandri *et al.*[6] stated that a proof existed that four was the maximum possible number of collisions; the present authors[7] published a brief outline giving all the steps of a complete proof. Now due to perceived present interest in the topic, and in the hope that more detail will be useful to those who may wish to extend our results, we present our proof in a fuller form with all details.

2. OVERVIEW

The strategy used in the proof is illustrated by the far simpler proof that in one dimension no more than three collisions can occur.

Let the central particle be denoted as 2; since the particles (or "rods") all lie on a line, it is evident that the outer particles 1 and 3 can never collide with one another. Since the particles travel uniformly at constant velocity between collisions, we need never consider a sequence of two successive collisions involving the same two particles. If we denote the outer particle which takes part in the first collision as 1, then the only sequence of three collisions which can occur is one in which first 1 collides with 2, then 2 with 3, and then 1 with 2 again. We use the notation (12)(23)(12) to denote this sequence, and refer to it as the "recollision sequence."

We choose the z axis to run from particle 2 to particle 1, and coordinates such that immediately after the first collision (12), particle 2 is stationary. Let the velocity of particle 1 at this time be called v_1 and that of particle 3 be called v_3 (Fig. 1). Evidently $v_1 > 0$, and if the second collision (23) is ever to occur, $v_3 > 0$ also. Now after the second collision particle 3 will be stationary and 2 will have velocity v_3 (the particles exchange velocities). If 2 is ever to catch up with 1 so that the third collision (12) can occur, it is necessary that $v_3 > v_1$. After the *third* collision 1 will have velocity v_3 and 2 will have velocity v_1; $v_1 > 0$, so 2 will not subsequently strike 3 (since 3 is still stationary and 2 is moving away), and $v_1 > v_3$, so 2 will not strike 1 either. Therefore no more collisions will occur.

The approach for the multidimensional case is similar. We will enumerate all sequences of a certain length containing no subsequence which has previously been proved to be impossible. For each enumerated sequence which we wish to prove impossible we will construct a separate geometric proof.

We denote the particle which takes part in both the first and the second collisions as 2 and the other particle which takes part in the first collision as 1. All sequences therefore begin with (12)(23). If, as in the one-dimensional case, the first three collisions form a "recollision sequence," one imaginable *four*-collision sequence is

I. (12)(23)(12)(23)

Note that the final three of the four collisions also form a recollision sequence (only the numbering is different). In the multidimensional case, however, another three-collision sequence is possible: (12)(23)(31), which we refer to as a "cyclic sequence." This is possible because unlike the one-dimensional case, 3 may collide with 1, as 2 does not necessarily lie between them. If the first three collisions of a four-collision sequence form

Fig. 1. Positions of three hard rods in the one-dimensional case.

822/71/5-6-15

a recollision sequence but the last three form a cyclic sequence, we have the distinct case

F. (12)(23)(12)(31)

This is the sequence for which initial conditions were obtained by Foch.

Suppose the first three collisions of a four-collision sequence form a cyclic sequence and the last three form a recollision sequence. According to our numbering convention this would be denoted

F'. (12)(23)(31)(23)

By time-reversal invariance, however, this does *not* constitute a distinct case. This can easily be seen by reading the sequence backward, substituting 1 for 2, 2 for 3, and 3 for 1.

Finally, suppose both the first three and the last three collisions form cyclic sequences. We then have the distinct case

II. (12)(23)(31)(12)

We will prove that neither sequence ***I*** nor sequence ***II*** can occur, so that any four-collision sequence must be ***F*** (or ***F'***). Any possible sequence of *five* collisions, therefore, must both begin and end with either sequence ***F*** or its time-reversed variant ***F'***. Since in ***F*** the first and third collisions involve the same pair of particles but the second and fourth do not, the two included four-collision sequences cannot both be ***F***; since in ***F'*** the second and fourth collisions involve the same pair of particles but the first and third do not, the two included four-collision sequences cannot both be ***F'***. Therefore either the first four are ***F'*** and the second four ***F***:

III. (12)(23)(31)(23)(12)

or the first four are ***F*** and the second four ***F'***:

IV. (12)(23)(12)(31)(12)

To see that these are distinct cases, it suffices to note that only in case ***IV*** do the same pair of particles take part in the first, third, and fifth collisions.

We will prove that neither sequence ***III*** nor sequence ***IV*** can occur; therefore, there can be no more than four collisions.

The four proofs are geometrically based and are all quite distinct. All have, however, points in common with the one-dimensional proof given above. We again choose a coordinate frame in which one of the particles is stationary between two of the collisions. We again choose a cylindrical coordinate axis (z axis) connecting the centers of two of the particles in contact at the time of one of the intermediate collisions—*not* the first or the last collision—so that the geometry of subsequent events (and that of preceding events) is relatively uncomplicated. The strategy once more is to show that some condition which must hold at the time of an intermediate collision in order for the last collision to occur in the future is incompatible with some other condition which must hold at that time in order for the first collision to have occurred in the past.

In addition to the possibility of cyclic three-collision sequences, a difference with the one-dimensional case is that positions and velocities must be expressed as vectors rather than as scalars. However, we will be able to restrict ourselves to mentioning only the component of each vector parallel to a given axis and a single component perpendicular to that axis, so that the results hold for any number of dimensions greater than one.

In our notation, we will call the location of particle n, its velocity, and their projections on the z axis $\mathbf{r}_n$, $\mathbf{v}_n$, $r_{nz}\hat{\mathbf{z}}$, and $v_{nz}\hat{\mathbf{z}}$, respectively, where $\hat{\mathbf{z}}$ is a unit vector along the z axis. We call the distance of particle n from the z axis $r_{n\rho}$ and the speed with which particle n moves *away* from the z axis $v_{n\rho}$. (Formally, $r_{n\rho} = |\mathbf{r}_n - r_{nz}\hat{\mathbf{z}}|$ and $v_{n\rho}$ times a unit vector in the direction of $\mathbf{r}_n - r_{nz}\hat{\mathbf{z}}$ is the projection of $\mathbf{v}_n$ on $\mathbf{r}_n - r_{nz}\hat{\mathbf{z}}$ unless $r_{n\rho} = 0$, in which case $v_{n\rho} = |\mathbf{v}_n - v_{nz}\hat{\mathbf{z}}|$.) See Fig. 2. The particle diameters are taken to be unity. The collisions are referred to as I, II, III,... and take place at times t_{I}, t_{II},...; $t-$ and $t+$ denote times immediately before and after t, respectively.

3. LEMMAS

Although our four proofs are not closely related, several common facts are used frequently:

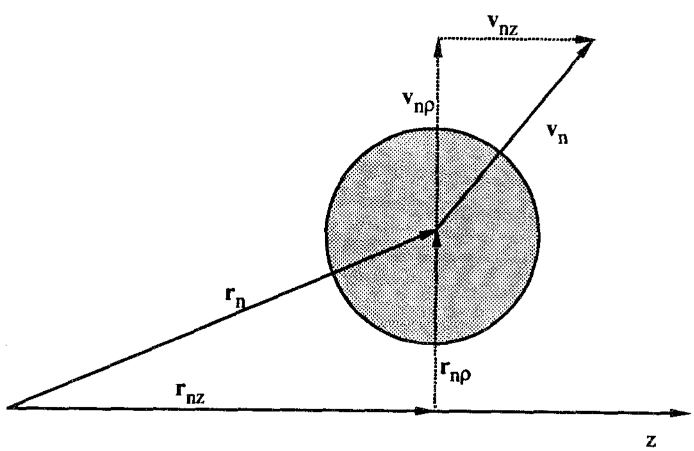

Fig. 2. Vector definitions.

Lemma A. If particle n strikes particle m in the $+x$ hemisphere of n, where $\hat{\mathbf{x}}$ denotes any axis in space, v_{nx} is decreased. (In other words, if a particle is struck "in the front," it slows down.) This should be intuitively clear.

Proof. Choose a coordinate frame in which m is stationary at $t-$. Let the z axis run from n to m at the time t of the collision and let θ be the angle from the z axis to the x axis (see Fig. 3). Before the collision,

$$v_{nx}(t-) = v_{nz}(t-)\cos\theta + v_{np}(t-)\sin\theta$$

where v_{np} is the magnitude of the projection of $\mathbf{v}_{n\rho}$ on the xz plane. The first term is positive, since $v_{nz}(t-) > 0$ or the collision will not take place, and $\cos\theta > 0$, or the contact point will be in the $-x$ hemisphere of n. At the collision, the particles exchange their z components of velocity, making $v_{nz}(t+) = 0$, so that

$$v_{nx}(t+) = 0 + v_{np}(t-)\sin\theta < v_{nx}(t-)$$

Lemma B. In the recollision sequence (12)(23)(12), let the z axis run from its origin at $\mathbf{r}_2(t_{\mathrm{II}})$ to $\mathbf{r}_3(t_{\mathrm{II}})$, with $\mathbf{v}_2(t_{\mathrm{II}}+) = 0$ (see Fig. 4). Then

$$\text{(i)}\quad r_{1\rho}(t_{\mathrm{II}}) < 1; \qquad \text{(ii)}\quad r_{1z}(t_{\mathrm{II}}) < 0; \qquad \text{(iii)}\quad r_{1z}(t_{\mathrm{III}}) < 0$$

Proof. (i) From t_{I} to t_{III}, 2 lies on the z axis. Hence if $r_{1\rho}(t_{\mathrm{II}}) > 1$ and $v_{1\rho}(t_{\mathrm{II}}) > 0$, $r_{1\rho}$ increases, so III will not occur; and if $r_{1\rho}(t_{\mathrm{II}}) > 1$ and $v_{1\rho}(t_{\mathrm{II}}) \leqslant 0$, then looking backward in time, $r_{1\rho}$ increases, so I did not occur.

(ii) The dynamical condition that two particles are moving closer together is that their relative velocity be opposed to their relative position; that is, $(\mathbf{r}_b - \mathbf{r}_a)\cdot(\mathbf{v}_b - \mathbf{v}_a) < 0$.

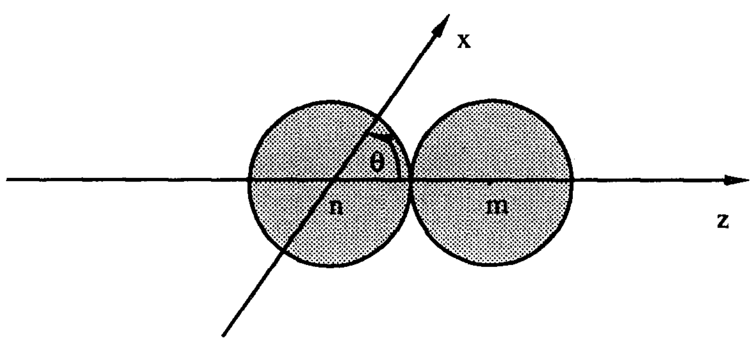

Fig. 3. Geometry of particles in Lemma A.

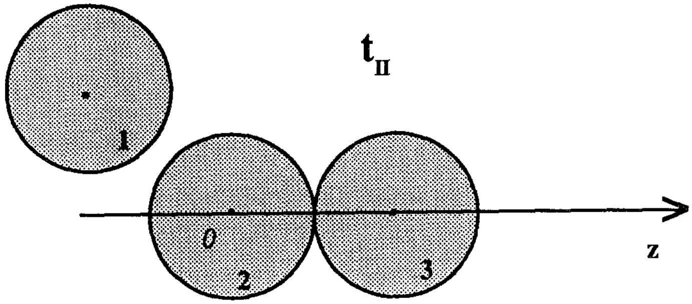

Fig. 4. Positions of the particles at t_{II} (Lemma B).

At $t_{II}+$, the corresponding condition for 1 to be approaching 2 (so that III can occur) is

$$\mathbf{r}_1 \cdot \mathbf{v}_1 = r_{1z} v_{1z} + r_{1\rho} v_{1\rho} < 0 \tag{1}$$

since $\mathbf{r}_2 = 0$ and $\mathbf{v}_2 = 0$.

At $t_{II}-$, 1 must be moving away from 2 (so that I can have occurred), so

$$\mathbf{r}_1 \cdot (\mathbf{v}_1 - \mathbf{v}_2) > 0 \qquad [\text{or} \quad -\mathbf{r}_1 \cdot (\mathbf{v}_1 - \mathbf{v}_2) < 0]$$

since $\mathbf{r}_2$ is still zero. $v_{2\rho}$ also is still zero, but now $v_{2z}(t_{II}-)$ is nonzero, so multiplying out the dot product in the equation above, we have

$$-r_{1z}(v_{1z} - v_{2z}(t_{II}-)) - r_{1\rho} v_{1\rho} < 0 \tag{2}$$

Adding this to Inequality (1), we obtain $r_{1z}(t_{II}) v_{2z}(t_{II}-) < 0$; but $v_{2z}(t_{II}-) > 0$ or II would not occur, so $r_{1z}(t_{II}) < 0$.

(iii) This part follows directly from (i) and (ii), since $\mathbf{r}_2 = 0$ between II and III (1 cannot "get past" 2; see Fig. 4).

4. PROOFS

Theorem I. (12)(23)(12)(23) is impossible.

Proof. It will be shown that given II, the conditions for IV to occur, together with the conditions for I to have occurred, contradict a condition necessary for III to occur. The coordinates used will be the same as those used in Lemma B, and positions and velocities refer to t_{II} unless otherwise specified (see Fig. 4).

As in the proof of Lemma B, the condition for 1 to be moving away from 2 (so that I can have occurred) is given by Inequality (2), which we rewrite as

$$r_{1z}(v_{1z} - v_{2z}(t_{\mathrm{II}}-)) + r_{1\rho}v_{1\rho} > 0$$

Since particle 3 is not involved in collision III, $v_{3z}(t_{\mathrm{III}}+) = v_{3z}(t_{\mathrm{II}}+)$. Also, at collision II, particles 2 and 3 exchange their z components of velocity, so that $v_{3z}(t_{\mathrm{II}}+) = v_{2z}(t_{\mathrm{II}}-)$. A necessary condition for IV to occur is $v_{2z}(t_{\mathrm{III}}+) > v_{3z}(t_{\mathrm{III}}+)$, so that 2 can "catch up" with 3; since $v_{3z}(t_{\mathrm{III}}+) = v_{2z}(t_{\mathrm{II}}-)$, this means $v_{2z}(t_{\mathrm{III}}+) > v_{2z}(t_{\mathrm{II}}-)$. Substituting this in the rewritten Inequality (2) and noting that $r_{1z} < 0$ (Lemma B), we obtain

$$r_{1z}(v_{1z} - v_{2z}(t_{\mathrm{III}}+)) + r_{1\rho}v_{1\rho} > 0 \tag{3}$$

We now eliminate $v_{2z}(t_{\mathrm{III}}+)$, r_{1z}, and $r_{1\rho}$ by writing them in terms of v_{1z}, $v_{1\rho}$, and the angle θ from the z axis to the vector $-\mathbf{r}_1(t_{\mathrm{III}})$ (see Fig. 5).

Since $v_{2z}(t_{\mathrm{III}}+)$ is just the z component of the velocity transferred from 1 to 2 at t_{III}, as $\mathbf{v}_2$ is zero up to that time, it is given by

$$v_{2z}(t_{\mathrm{III}}+) = (v_{1z}\cos\theta - v_{1\rho}\sin\theta)\cos\theta$$

Also,

$$r_{1z} = -\cos\theta - v_{1z}(t_{\mathrm{III}} - t_{\mathrm{II}})$$

and

$$r_{1\rho} = \sin\theta - v_{1\rho}(t_{\mathrm{III}} - t_{\mathrm{II}})$$

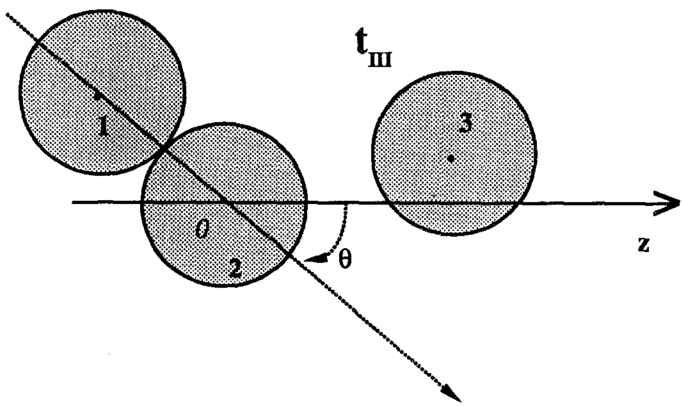

Fig. 5. Geometry of the particles at t_{III} (Theorem I).

Substituting these three expressions into Inequality (3) and using that $\cos\theta > 0$ (since $r_{1z} < 0$), we find that Inequality (3) contradicts the necessary condition for III to occur, i.e.,

$$v_{1z}\cos\theta > v_{1\rho}\sin\theta \tag{4}$$

Details are given in Appendix B.

Theorem II. (12)(23)(31)(12) is impossible.

Proof. Again, we will show that a necessary condition for III to occur is contradicted by the requirements that IV occur and that I has occurred. We choose the z axis to run from the origin at $\mathbf{r}_1(t_{\mathrm{III}})$ to $\mathbf{r}_3(t_{\mathrm{III}})$, in a reference frame such that $\mathbf{v}_2(t_{\mathrm{I}}+)=0$. We construct around $\mathbf{r}_2(t_{\mathrm{I}})$ an "action sphere" of unit radius whose surface we call S (see Fig. 6). For clarity of presentation, the proof will be given in several steps:

(a) We will show in (b) that the condition for IV, given I, requires that both $\mathbf{r}_1(t_{\mathrm{I}})$ and $\mathbf{r}_3(t_{\mathrm{II}})$ be on the $+z$ hemisphere of S. This implies that the distance along the z axis $|r_{1z}(t_{\mathrm{I}}) - r_{3z}(t_{\mathrm{II}})| < 1$ (see Fig. 6). Since $r_{3z}(t_{\mathrm{III}}) - r_{1z}(t_{\mathrm{III}}) = 1$, this in turn implies $|r_{3z}(t_{\mathrm{III}}) - r_{3z}(t_{\mathrm{II}})| > |r_{1z}(t_{\mathrm{III}}) - r_{1z}(t_{\mathrm{I}})|$ (see Fig. 6). Unless $v_{3z}(t_{\mathrm{III}}-) > v_{1z}(t_{\mathrm{III}}-)$ this is impossible, since $|r_{1z}(t_{\mathrm{III}}) - r_{1z}(t_{\mathrm{I}})| > |r_{1z}(t_{\mathrm{III}}) - r_{1z}(t_{\mathrm{II}})|$ (1 travels in a straight line between I and III), so that $|r_{3z}(t_{\mathrm{III}}) - r_{3z}(t_{\mathrm{II}})| > |r_{1z}(t_{\mathrm{III}}) - r_{1z}(t_{\mathrm{II}})|$, implying $v_{3z}(t_{\mathrm{III}}-) > v_{1z}(t_{\mathrm{III}}-)$. Contradicting this, however, is the fact that by the construction of our coordinate system $v_{3z}(t_{\mathrm{III}}-) < v_{1z}(t_{\mathrm{III}}-)$ is required for III to occur.

(b) It remains to show that $\mathbf{r}_1(t_{\mathrm{I}})$ and $\mathbf{r}_3(t_{\mathrm{II}})$ are on the $+z$ hemisphere of S. The fact that 2 is stationary between I and II $[\mathbf{v}_2(t_{\mathrm{I}}+)=0]$

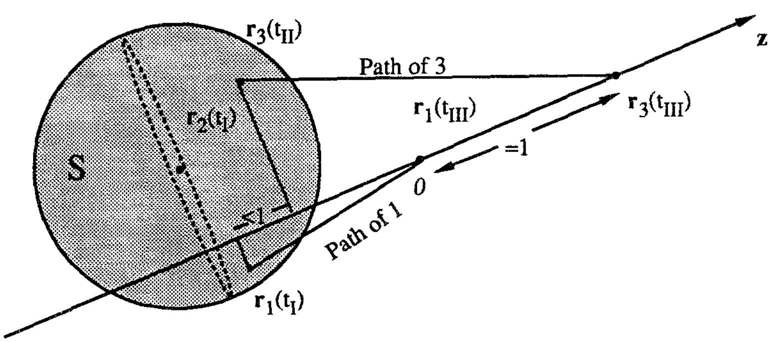

Fig. 6. The action sphere and positions of particles used in the proof of Theorem II.

requires that $\mathbf{r}_1(t_{\mathrm{I}})$ and $\mathbf{r}_3(t_{\mathrm{II}})$ are both on S. From $\mathbf{v}_2(t_{\mathrm{I}}+)=0$ and the fact that 1 travels in a straight line between I and III, it follows that after I the path of 1 cannot pass through S (particle 2 would be "in its way"); hence, $\mathbf{r}_1(t_{\mathrm{III}})$ is outside S. We will show in (c) that $r_{2z}(t_{\mathrm{I}})<0$ and in (e) that the z axis passes through S. From this and the fact that the path of 3 lies on a tangent to S between II and III, it follows that both $\mathbf{r}_1(t_{\mathrm{I}})$ and $\mathbf{r}_3(t_{\mathrm{II}})$ are indeed on the $+z$ hemisphere of S (see Fig. 6).

(c) It still remains to show that $\mathbf{r}_{2z}(t_{\mathrm{I}})<0$ and that the z axis passes through S. To show the first, we construct a z' axis with the same origin as the z axis and which runs to that origin from the center of S (see Fig. 7). Now if, as we will show in (d), $r_{3z'}(t_{\mathrm{III}})>0$, then $\mathbf{r}_3(t_{\mathrm{III}})$ and $\mathbf{r}_2(t_{\mathrm{I}})$ are on opposite sides of the origin $\mathbf{r}_1(t_{\mathrm{III}})$ on the z' axis, hence also on the z axis. The latter yields $r_{2z}(t_{\mathrm{I}})<0$.

(d) We now show that $r_{3z'}(t_{\mathrm{III}})>0$ is implied by the condition that IV occur. Since $\mathbf{r}_3(t_{\mathrm{III}})$ is within unit distance of the z' axis, $\mathbf{r}_3(t_{\mathrm{II}})$ must lie on the $+z'$ hemisphere of S. But then by Lemma A, since $v_{2z'}(t_{\mathrm{II}}-)=0$, $v_{2z'}(t_{\mathrm{II}}+)<0$, which implies that $v_{1z'}(t_{\mathrm{III}}+)<0$ also or else IV could not occur (1 would not be moving toward 2). Now from the definition of the z' axis and the fact that the path of 1 cannot pass through S, it follows that $v_{1z'}(t_{\mathrm{I}}+)>0$. But $v_{1z'}(t_{\mathrm{III}}-)=v_{1z'}(t_{\mathrm{I}}+)$ and $v_{1z'}(t_{\mathrm{III}}+)<0$, so $v_{1z'}$ must be decreased by III; Lemma A then implies that at t_{III} 3 strikes 1 in the $+z'$ hemisphere of 1, and then since $r_{1z'}(t_{\mathrm{III}})=0$ we have that indeed $r_{3z'}(t_{\mathrm{III}})>0$.

(e) It finally remains to show that the z axis passes through S. To do this, we will show that the z axis makes a smaller angle with the z' axis than does the path of 1, which intersects S at $\mathbf{r}_1(t_{\mathrm{I}})$ (see Fig. 8).

In what follows the positions and velocities refer to $t_{\mathrm{III}}-$ unless otherwise specified.

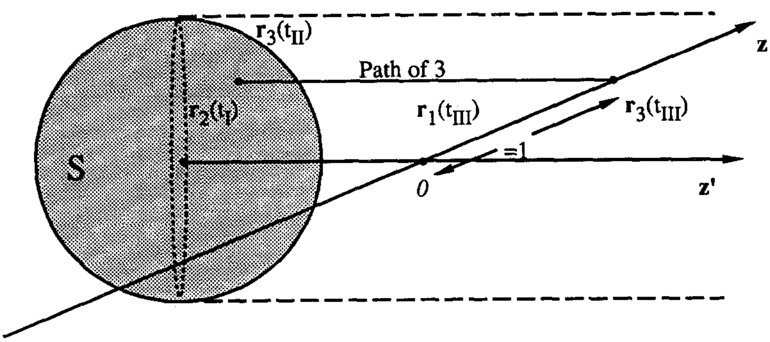

Fig. 7. Definition of the z' axis used in the proof of Theorem II.

The vector $-\mathbf{v}_1$ leads from the origin to S. Call its component parallel to the z axis $-\mathbf{v}_{1_z}$ and the rest $-\mathbf{v}_{1_\rho}$. It suffices to show that $-\mathbf{v}_{1_\rho}$ is in the $+z'$ direction (see Fig. 8). For IV to occur, $\mathbf{v}_1(t_{\rm III}+)$ must be in the $-z'$ direction, as was shown above; but $\mathbf{v}_1(t_{\rm III}+)=\mathbf{v}_{1_\rho}+\mathbf{v}_{3_z}$ (1 and 3 exchange their z velocities at $t_{\rm III}$). Since $-\mathbf{v}_{1_\rho}=\mathbf{v}_{3z}-\mathbf{v}_1(t_{\rm III}+)$ and $-\mathbf{v}_1(t_{\rm III}+)$ is in the $+z'$ direction, it remains only to show that $\mathbf{v}_{3_z}$ is in the $+z'$ direction. Clearly, unless $v_{3_z}>0$, $-\mathbf{v}_3$ cannot intersect S (see Fig. 7) and II could not have occurred. Since (as shown above) $r_{3_{z'}}>0$, the angle between the z and z' axes is acute; hence $v_{3_z}>0$ implies that $\mathbf{v}_{3_z}$ is in the $+z'$ direction, completing the proof.

Theorem III. (12)(23)(31)(23)(12) is impossible.

Proof. Once again we show that the conditions for the last collision to occur and for the first collision to have occurred are incompatible with the requirement that III occurs. We choose a frame of reference in which 3 is stationary at $t_{\rm III}+$ and run the z axis from $\mathbf{r}_3(t_{\rm III})$ to $\mathbf{r}_1(t_{\rm III})$ (see Fig. 9).

We first apply Lemma B(iii) to the recollision sequence II, III, IV to get $r_{2z}(t_{\rm IV})<0$ (see Fig. 9) and hence by Lemma A, $v_{2z}(t_{\rm IV}+)<v_{2z}(t_{\rm IV}-)$. But $v_{2z}(t_{\rm IV}-)=v_{2z}(t_{\rm III})$, so $v_{2z}(t_{\rm IV}+)<v_{2z}(t_{\rm III})$. However, $r_{1z}(t_{\rm IV})>1$, since $v_{1z}(t_{\rm IV})>0$ [it is just the velocity $v_{3z}(t_{\rm III}-)$ transferred from 3 to 1 at III if III occurs]. Therefore for 2 to "catch up" with 1 (so that V occurs) we must have $v_{2z}(t_{\rm IV}+)>v_{1z}(t_{\rm IV})$. Therefore, since $v_{2z}(t_{\rm IV}+)<v_{2z}(t_{\rm III})$, it follows that $v_{2z}(t_{\rm III})>v_{1z}(t_{\rm IV})$. But $v_{1z}(t_{\rm IV})=v_{3z}(t_{\rm III}-)$, so that $v_{2z}(t_{\rm III})>v_{3z}(t_{\rm III}-)$.

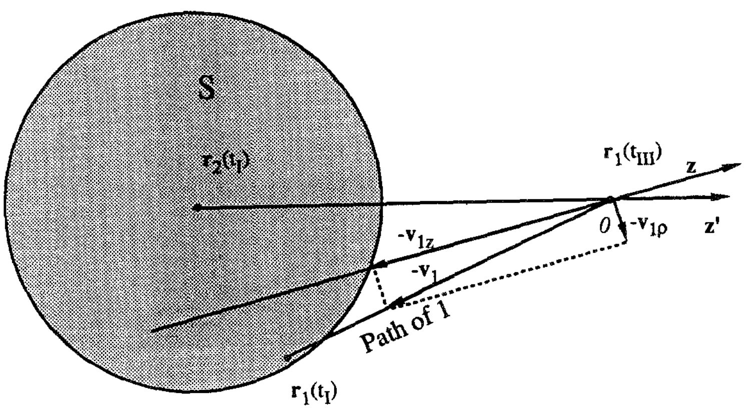

Fig. 8. The path of particle 1 and its velocity at $t_{\rm III}-$, as used in part (e) of the proof of Theorem II.

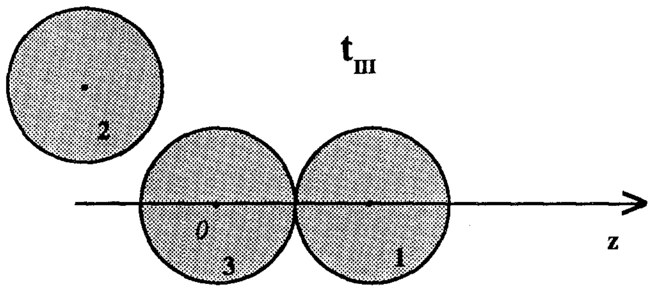

Fig. 9. Positions of the particles at t_{III} (Theorem III).

However, we will now show that if $v_{2z}(t_{\mathrm{III}}) > v_{3z}(t_{\mathrm{III}}-)$ as required for V to occur, then I cannot have occurred.

First, by Lemma B we have $r_{2z}(t_{\mathrm{III}}) < 0 = r_{3z}(t_{\mathrm{III}})$. Tracing back in time to II with $v_{2z}(t_{\mathrm{III}}) > v_{3z}(t_{\mathrm{III}}-)$ then yields $r_{2z}(t_{\mathrm{II}}) < r_{3z}(t_{\mathrm{II}})$. Then using again Lemma A, one obtains

$$v_{2z}(t_{\mathrm{II}}-) > v_{2z}(t_{\mathrm{II}}+) \tag{5}$$

However, $v_{2z}(t_{\mathrm{II}}+) = v_{2z}(t_{\mathrm{III}})$ and $v_{2z}(t_{\mathrm{III}}) > v_{1z}(t_{\mathrm{IV}})$, so that with $v_{1z}(t_{\mathrm{IV}}) > 0$ one has $v_{2z}(t_{\mathrm{II}}+) > 0$ and [by Inequality (5)] $v_{2z}(t_{\mathrm{II}}-) > 0$.

Next we show that these conditions imply that I cannot have occurred. For, by construction we have $r_{1z}(t_{\mathrm{III}}) = 1$ and $v_{3z}(t_{\mathrm{III}}+) = 0$, and since the velocity transferred from 1 to 3 at t_{III} is $v_{1z}(t_{\mathrm{III}}-) = v_{3z}(t_{\mathrm{III}}+)$, we have $v_{1z}(t_{\mathrm{III}}-) = 0$; therefore also $v_{1z}(t_{\mathrm{II}}) = 0$ and thus $r_{1z}(t_{\mathrm{II}}) = r_{1z}(t_{\mathrm{III}}) = 1$. On the other hand, by Lemma B(ii), $r_{2z}(t_{\mathrm{III}}) < 0$ (see Fig. 9), and then, since $v_{2z}(t_{\mathrm{II}}+) > 0$, we have also $r_{2z}(t_{\mathrm{II}}) < 0$. Therefore, because of the relative positions of 1 and 2 at time II (see Fig. 9), $v_{2z}(t_{\mathrm{II}}-) > 0$ implies that 1 cannot have occurred.

Theorem IV. (12)(23)(12)(31)(12) is impossible.

Proof. Again we start at III and consider the conditions for V to occur in the future and for I to have occurred in the past. We choose a frame of reference in which 1 is stationary at $t_{\mathrm{III}}+$ and run the z axis from $\mathbf{r}_1(t_{\mathrm{III}})$ to $\mathbf{r}_2(t_{\mathrm{III}})$ (see Fig. 10).

We introduce the velocity $\varepsilon = v_{1z}(t_{\mathrm{III}}-) = v_{2z}(t_{\mathrm{III}}+)$, which characterizes the importance of III in this collision sequence, since the condition for III to occur is $\varepsilon > 0$. Suppose now that we change ε without changing anything else at time t_{III}. Then collision IV (looking forward in time from III) and collision II (looking backward in time from III) will not be affected, since each collision involves only 3 and that particle whose z velocity is zero (1 in the case of IV and 2 in the case of II).

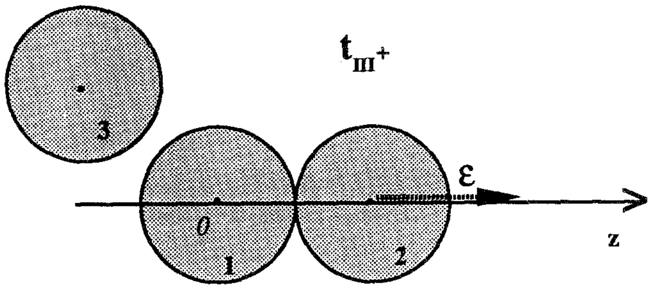

Fig. 10. Positions of the particles at t_{III} (Theorem IV).

We will show in the next paragraph that if for some ε, for which I did occur and V will occur, we decrease the value of ε without changing anything else at time t_{III}, I will still have occurred in the past and V will still occur in the future. Thus ε can be brought down to zero and the first and last collisions will still occur. At $\varepsilon = 0$, however, III does not actually occur (this is a so-called "grazing collision"), so that the sequence of collisions is (12)(23)(31)(12), which cannot take place according to Theorem II.[3] Therefore there cannot be an ε for which I and V both occur.

To determine at t_{II} (looking backward in time) whether I occurs, and to determine at t_{IV} (looking forward) whether V occurs, we use the formula $|\mathbf{R} + \mathbf{V}t|$ for the distance at time t between particles m and n, where $\boldsymbol{R} \equiv \mathbf{r}_n(t=0) - \mathbf{r}_m(t=0)$ and $\mathbf{V} \equiv \mathbf{v}_n(t=0) - \mathbf{v}_m(t=0)$. Let $R \equiv |\mathbf{R}|$ and $V \equiv |\mathbf{V}|$. Particles m and n will then collide at a time t such that $|\mathbf{R} + \mathbf{V}t| = 1$. Squaring and solving for t gives

$$t = \{-\mathbf{R}\cdot\mathbf{V} - [(\mathbf{R}\cdot\mathbf{V})^2 - V^2(R^2-1)]^{1/2}\}/V^2$$

The minus sign for the square root is used since the collision takes place at the *earliest* time at which $|\mathbf{R} + \mathbf{V}t| = 1$. If the collision is to take place, t must be real, so that $(\mathbf{R}\cdot\mathbf{V})^2 > V^2(R^2-1)$. We have already noted that for the collision to take place in the "future" the particles must be approaching each other, so that $\mathbf{R}\cdot\mathbf{V} < 0$; hence a necessary and sufficient condition for the collision to occur is $-\mathbf{R}\cdot\mathbf{V} > V(R^2-1)^{1/2}$ or

$$f \equiv -\mathbf{R}\cdot\mathbf{V} - V(R^2-1)^{1/2} > 0 \tag{6}$$

We now compute $\mathbf{R}$ and $\mathbf{V}$ in this formula for our two cases.

At $t_{II}-$ the condition for I to have occurred is $f_1(\varepsilon) > 0$ with $\mathbf{R} = \mathbf{r}_1(t_{II}) - \mathbf{r}_2(t_{II})$ and $\mathbf{V} = -[\mathbf{v}_1(t_{II}) - \mathbf{v}_2(t_{II}-)]$. (The minus sign is due to the

[3] Thus, if there is a counterexample to Theorem IV, there must also be one to Theorem II.

fact that we are looking backward in time.) Since $v_{1z}(t_{\rm II})=v_{1z}(t_{\rm III}-)=\varepsilon$ and $v_{2z}(t_{\rm III}-)=v_{1z}(t_{\rm III}+)=0$, it follows that $V_z=v_{2z}(t_{\rm II}-)-\varepsilon$ and $R_z=-[1+\varepsilon(t_{\rm III}-t_{\rm II})]$. [Here we used that $\mathbf{R}(t_{\rm II})=\mathbf{R}(t_{\rm III})-\mathbf{V}(t_{\rm III}-)(t_{\rm III}-t_{\rm II})$ and that at $t_{\rm III}$, $r_{1z}=0$ and $r_{2z}=1$.]

Similarly, at $t_{\rm IV}+$ the condition for V to occur is $f_2(\varepsilon)>0$ with $\mathbf{R}=\mathbf{r}_1(t_{\rm IV})-\mathbf{r}_2(t_{\rm IV})$ and $\mathbf{V}=\mathbf{v}_1(t_{\rm IV}+)-\mathbf{v}_2(t_{\rm IV})$. Since $v_{2z}(t_{\rm IV})=v_{2z}(t_{\rm III}+)=\varepsilon$ and $v_{1z}(t_{\rm III}+)=v_{2z}(t_{\rm III}-)=0$, it follows that $V_z=v_{1z}(t_{\rm IV}+)-\varepsilon$ and $R_z=-[1+\varepsilon(t_{\rm IV}-t_{\rm III})]$. [Here we used that $\mathbf{R}(t_{\rm IV})=\mathbf{R}(t_{\rm III})+\mathbf{V}(t_{\rm III}+)(t_{\rm VI}-t_{\rm III})$ and that at $t_{\rm III}$, $r_{1z}=0$ and $r_{2z}=1$.]

In both cases V_z is of the form $w-\varepsilon$ and R_z is of the form $-(1+\varepsilon t)$, with $\varepsilon>0$ and $t>0$. Here w, t, and those components of $\mathbf{R}$ and $\mathbf{V}$ perpendicular to the z axis are all independent of ε. Substituting these expressions into Inequality (6) and using that in both cases $R^2<2$ (which we will prove below), we find that f_1 and f_2 are monotonically decreasing functions of ε (details are given in Appendix C). Then, if $f_1>0$ and $f_2>0$ hold for any $\varepsilon>0$, they hold for $\varepsilon=0$; thus the necessary and sufficient conditions for collisions I and V require that Theorem II be violated.

It remains to prove that $R^2<2$ at $t_{\rm II}$ and $t_{\rm IV}$ in the sequence (12)(23)(12)(31) (as stated by Sandri *et al.*[(6)]).

At $t_{\rm II}$ we use the same coordinates as in Lemma B (Fig. 4). By this lemma $r_{1\rho}(t_{\rm II})<1$, so we need only to show that $-r_{1z}(t_{\rm II})<1$. Again by Lemma B, $\mathbf{r}_{1z}(t_{\rm III})<0$, so that Lemma A requires $v_{1z}(t_{\rm II})=v_{1z}(t_{\rm III}-)>v_{1z}(t_{\rm III}+)$. But unless $v_{1z}(t_{\rm III}+)>v_{3z}(t_{\rm III}+)$, 1 will never "catch up" with 3 and IV will not occur; this implies that $v_{1z}(t_{\rm III}+)>v_{3z}(t_{\rm II}+)$. [Here we used that 3 does not participate in III, so $v_{3z}(t_{\rm III}+)=v_{3z}(t_{\rm II}+)$.] However, $v_{3z}(t_{\rm II}+)=v_{2z}(t_{\rm II}-)$, so IV requires $v_{1z}(t_{\rm II})>v_{2z}(t_{\rm II}-)$, or in other words $-v_{1z}(t_{\rm II})<-v_{2z}(t_{\rm II}-)$. On the other hand, this condition (1 is "fleeing" 2) plus the fact that Lemma B requires $\mathbf{r}_{1z}(t_{\rm II})<0$ imply that indeed $-r_{1z}(t_{\rm II})<1$, since otherwise I could not have occurred.[4]

The above proof that $R^2<2$ at $t_{\rm II}$ proves also that $R^2<2$ at $t_{\rm IV}$, since the final four collisions, reading backward and renumbering, are again (12)(23)(12)(31) and $\mathbf{R}$ is again defined at the time of the "second" collision.

5. DISCUSSION

We now make some remarks concerning extensions of the present results.

[4] Note that the proof that $R^2<2$ at $t_{\rm II}$ is independent of whether collision V occurs; see point 3 in the Discussion below.

1. The one-dimensional case is far simpler than the case of two or more dimensions, as in one dimension the collisions simply "sort" the velocities until $r_i < r_j$ implies $v_i < v_j$, after which the particles are all moving apart. In the case of equal masses, the collisions act according to the binary sort algorithm (if for a neighboring pair i, j of particles $r_i < r_j$ but $v_i > v_j$, the pair must eventually collide and exchange their velocities). The number of collisions, therefore, is just the number of pairs i, j with $r_i < r_j$ but $v_i > v_j$, so that the maximum number of collisions is $\binom{n}{2}$. This is so regardless of the diameters of the particles, which may be unequal. A detailed proof is given in Appendix A.

2. In kinetic theory, because of the cluster expansions used, one must take into account correlations among particles resulting not only from sequences of collisions which actually take place (real or "interacting" collisions), but also from sequences which *would have* taken place had it not been for an intervening (real) collision. Such sequences can be accounted for by considering sequences of collisions such that for some of the collisions the particles do not interact ("noninteracting" collisions, in which the particles simply continue their uniform motion "through each other").[8] Fortunately, for a given total number of interacting and noninteracting collisions, the geometry is much simpler when one or more collisions are noninteracting. Sengers *et al.*[9] proved that the maximum number of collisions remains four, even if one includes noninteracting collisions.

3. The various restrictions on the motion of the three hard spheres which appear in our proofs may find application in the calculation of the numerical effects of certain collision sequences on the transport properties of a hard-sphere gas. For example, the results of Sengers *et al.*[3] for a moderately dense gas of hard spheres show that the contributions of the four-collision sequences to the viscosity and thermal conductivity of such a gas are four orders of magnitude smaller than those from typical three-collision sequences. In addition, these restrictions may also have a bearing on whether certain sequences of collisions among *more* than three particles are possible. For example, the position of particle 1 at the time of collision II in the sequence (12)(23)(12)(31) is severely restricted: in the proof of Theorem IV we saw that at time II, $R = |\mathbf{r}_1 - \mathbf{r}_2| < \sqrt{2}$ was required; on the other hand, Lemma B(i) requires that at the same time $|\mathbf{r}_1 - \mathbf{r}_3| > \sqrt{2}$ if the first three collisions are to occur (see Fig. 4).

4. The fact that our proofs are independent of the dimensionality of the system (provided it is greater than one) leads us to the following conjecture: the maximum number of collisions which can take place among n identical hard spheres is independent of the dimensionality d of the system, provided $d \geqslant n - 1$. (This is of course trivially true for two spheres.) The

conjecture is reinforced by the consideration that the introduction of each additional identical sphere after the first introduces one more quantity with dimension "length": its distance from the center of mass of the spheres already present. The additional angular degrees of freedom introduced may in a certain sense be ignorable coordinates. Thus we conjecture for example that the maximum number of collisions among four identical spheres may be greater in three dimensions than in two, but should be the same in four or more dimensions as in three.

5. Finally, we note that no general line appears in our four proofs which would yield a clue as to how to generalize them to more complicated cases such as collision sequences among four spheres. It would appear that each collision sequence has its own particular geometry, so that each sequence (all of whose subsequences are possible) may have to be examined individually.

APPENDIX A

Here we prove that n classical Newtonian hard particles of arbitrary diameters but equal mass constrained to move in one dimension can undergo at most $\binom{n}{2}$ collisions, and that for any set of diameters there are initial velocities which will bring about $\binom{n}{2}$ collisions.

Let the positions r_i of the particles increase from left to right; let the velocity of the leftmost particle *at time zero* be called v_1, that of the second-leftmost v_2, etc. Let $r_1(t)$ denote the position at time t of the center of that particle which at time t has velocity v_1, etc. Note that the v_i *never change*; they are merely associated with different particles. There is no need to number the particles, only the velocities.

Let $i<j$ without loss of generality. Then at time zero the "total gap" $\Delta = r_j - r_i - \Sigma > 0$, where $\Sigma(t)$ is the sum of half the diameter of the particle with velocity v_i, half the diameter of the particle with velocity v_j, and the sum of the diameters of all particles between them. (Particles cannot overlap.)

Suppose $v_i < v_j$. Then Δ will always increase (at a constant rate); for $r_j - r_i$ increases unless one of the two particles undergoes a collision; but any decrease in $r_j - r_i$ due to the instantaneous transfer of velocity from one particle to another (Enskog's "collisional transfer")[(2)] is canceled by the corresponding decrease in Σ. For instance, if a particle with velocity $v_k > v_j$ hits the particle v_j from the left, $r_j - r_i$ instantaneously decreases by the sum of the radii of the colliding particles, but Σ instantaneously decreases by the same amount, since now there is one fewer particle between the particle with velocity v_i and the particle with velocity v_j.

In the above case there will be exactly zero collisions between a particle with velocity v_i and a particle with velocity v_j.

Suppose, on the other hand, $v_i > v_j$. Then Δ will decrease (at a constant rate) until there are no particles between the particle with velocity v_i and that with velocity v_j; it will continue to decrease (at the same rate) until the particle with velocity v_i collides with the particle with velocity v_j. *After* the collision the new Δ $(r_i - r_j - \Sigma)$ will thereafter increase indefinitely (at the same rate at which the old Δ decreased) by the argument above.

In this case there will be exactly one collision between a particle with velocity v_i and a particle with velocity v_j.

Thus there can be at most one collision between some particle with velocity v_i and some particle with velocity v_j, and the total number of collisions will be equal to the number of $i<j$ pairs with $v_i > v_j$. Then the maximum number of collisions altogether is $\binom{n}{2}$, where n is the number of particles. Furthermore, this maximum can be realized: merely let the velocities at time zero decrease monotonically from left to right.

APPENDIX B

We show that Inequality (3) in the proof of Theorem I cannot hold. Making the indicated substitutions in Inequality (3) yields

$$[-\cos\theta - v_{1z}(t_{\mathrm{III}} - t_{\mathrm{II}})][v_{1z} - v_{1z}\cos^2\theta + v_{1\rho}\sin\theta\cos\theta] + [\sin\theta - v_{1\rho}(t_{\mathrm{III}} - t_{\mathrm{II}})] > 0$$

Simplifying, we obtain

$$\sin^2\theta(v_{1\rho}\sin\theta - v_{1z}\cos\theta) - (t_{\mathrm{III}} - t_{\mathrm{II}})(v_{1z}^2\sin^2\theta + v_{1z}v_{1\rho}\sin\theta\cos\theta + v_{1\rho}^2) > 0 \qquad \text{(A1)}$$

This, however, contradicts Inequality (4) in the proof of Theorem I:

$$v_{1z}\cos\theta > v_{1\rho}\sin\theta$$

For, if Inequality (4) holds, the first term in Inequality (A1) is negative, requiring

$$v_{1z}^2\sin^2\theta + v_{1z}v_{1\rho}\sin\theta\cos\theta + v_{1\rho}^2 < 0$$

However, since $\cos\theta > 0$, $v_{1z}v_{1\rho}\sin\theta$ would then have to be negative, and as $\cos\theta < 2$,

$$v_{1z}v_{1\rho}\sin\theta\cos\theta > 2v_{1z}v_{1\rho}\sin\theta$$

requiring $v_{1z}^2\sin^2\theta + 2v_{1z}v_{1\rho}\sin\theta + v_{1\rho}^2 < 0$, which is not possible (the left-hand side is a complete square).

APPENDIX C

We show that f in the proof of Theorem IV is a monotonically decreasing function of ε. We have

$$f \equiv -\mathbf{R}\cdot\mathbf{V} - V(R^2-1)^{1/2}$$

with

$$R_z = -(1+\varepsilon t), \qquad V_z = w - \varepsilon, \qquad t > 0, \quad \varepsilon \geqslant 0, \quad R^2 < 2$$

We call the components of $\mathbf{R}$ and $\mathbf{V}$ orthogonal to the z axis $\mathbf{R}_\rho \equiv \mathbf{R} - R_z\hat{\mathbf{z}}$ and $\mathbf{V}_\rho \equiv \mathbf{V} - V_z\hat{\mathbf{z}}$ with $R_\rho \equiv |\mathbf{R}_\rho|$ and $V_\rho \equiv |\mathbf{V}_\rho|$. Then $f = -R_z V_z - \mathbf{R}_\rho \cdot \mathbf{V}_\rho - [(V_z^2 + V_\rho^2)(R_z^2 + R_\rho^2 - 1)]^{1/2}$ and

$$\frac{df}{d\varepsilon} = \left[-(1+\varepsilon t)\frac{V}{(R^2-1)^{1/2}} + (w-\varepsilon)\right]\left(t + \frac{(R^2-1)^{1/2}}{V}\right)$$

Now $(R^2-1)^{1/2} < 1$ and $|w-\varepsilon| < V$, so $(w-\varepsilon) - V/(R^2-1)^{1/2}$ is negative; hence $df/d\varepsilon < 0$.

ACKNOWLEDGMENT

One of us (E.G.D.C.) gratefully acknowledges financial support of the Department of Energy under contract number DE-FG02-88-ER13847.

REFERENCES

1. J. V. Sengers, *Phys. Fluids* **9**:1333 (1966); J. R. Dorfman and E. G. D. Cohen, *J. Math. Phys.* **8**:282 (1967).
2. J. R. Dorfman and H. van Beijeren, In *Statistical Mechanics*, Part B, B. J. Berne, ed. (Plenum Press, New York, 1977), p. 65.
3. J. V. Sengers, D. T. Gillespie, and J. J. Perez-Esandi, *Physica* **90A**:365 (1978).
4. W. Thurston and G. Sandri, *Bull. Am. Phys. Soc.* **9**:386 (1964).
5. E. G. D. Cohen, in *Statistical Mechanics of Equilibrium and Non-Equilibrium*, J. Meixner, ed. (North-Holland, Amsterdam, 1965), p. 142.
6. G. Sandri, R. D. Sullivan, and P. Norem, *Phys. Rev. Lett.* **13**:743 (1964); G. Sandri and A. H. Kritz, *Phys. Rev.* **150**:92 (1966).
7. E. G. D. Cohen, In *Lectures in Theoretical Physics*, VIIIA, W. E. Brittin, ed. (University of Colorado Press, Boulder, Colorado, 1966), p. 167.
8. W. R. Hoegy and J. V. Sengers, *Phys. Rev. A* **2**:2463 (1970).
9. J. V. Sengers, D. T. Gillespie, and W. R. Hoegy, *Phys. Lett. A* **32**:387 (1970).