

# Dynamics of Hard Rods in One Dimension

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We examine a system consisting of  $N$  classical, Newtonian, perfectly elastic hard rods constrained to move on a line. The mass and length of each rod are arbitrary. We develop an algorithm which gives, after any given possible sequence of collisions, the new velocities of the  $N$  rods and a necessary condition for any given pair of rods to be involved in the next collision, all in terms of the initial velocities of the rods. These results are then used to prove that for the case where there are exactly three rods on the line, the maximum possible number of collisions among them is the largest integer  $n$  such that  $m_2 < (\mu_{12}\mu_{23})^{1/2}/\cos[\pi/(n-1)]$ , where  $m_2$  is the mass of the central particle and  $\mu_{12}$  and  $\mu_{23}$  are the reduced masses of the left and right particle pairs. We further derive for this three-particle case a condition on the initial velocities which is necessary and sufficient for  $k$  collisions,  $1 < k \leq n$ , to occur, as well as explicit expressions for the velocities after each collision in terms of the initial velocities.

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**KEY WORDS:** Collisions; maximum collision number; classical dynamics; one-dimensional systems; hard spheres; hard rods.

## 1. INTRODUCTION

The description of the nonequilibrium properties of dilute gases involves knowledge of the dynamical properties of isolated subsystems consisting of a small number of gas particles.<sup>(1,2)</sup> For a subsystem of two particles interacting through a central force, calculation of the dynamics is straightforward, but even for the three-body problem the calculation becomes quite complex, even in the relatively simple case of classical, Newtonian, perfectly elastic hard spheres. Little is known even about the question of which sequences of collisions are possible among such spheres when their masses and diameters are equal.

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There are, however, known initial conditions which lead to four collisions among an isolated set of three such identical spheres, and it is known that more than four collisions among them are not possible.<sup>(3,4)</sup>

While it is the results for particles moving in three dimensions that are of immediate physical interest,<sup>(2)</sup> it is useful to study the one-dimensional case, as some of the results may point the way to progress in the three-dimensional case. We call the one-dimensional equivalent of hard spheres "hard rods," and it is exclusively with classical, Newtonian, perfectly elastic hard rods that we deal in this paper.

A set of such particles will undergo collisions until the particles are arranged on the line running from left to right in order of increasing velocity to the right, so that no particle is approaching any other particle. From that point on no further collisions can occur. It is known<sup>(4)</sup> for a set of  $i$  such particles (of arbitrary lengths, which may differ for different particles) that if all their masses are equal, the maximum possible number of collisions is  $\binom{i}{2} = i(i-1)/2$ . (For point particles, this has long been well known; see, e.g., ref. 5). This is so because in this particular case the particles upon collision simply exchange their velocities, and so the set of particles simply sorts their velocities according to the binary sort algorithm.<sup>(4)</sup>

We wish to find corresponding results for the case of unequal masses. Let us first give a nonrigorous, qualitative account of the results we expect. Let us consider a subset of three neighboring particles on the line such that the left-hand particle is approaching the right-hand particle, and both are approaching the central particle. Elementary considerations suggest that the sequence of collisions cannot terminate until the central particle of the three has transferred enough momentum from the left-hand particle to the right-hand particle so that the distance between the two outer particles is increasing. For the case of equal masses this requires at least three collisions among the three particles. This follows from the number of exchanges of the original particle velocities required to properly order the three particle velocities, plus the fact that if there are collisions with particles outside the subset of three, the effect of the additional collisions will be to cause the pair of outer particles to approach one another with still greater speed, requiring transfer of still more momentum from the left-hand particle to the right-hand particle.

If, however, the central particle is more massive than the two outer particles, the transfer of momentum from the left-hand particle to the right-hand particle is more efficient, so that we may expect fewer collisions to be needed to transfer the necessary amount of momentum. If, on the other hand, the central particle of the subset is lighter than the outer particles, we expect more collisions among the three to be needed to transfer the

necessary amount of momentum. As the mass of the central particle approaches zero with the mass of the other particles and the initial velocities remaining constant, we expect the central particle to have to "rattle around" transferring momentum between the outer particles, so that the required number of collisions increases indefinitely.

For the case of only three particles on the line, this means that for equal masses we know that a maximum of three collisions is possible; that if the mass of the central particle is larger than that of either of the outer two particles, we expect that fewer collisions may occur for the same set of initial velocities; and that if the mass of the central particle approaches zero with the masses of the two other particles and the initial velocities remaining constant, the number of possible collisions increases indefinitely.

We now proceed to calculate quantitative results for arbitrary sets of masses (and lengths).

## 2. DYNAMICS OF HARD RODS ON A LINE

We now give an algorithm for calculating the velocities of each of a given number  $N$  of hard rods on a line after a given sequence of collisions, and a necessary condition for a specific particle pair to take part in the next collision after the given sequence. The algorithm requires no knowledge of the lengths or positions of the particles, and is useful in examining systems with any number of particles; we will also use it in the following sections to determine the total number of collisions which take place in the three-particle case.

We let the  $x$  direction run from left to right and number the particles 1, 2, ... from left to right. We write  $m_k$  for the mass of particle  $k$ ; the particle velocities remain constant between collisions, so we write  $v_k^{(j)}$  for the velocity of particle  $k$  between the  $j$ th and  $(j+1)$ st collision.

One of the simplifying features of the one-dimensional case is that the particles always remain in the same order, so that each collision is between some particle which we call  $i$  and the particle  $i+1$  to its right. In examining the dynamics of a collision, we therefore need to consider only the masses and velocities of adjacent particles  $i$  and  $i+1$ . We define the reduced masses and relative velocities after the  $j$ th collision by

$$\mu_{i,i+1} \equiv \frac{m_i m_{i+1}}{m_i + m_{i+1}}, \quad v_{i,i+1}^{(j)} \equiv v_i^{(j)} - v_{i+1}^{(j)}$$

After the  $j$ th collision particle  $i$  is approaching particle  $i+1$  if and only if  $v_{i,i+1}^{(j)} > 0$ . This is therefore a necessary condition that the next collision occur between particles  $i$  and  $i+1$ ; it is, however, not a sufficient

condition (except in the case of three particles when at least one collision has already occurred; see below), since another collision may occur before particle  $i$  reaches particle  $i + 1$ . Whether this occurs depends in general on the lengths and initial positions of all the particles as well as on their initial velocities, complicating the characterization of the region in phase space that leads to a given sequence of collisions among four or more particles.

If the  $(j + 1)$ st collision does indeed occur between particles  $i$  and  $i + 1$ , the laws of conservation of momentum and energy give us the velocities of  $i$  and  $i + 1$  after the  $(j + 1)$ st collision in terms of their velocities before the collision (see, e.g., ref. 6):

$$v_i^{(j+1)} = v_i^{(j)} - 2 \frac{\mu_{i,i+1}}{m_i} v_{i,i+1}^{(j)}$$

$$v_{i+1}^{(j+1)} = v_{i+1}^{(j)} + 2 \frac{\mu_{i,i+1}}{m_{i+1}} v_{i,i+1}^{(j)}$$

The key quantities in the determination of the evolution of the system, however, are not the velocities of the individual particles, but rather the relative velocities of adjacent particle pairs. As the velocities of the particles not involved in the collision between particles  $i$  and  $i + 1$  do not change, the only relative velocities which change are those involving either particle  $i$  or particle  $i + 1$ . The relative velocities which do change are given by subtraction:

$$v_{i-1,i}^{(j+1)} = v_{i-1,i}^{(j)} + 2 \frac{\mu_{i,i+1}}{m_i} v_{i,i+1}^{(j)}$$

$$v_{i,i+1}^{(j+1)} = -v_{i,i+1}^{(j)} \quad (1)$$

$$v_{i+1,i+2}^{(j+1)} = v_{i+1,i+2}^{(j)} + 2 \frac{\mu_{i,i+1}}{m_{i+1}} v_{i,i+1}^{(j)}$$

If it is known that a given sequence of  $j$  collisions occurs, the final velocities of all the particles can be calculated by repeated application of (1), giving them as linear combinations of the set of initial velocities  $v_{k,k+1}^{(0)}$ ; the coefficients will be functions of the particle masses. If any of the  $v_{k,k+1}^{(j)}$  are then positive, at least one more collision will occur; if, however, more than one  $v_{k,k+1}^{(j)}$  is positive, it is necessary to use the initial positions and lengths of the particles and follow their trajectories to determine which collision will occur next. Since this latter complication does not arise after the first collision in the case of three particles, as we will see in the following section, we devote the rest of this paper to the case of three particles.

### 3. THE THREE-PARTICLE CASE

For the case of three particles we assume that at least one collision occurs (the distance between the central particle and at least one outer particle is decreasing) and assume without loss of generality that the outer particle which takes part in the first collision is on the left (particle 1). Then the first collision is between particles 1 and 2, and  $v_{12}^{(0)} > 0$  necessarily in all that follows.

For the three-particle case the only possible sequences of collisions are those which alternate between collisions involving particles 1 and 2 and those involving particles 2 and 3. This is so since each of the two particle pairs is moving apart after a mutual collision so that if  $j > 0$ ,  $v_{k,k+1}^{(j)}$  can be positive for at most one value of  $k$ . This greatly simplifies the problem of determining the number of collisions which occur as well as the relative velocities after the  $j$ th collision, as the lengths and initial positions of the particles become irrelevant, as do any velocities other than the relative velocities of the two pairs 1, 2 and 2, 3 (the motion of the center of mass is irrelevant). We will therefore describe the initial conditions by specifying only  $v_{12}^{(0)}$  and  $v_{23}^{(0)}$ . Then, according to (1), the velocities  $v_{i,i+1}^{(j)}$  after the  $j$ th collision are given by

$$\begin{aligned}
 v_{12}^{(j)} &= -v_{12}^{(j-1)} \\
 v_{23}^{(j)} &= v_{23}^{(j-1)} + 2 \frac{\mu_{12}}{m_2} v_{12}^{(j-1)} = v_{23}^{(j-1)} + x \left( \frac{\mu_{12}}{\mu_{23}} \right)^{1/2} v_{12}^{(j-1)}
 \end{aligned}
 \tag{2}$$

when  $j$  is odd (collision between 1 and 2); and by

$$\begin{aligned}
 v_{12}^{(j)} &= v_{12}^{(j-1)} + 2 \frac{\mu_{23}}{m_2} v_{23}^{(j-1)} = v_{12}^{(j-1)} + x \left( \frac{\mu_{23}}{\mu_{12}} \right)^{1/2} v_{23}^{(j-1)} \\
 v_{23}^{(j)} &= -v_{23}^{(j-1)}
 \end{aligned}
 \tag{3}$$

when  $j$  is even (collision between 2 and 3). Here we define  $x$ , an important dimensionless parameter which characterizes the system, as the ratio of twice the geometric mean of the reduced masses of the left-hand and right-hand particle pairs to the central mass:  $x \equiv 2(\mu_{12}\mu_{23})^{1/2}/m_2$ . Note for later reference that  $0 < x < 2$ ; that  $x = 1$  if all three masses are equal; that  $x \rightarrow 0$  corresponds to a central mass much larger than the outer masses; and that  $x \rightarrow 2$  corresponds to a central mass much smaller than the outer masses, so that, as mentioned in the Introduction, a large number of collisions is possible.

Now if we iterate Eqs. (2) and (3) starting with  $v_{12}^{(0)}$  and  $v_{23}^{(0)}$ , we obtain the  $v_{i,i+1}^{(j)}$  as linear combinations of  $v_{12}^{(0)}$  and  $v_{23}^{(0)}$ , with coefficients equal to 1,  $(\mu_{12}/\mu_{23})^{1/2}$ , or  $(\mu_{23}/\mu_{12})^{1/2}$  times some polynomial in  $x$ .

We therefore will now discuss the properties of the particular polynomials involved.

#### 4. THE CHEBYSHEV POLYNOMIALS<sup>2</sup>

For  $0 < x < 2$  and  $k \geq 0$ , we define the function  $S_k(x)$  by  $S_k(2 \cos \theta) = \sin(k+1)\theta/\sin \theta$ . For integer  $k$ , a classic result<sup>(7)</sup> is that the  $S_k(x)$  are polynomials in  $x$ , known as "the Chebyshev polynomials of the first kind," which can be given by the recursion relation  $S_k(x) = xS_{k-1}(x) - S_{k-2}(x)$  with  $S_0 = 1$  and  $S_1 = x$ . The zeros of  $S_k(x)$  lie at  $x = 2 \cos[m\pi/(k+1)]$  where  $m$  is a positive integer. As  $x$  increases from 0 to 2,  $\theta \equiv \arccos(x/2)$  decreases from  $\pi/2$  to 0. The greatest zero of  $S_k$  is at  $x = 2 \cos[\pi/(k+1)]$ . As we will show that the maximum number of collisions among three hard rods depends on the value of  $x$  relative to these greatest zeros for integer  $k$ , we plot in Fig. 1 some values of  $x$  such that  $S_k(x) = 0$  when  $k = 1, 2, \dots$ , and the corresponding values of  $(\pi/\theta) + 1$ .

We will now give two lemmas concerning the Chebyshev polynomials which we will need in the determination of the motion of three hard rods.

**Lemma I.** If  $x$  is greater than the greatest zero of  $S_k$  but less than the greatest zero of  $S_{k+1}$ ,  $k > 0$ , then (i)  $S_{k+1}(x) < 0$ ; (ii)  $S_{k+2} < 0$ ; and (iii) for  $j \leq k$ ,  $S_j(x) > 0$ . See Fig. 1.

*Proof.*  $x$  is greater than the greatest zero of  $S_k$  if and only if  $\theta \equiv \arccos(x/2) < \pi/(k+1)$ . We therefore have  $\pi/(k+2) < \theta < \pi/(k+1)$ , so that:

- (i)  $\pi < (k+2)\theta < [(k+2)/(k+1)]\pi < 2\pi$ ,  
and therefore  $S_{k+1} = \sin(k+2)\theta/\sin \theta < 0$ .
- (ii)  $\pi < [(k+3)/(k+2)]\pi < (k+3)\theta < [(k+3)/(k+1)]\pi \leq 2\pi$ ,  
and therefore  $S_{k+2} = \sin(k+3)\theta/\sin \theta < 0$ .
- (iii)  $0 < [(j+1)/(k+2)]\pi < (j+1)\theta < [(j+1)/(k+1)]\pi \leq \pi$ ,  
and therefore  $S_j = \sin(j+1)\theta/\sin \theta > 0$  if  $j \leq k$ .

**Lemma II.** If  $x$  is greater than the greatest zero of  $S_{k-2}(x)$ , then the sequence  $\{-S_{j-1}/S_{j-2}\}$  with  $j = k, k-1, k-2, \dots, 2$  decreases monotonically as  $j$  decreases.

<sup>2</sup>"The Chebyshev polynomial is like a fine jewel that reveals different characteristics under illumination from varying positions" (Rivlin<sup>(8)</sup>).

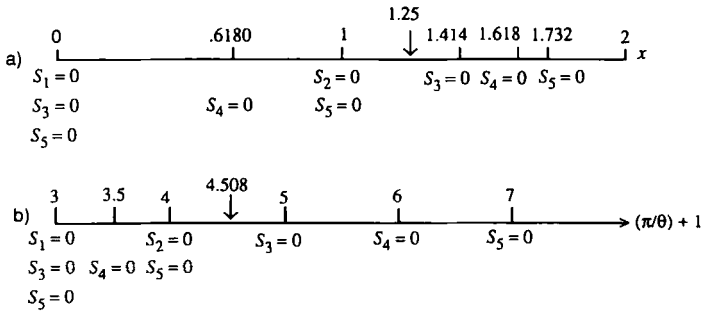


Fig. 1. (a) Values of  $x \geq 0$  such that  $S_k(x) = 0$  for  $1 \leq k \leq 5$ . The  $S_k$  that equal zero for each value of  $x$  are listed below the line; if an  $S_k$  appears in the  $m$ th row, the zero is the  $m$ th greatest zero for that value of  $k$ . The arrow corresponds to the value of  $x$  obtained when the masses of the two outer particles are equal and the mass of the central particle equals  $3/5$  that of an outer particle (see point 3 of the Discussion); for this value of  $x$  a maximum of four collisions is possible. Note for comparison with Lemma I that  $x$  is greater than the greatest zero of  $S_2$ , is less than the greatest zero of  $S_3$ , and lies between the two greatest zeros of  $S_3$  as well as those of  $S_4$ . (b) Values of  $(\pi/\theta) + 1$ ,  $\theta \leq \pi/2$ , such that  $S_k(2 \cos \theta) = 0$  for  $1 \leq k \leq 5$ . The arrow corresponds to the value of  $x$  in part (a). This part of the figure is given to show more clearly the relationship between the masses and the maximum number of collisions; for each  $m$  the  $m$ th greatest zeros of the  $S_k$  are equally spaced a distance  $1/m$  apart. The maximum number of collisions is the integer value to the left of the arrow (four in this case). See point 1 of the Discussion.

*Proof.* If  $x$  is less than the greatest zero of  $S_{k-1}$ , we must treat the first term in the sequence [with  $j = k$ ] as a special case. We therefore divide the proof into two parts: (i) the case where  $x$  is less than the greatest zero of  $S_{k-1}$ , and (ii) the case where  $x$  is greater than the greatest zero of  $S_{k-1}$ . We further subdivide case (i) into two parts: in (a) we show that the first term in the sequence is greater than any other term, and in (b) we show that the terms other than the first decrease as  $j$  decreases.

(i) We first let  $x$  be less than the greatest zero of  $S_{k-1}$ .

(a) By Lemma I, the first term (with  $j = k$ ) in the sequence of  $\{-S_{j-1}/S_{j-2}\}$  is positive and so is greater than any negative terms. Also by Lemma I, for  $j < k$  we have  $S_{j-1} > 0$  and  $S_{j-2} > 0$ . All terms in the sequence except  $j = k$  are therefore negative, so the lemma follows for this special case.

(b) For  $j < k$ , we note that  $x$  is greater than the greatest zero of  $S_{k-2}$  if and only if  $\theta < \pi/(k-1)$ . Then, since  $j \leq k-1$  and  $\theta < \pi/(k-1)$ , we have that  $j\theta < \pi$  and  $(j-1)\theta < \pi$ . But then

$$\frac{d}{dj} \left( \ln \frac{S_{j-1}}{S_{j-2}} \right) = \theta [\cot j\theta - \cot(j-1)\theta] < 0$$

since the cotangent is a monotonically decreasing function of its argument between 0 and  $\pi$ . Therefore  $\{-S_{j-1}/S_{j-2}\}$  is a monotonically increasing function of  $j$ , and for integral values of  $j$  the lemma then follows for this case.

(ii) We now treat the case where  $x$  is greater than the greatest zero of  $S_{k-1}$ .

We note that  $x$  greater than the greatest zero of  $S_{k-1}$  if and only if  $\theta < \pi/k$ . Then since  $j \leq k$  and  $\theta < \pi/k$ , we again have that  $j\theta < \pi$  and  $(j-1)\theta < \pi$ , and therefore that

$$\frac{d}{dj} \left( \ln \frac{S_{j-1}}{S_{j-2}} \right) = \theta [\cot j\theta - \cot(j-1)\theta] < 0$$

as above, and for integral values of  $j$  the lemma then follows in the same fashion for this case as well.

### 5. THEOREM

The theorem consists of three parts:

(A) A necessary and sufficient condition that initial conditions exist for three hard rods of arbitrary masses moving on a line to undergo  $n$  collisions with  $n > 3$  is that  $x$  be greater than the largest zero of  $S_{n-2}(x)$ , that is,<sup>3</sup>

$$\frac{2}{m_2} (\mu_{12}\mu_{23})^{1/2} > 2 \cos \frac{\pi}{n-1}$$

or

$$m_2 < \frac{(\mu_{12}\mu_{23})^{1/2}}{\cos[\pi/(n-1)]}$$

Initial conditions always exist for which the rods undergo three collisions.

(B) Assuming that, according to (A),  $n$  collisions are possible but  $n + 1$  collisions are not possible, the initial conditions mentioned in (A) are given by the following:  $k$  collisions will occur,  $1 < k \leq n$ , if and only if

$$v_{23}^{(0)} > -\frac{S_{k-1}}{S_{k-2}} \left( \frac{\mu_{12}}{\mu_{23}} \right)^{1/2} v_{12}^{(0)}$$

<sup>3</sup> Gal'perin<sup>(9)</sup> quotes Zemljakov<sup>(10)</sup> as giving this formula as an upper bound for point particles.



(C) After the  $j$ th collision the relative velocities  $v_{i,i+1}^{(j)}$  are given by

$$\begin{aligned}
 v_{12}^{(j)} &= -S_{j-1}v_{12}^{(0)} - S_{j-2} \left( \frac{\mu_{23}}{\mu_{12}} \right)^{1/2} v_{23}^{(0)} \\
 v_{23}^{(j)} &= S_{j-1}v_{23}^{(0)} + S_j \left( \frac{\mu_{12}}{\mu_{23}} \right)^{1/2} v_{12}^{(0)}
 \end{aligned}
 \tag{4}$$

when  $j$  is odd, except that  $v_{12}^{(1)} = -S_0v_{12}^{(0)}$ ; and by

$$\begin{aligned}
 v_{12}^{(j)} &= S_jv_{12}^{(0)} + S_{j-1} \left( \frac{\mu_{23}}{\mu_{12}} \right)^{1/2} v_{23}^{(0)} \\
 v_{23}^{(j)} &= -S_{j-2}v_{23}^{(0)} - S_{j-1} \left( \frac{\mu_{12}}{\mu_{23}} \right)^{1/2} v_{12}^{(0)}
 \end{aligned}
 \tag{5}$$

when  $j$  is even.

*Proof.* The proof is by induction. The theorem is first proved for  $j=1$  and  $j=2$ . Then the theorem follows [part (i) below] for each odd  $j'$  from (5), which is assumed to hold for the even value  $j=j'-1$ , and [part (ii) below] for each even  $j'$  from (4), which is assumed to hold for the odd value  $j=j'-1$ . Note that whenever we give a proof for a particular  $k$  that (B) holds, we have proved that the condition in (A) is a sufficient condition, that is, that initial conditions exist for  $k$  collisions to occur. In following the proof, it is useful to keep in mind that odd-numbered collisions are between particles 1 and 2 and that even-numbered collisions are between particles 2 and 3.

For  $j=1$ , we need prove only (C), as (B) and (A) are not relevant here. After the first collision, (2) gives  $v_{12}^{(1)} = -v_{12}^{(0)} = -S_0(x)v_{12}^{(0)}$  and

$$v_{23}^{(1)} = v_{23}^{(0)} + x \left( \frac{\mu_{12}}{\mu_{23}} \right)^{1/2} v_{12}^{(0)} = S_0(x)v_{23}^{(0)} + S_1(x) \left( \frac{\mu_{12}}{\mu_{23}} \right)^{1/2} v_{12}^{(0)}$$

which proves (4) in (C) for  $j=1$ .

We next prove the theorem for  $j=2$ . The necessary and sufficient condition for the second collision is that particles 2 and 3 be approaching one another, i.e.,  $v_{23}^{(1)} > 0$  or  $S_0(x)v_{23}^{(0)} > -S_1(x)(\mu_{12}/\mu_{23})^{1/2}v_{12}^{(0)}$ , which proves (B) and therefore (A) for this case.<sup>4</sup>

<sup>4</sup> Note for later comparison with the case of general  $j$  that since  $S_0 > 0$  and  $S_1 > 0$ , in this case  $v_{23}^{(0)}$  may be  $< 0$ .

We now assume that the second collision has occurred and proceed to prove (C) for this case. After the second collision, (3) gives

$$v_{12}^{(2)} = (xS_1 - S_0)v_{12}^{(0)} + S_1 \left( \frac{\mu_{23}}{\mu_{12}} \right)^{1/2} v_{23}^{(0)} = S_2 v_{12}^{(0)} + S_1 \left( \frac{\mu_{23}}{\mu_{12}} \right)^{1/2} v_{23}^{(0)}$$

$$v_{23}^{(2)} = -S_0 v_{23}^{(0)} - S_1 \left( \frac{\mu_{12}}{\mu_{23}} \right)^{1/2} v_{12}^{(0)}$$

which proves (5) in (C) for  $j = 2$ .<sup>5</sup>

(i) We now prove the theorem for all odd  $(j + 1)$ . Suppose that it has been proven for a given even value of  $j$  that  $j$  collisions have occurred and that (5) in (C) holds. In order to first prove that the condition in (A) is necessary, and then prove (B) [and therefore that the condition in (A) is sufficient], we consider separately the two possibilities: (a)  $x$  is less than the greatest zero of  $S_{j-1}$  ( $j > 2$  necessarily); (b)  $x$  is greater than the greatest zero of  $S_{j-1}$ .

(a) Suppose first that  $x$  is less than the greatest zero of  $S_{j-1}$ . Then by Lemma I,  $S_{j-1} < 0$  and  $S_j < 0$ , since, as will be shown below in (ii), the  $j$ th collision could have occurred only if  $x$  is greater than the greatest zero of  $S_{j-2}$ . We will also show below in (ii) that for  $S_{j-1} < 0$ , the  $j$ th collision could have occurred only if  $v_{23}^{(0)} > 0$ . But then the condition that particles 1 and 2 be approaching one another, i.e.,  $v_{12}^{(j)} > 0$ , cannot be satisfied [both terms in  $v_{12}^{(j)}$  in (5) are negative] and the  $(j + 1)$ st collision cannot occur, proving (A) for this case.

(b) Suppose instead that  $x$  is greater than the greatest zero of  $S_{j-1}$ , so that  $S_{j-1} > 0$ . Then the necessary and sufficient condition for the  $(j + 1)$ st collision, that particles 1 and 2 be approaching one another, i.e.,  $v_{12}^{(j)} > 0$  or, by (5),  $S_{j-1} v_{23}^{(0)} > -S_j (\mu_{12}/\mu_{23})^{1/2} v_{12}^{(0)}$ , can be satisfied. To prove (B) for this case, we then need only divide the last inequality by  $S_{j-1}$  and invoke Lemma II, which proves that if  $v_{23}^{(0)}$  is great enough to satisfy the condition that the  $(j + 1)$ st collision occur, it also is great enough to satisfy the condition that all previous collisions occurred.

Before we proceed to prove (C), in order to establish a condition needed for part (ii) of the proof (below), we now suppose that while  $x$  is greater than the greatest zero of  $S_{j-1}$ , it is less than the greatest zero of  $S_j$ , so that  $S_j < 0$  by Lemma I. Since  $S_j/S_{j-1} < 0$ , the condition  $v_{12}^{(j)} > 0$  can be satisfied only if  $v_{23}^{(0)} > 0$ , the requirement we will use below in (ii).

(c) We now prove (C) for  $v_{i,i+1}^{(j+1)}$  for the case that the  $(j + 1)$ st colli-

<sup>5</sup> Note for later comparison with the case of general  $j$  that in this case  $S_1 > 0$ .

sion occurs. After the  $(j + 1)$ st collision, (2) applied to (5) immediately yields (4) for  $v_{12}^{(j+1)}$ ; for  $v_{23}^{(j+1)}$  if yields

$$v_{23}^{(j+1)} = (xS_{j-1} - S_{j-2})v_{23}^{(0)} + (xS_j - S_{j-1})\left(\frac{\mu_{12}}{\mu_{23}}\right)^{1/2} v_{12}^{(0)}$$

which in turn, by the recursion relation for the Chebyshev polynomials, yields (4) for  $v_{23}^{(j+1)}$ .

(ii) We now prove the theorem for all even  $(j - 1)$  with  $j > 1$ . Suppose that it has been proven for a given odd value of  $j$  that  $j$  collisions have occurred and that (4) in (C) holds. In order to first prove that the condition in (A) is necessary, and then prove (B) [and therefore that the condition in (A) is sufficient], we consider separately the two possibilities: (a)  $x$  is less than the greatest zero of  $S_{j-1}$ ; (b)  $x$  is greater than the greatest zero of  $S_{j-1}$ .

(a) Suppose first that  $x$  is less than the greatest zero of  $S_{j-1}$ . Then by Lemma I,  $S_{j-1} < 0$  and  $S_j < 0$ , since, as we have shown above in (i), the  $j$ th collision could have occurred only if  $x$  is greater than the greatest zero of  $S_{j-2}$ . We have also shown above in (i) that for  $S_{j-1} < 0$ , the  $j$ th collision could have occurred only if  $v_{23}^{(0)} > 0$ . But then the condition that particles 2 and 3 be approaching one another, i.e.,  $v_{23}^{(j)} > 0$ , cannot be satisfied [both terms in  $v_{23}^{(j)}$  in (4) are negative] and the  $(j + 1)$ st collision cannot occur, proving (A) for this case.

(b) Suppose instead that  $x$  is greater than the greatest zero of  $S_{j-1}$ , so that  $S_{j-1} > 0$ . Then the necessary and sufficient condition for the  $(j + 1)$ st collision, that particles 2 and 3 be approaching one another, i.e.,  $v_{23}^{(j)} > 0$  or, by (4),  $S_{j-1}v_{23}^{(0)} > -S_j(\mu_{12}/\mu_{23})^{1/2} v_{12}^{(0)}$ , can be satisfied. To prove (B) for this case, we then need only divide the last inequality by  $S_{j-1}$  and invoke Lemma II, which proves that if  $v_{23}^{(0)}$  is great enough to satisfy the condition that the  $(j + 1)$ st collision occur, it also is great enough to satisfy the condition that all previous collisions occurred.

Before we proceed to prove (C), in order to establish the condition needed for part (i) of the proof (above), we now suppose that while  $x$  is greater than the greatest zero of  $S_{j-1}$ , it is less than the greatest zero of  $S_j$  so that  $S_j < 0$  by Lemma I. Since  $S_j/S_{j-1} < 0$ , the condition  $v_{23}^{(j)} > 0$  can be satisfied only if  $v_{23}^{(0)} > 0$ , the requirement used above in (i).

(c) We now prove (C) for  $v_{i,i+1}^{(j+1)}$  for the case that the  $(j + 1)$ st collision occurs. After the  $(j + 1)$ st collision, (3) applied to (4) immediately yields (5) for  $v_{23}^{(j+1)}$ ; for  $v_{12}^{(j+1)}$  it yields

$$v_{12}^{(j+1)} = (xS_j - S_{j-1})v_{12}^{(0)} + (xS_{j-1} - S_{j-2})\left(\frac{\mu_{23}}{\mu_{12}}\right)^{1/2} v_{23}^{(0)}$$

which in turn, by the recursion relation for the Chebyshev polynomials, yields (5) for  $v_{12}^{(j+1)}$ , completing the proof.

**Corollary.** If  $v_{23}^{(0)} = 0$ , the number of collisions which will occur among three particles is one fewer than the maximum number permitted by their masses.

*Proof.* If  $(j+1)$  is the largest number of collisions permitted by part (A) of the theorem, then by (A),  $x$  is greater than the greatest zero of  $S_{j-1}$  but less than the greatest zero of  $S_j$ . Then by Lemma I,  $S_{j-1} > 0$  and  $S_{j-2} > 0$ , but  $S_j < 0$ . It follows that  $\{-S_{j-1}/S_{j-2}\} < 0$  but  $\{-S_j/S_{j-1}\} > 0$ , and for  $v_{23}^{(0)} = 0$  the condition given by part (B) of the theorem is satisfied for  $j$  collisions to occur but not for  $(j+1)$  collisions to occur.

## 6. DISCUSSION

We now make several remarks concerning our results.

1. The appearance of the Chebyshev polynomials in our calculations introduces an angle  $\theta$  into the problem. It becomes natural, therefore, to characterize a system of three particles by a complex mass  $\mathbf{m}$  which has magnitude  $m_2$ , lies in the first quadrant of the complex plane, and whose real part equals  $(\mu_{12}\mu_{23})^{1/2}$ , the geometric mean of the reduced masses of the particle pairs. The phase of this complex mass is then the angle  $\theta \equiv \arccos(x/2)$  we used above, and the maximum number of collisions possible is the largest integer  $n$  such that  $n < \pi/\theta + 1$  (see Fig. 1). It is not clear that this complex mass has any particular physical meaning, but it may prove useful in calculations involving four or more particles.

2. We note that our theorem gives the expected result for some special cases: (i) if the central particle is heavier than either outer particle,  $x < 1$ ,  $\theta > \pi/3$ , and only three collisions can occur; (ii) if all three masses are equal,  $x = 1$ ,  $\theta = \pi/3$ , and only three collisions can occur; and (iii) as the mass of the central particle approaches zero with the masses of the outer particles remaining constant,  $x \rightarrow 2$ ,  $\theta \rightarrow 0$ , and the number of collisions which can occur increases indefinitely.

3. As a concrete example, we consider the case represented by the arrow in Fig. 1. If the masses of the outer particles are equal, and the mass of the central particle is  $3/5$  that of an outer particle, then  $x = 5/4$ ,  $S_0 = 1$ ,  $S_1 = 5/4$ ,  $S_2 = 9/16$ , and  $S_3 = -35/64$ . By part (A) of the theorem, four collisions can occur, but five cannot. By part (B) of the theorem, exactly four collisions will occur if and only if  $v_{23}^{(0)}/v_{12}^{(0)} > 35/36$ .

4. The contribution of a given collision sequence to nonequilibrium properties of a gas mixture (such as transport coefficients) depends on,

among other things, the volume of phase space occupied by the set of initial conditions which lead to that sequence.<sup>(2)</sup> When part (A) of our theorem allows at most  $n$  collisions to occur, part (B) of the theorem provides the ratio of the phase space volume of initial conditions which leads to exactly  $j$  collisions to the volume which leads to exactly  $k$  collisions, where  $2 \leq j < n$  and  $2 \leq k < n$ ; namely, the ratio

$$\frac{\{-S_j/S_{j-1}\} - \{-S_{j-1}/S_{j-2}\}}{\{-S_k/S_{k-1}\} - \{-S_{k-1}/S_{k-2}\}}$$

This stems from the fact that the initial positions and the velocity of the center of mass are irrelevant to the number of collisions which occur, and that the time scale is also arbitrary, so that knowledge of the ratio  $v_{23}^{(0)}/v_{12}^{(0)}$  suffices to determine the number of collisions which occur. In the concrete example cited in 3 above and represented by the arrow in Fig. 1, the ratio of the phase-space volume leading to exactly three collisions to that leading to exactly two collisions is 16/9.

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