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Computer Study of Ergodicity and Mixing in a Two-Particle, Hard Point Gas System

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Computer experiments performed on the unequal-mass, two-particle hard point gas are discussed and shown to provide evidence for ergodic and mixing behavior when the two-particle mass ratio (m_2/m_1) in $\cos\theta = [1 - (m_2/m_1)]/[1 + (m_2/m_1)]$ is such that θ is an irrational multiple of π. Although this system appears to be ergodic and mixing, it is certainly not a C-system.

1. INTRODUCTION

In view of Sinai's proof [1] of ergodicity and mixing in the two-dimensional hard disc gas and in the three-dimensional hard sphere gas, it is worthwhile to inquire if ergodicity and mixing may not also occur in an even simpler one-dimensional hard point gas. Now, such is certainly not the case when the hard point gas has equal mass particles. This latter system is known to be integrable [2] (and hence, not ergodic and mixing) since it possesses analytic constants of the motion Φ which are in involution [2] of the type

$$\Phi_n = \sum_{k=1}^{N} P_k^{2n}, \tag{1}$$

where $n = 1, 2,..., N$, where N is the number of gas particles, and where P_k is the momentum of the kth particle. Indeed, a complete analytic solution for this equal mass case has recently been provided by Hobson and Cheng [3]. However, the question of ergodicity and mixing for a hard point gas having unequal masses remains open. Even the simplest unequal mass case having only two moving point particles is not completely decided, as has been recently emphasized by Lebowitz, [4] and it is on this simplest case that we focus our attention in this paper. In particular, we describe the results of an empirical computer study of the motion for two unequal mass points confined to move inside a one-dimensional box.

2. Mathematical Preliminaries

We first prove that this two-particle system is certainly not ergodic and mixing for every mass ratio. Let the left particle have mass m_1 and the right particle mass m_2. After a two-particle collision, the velocities v_1' and v_2' of particles one and two, respectively, are given by the matrix equation

$$v' = \begin{pmatrix} v_1' \\ v_2' \end{pmatrix} = \begin{pmatrix} \delta & (1-\delta) \\ (1+\delta) & -\delta \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = Bv, \tag{2}$$

where $\delta = (m_1 - m_2)/(m_1 + m_2)$, and v_1 and v_2 are the particle velocities before collision. Equally, a left wall collision by particle one may be written

$$v' = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = Lv, \tag{3}$$

while a right wall collision by particle two may be written

$$v' = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = Rv. \tag{4}$$

It is now convenient to introduce a change in the velocity variables given by $w_1 = v_1 \cos(\theta/2)$ and $w_2 = v_2 \sin(\theta/2)$, where $\delta = \cos\theta$. In terms of the new velocity variables, Eq. (2) may be written

$$w' = \begin{pmatrix} \cos\theta & \sin\theta \\ \sin\theta & -\cos\theta \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = Cw, \tag{5}$$

while Eqs. (3) and (4) become $w' = Lw$, and $w' = Rw$, since the reflection matrices L and R are invariant under this velocity transformation. Moreover, the matrices C, L, and R all preserve the quadratic relationship

$$[(w_1')^2 + (w_2')^2] = (w_1^2 + w_2^2). \tag{6}$$

As a consequence, the sequence of velocity-pairs (w_1, w_2) that occurs along any specified system trajectory must lie on a circle in the (w_1, w_2)-plane. Thus, this system can retain the possibility of being ergodic and mixing only if the set of distinct velocity-pairs (w_1, w_2) occurring along almost every trajectory is countably infinite and densely fills the associated velocity circle. However, as we now show when the mass ratio (m_2/m_1) yields a value of θ that is a rational multiple of π, only a finite number of distinct velocity-pairs (w_1, w_2) can occur along each trajectory, thus, precluding ergodicity and mixing for at least a dense, but countable set of mass ratios (m_2/m_1).

Consider now any finite sequence of velocity-pairs that occurs along an arbitrarily chosen trajectory, and let (w_{10}, w_{20}) be the initial velocity-pair on the chosen trajectory. Then, the specified velocity sequence may always be written as the matrix product

$$CRCL \cdots RCLR \begin{pmatrix} w_{10} \\ w_{20} \end{pmatrix}, \tag{7}$$

where successive velocity-pairs are obtained by sequential matrix operations. By noting that $L = -R$ and that $L^2 = R^2 = C^2 = I$, where I is the unit matrix, one may always reduce any finite velocity sequence such as sequence (7) to one of the forms $\pm(CR)^k$, $\pm(RC)^k$, $\pm(CR)^k R$, or $\pm(RC)^k R$, where k is zero or some positive integer. Thus, since (CR) merely rotates the velocity vectory through the angle θ, while (RC) merely performs the inverse rotation, the final velocity-pair (w_{1f}, w_{2f}) of any finite velocity sequence is obtained from (w_{10}, w_{20}) by rotating (w_{10}, w_{20}) through the angle $\pm(k\theta)$ or by first reflecting it and then rotating it through $\pm(k\theta)$. Obviously, then, when θ is a rational multiple of π, as is the case for a denumerable set of mass ratios, only a finite number of distinct velocity-pairs can occur [5] along every trajectory. In particular if $\theta = (m\pi/n)$, where m and n are integers with $m < n$, there are at most $4n$ distinct velocity-pairs allowed; while if $\theta = m\pi/n$ with m and n having no common divisor, there are precisely $4n$ distinct velocity-pairs allowed.

On the other hand, when θ is an irrational multiple of π, as occurs for mass ratios forming a dense set of positive measure, the allowed velocity-pairs become uniformly dense [5] on the velocity circle. As a consequence, it is at least possible for the two-particle hard point gas having "irrational" θ to be ergodic in velocity space. In the next section, we present computer generated evidence that indicates that this type ergodic behavior actually occurs, and, in Section IV, we present evidence supporting ergodicity over the full phase space (actually over the energy hypersurface) for this system in the form of Poincaré surfaces of section [6]. These Poincaré surfaces of section are two-dimensional planes chosen to intersect the three-dimensional energy "volume." An ergodic trajectory for this system, if it exists, would be expected to intersect a surface of section plane at a set of uniformly dense points covering the allowed region of this plane. The computer generated evidence indicates that this is indeed the case for irrational θ. Finally, we integrate a set of initially close trajectories for this system and demonstrate that the initial phase space points spread in time, rather uniformly covering the allowed phase space region. Thus, the hard point gas is apparently mixing [7] as well as ergodic when θ is irrational.

In summary, the evidence to be presented here indicates that the unequal-mass, hard point gas can, under suitable restrictions, exhibit ergodicity and mixing just as do its more sophisticated hard disc and hard sphere cousins. Nonetheless, in contrast to these more sophisticated systems, the hard point gas is not a C-system [8] because for it, initially close trajectories do not, as we show in the following, separate exponentially with time. This lack of C-system behavior probably means [9] that the hard point gas will prove of greater interest to mathematicians than to physicists.

3. Presentation of Computer Results

For the two-particle, hard point gas, a mass ratio (m_2/m_1) yielding an irrational θ-value at least allows the possibility for most trajectories to possess countable infinite dense sets of distinct velocity-pairs that uniformly cover their associated velocity circles. By consequence, a proof for this type of ergodicity is thus reduced to showing that the allowed velocity-pairs actually occur. Clearly, the finite arithmetic of a computer precludes the calculation of a dense set of velocity-pairs; however, a computer can establish whether or not each member of the finite set of $4n$ velocity-pairs allowed by a "rational" θ-value ($\theta = m\pi/n$ with m and n integers having no common divisor) is in fact observed to occur. Thus, a computer can provide evidence supporting ergodic behavior for irrational θ by demonstrating that an increasing number $4n$ of allowed velocities is actually observed for a sequence of rational θ approaching the irrational θ-value.

In our computer experiments, rather than approaching an irrational θ-value via a sequence of rationals, we chose to investigate (among others) the sequence of θ-values given by $\theta = 2\pi/n$ for $n = 5, 7, 11, 15, 17, 23, 25, 33, 41$, or 67, and the sequence of θ-values given by $\theta = (n-1)\pi/2n$ for the same n-values. For each of these θ-values, all $4n$ of the allowed velocity-pairs were indeed observed to occur, thus indicating that irrational θ-values would yield ergodic behavior on the associated velocity circle. The only surprise in these calculations, to us at least, was the rather large total number of collisions (including both wall and particle–particle collisions) required to observe all $4n$ velocity-pairs. Indeed, initially we believed that some unsuspected constant of the motion was preventing the occurrence of all $4n$ velocity-pairs. However, we soon realized that the matrix properties $C^2 = L^2 = R^2 = I$ yield a type of oscillatory behavior in the velocity-pair sequences and that, as a consequence, the k in $\pm(CR)^k$, for example, increases very slowly.

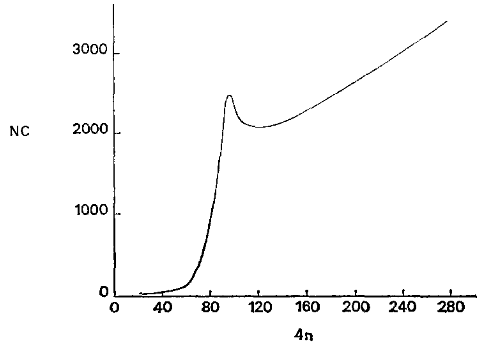

FIG. 1. A plot of the total collision number NC versus the number of allowed velocity-pairs $4n$. NC is the total number of collisions required to observe all 4n allowed velocity-pairs. The curve in this figure is highly sensitive to initial conditions.

An indication of this problem is pictured in Fig. 1, where we graph a curve of total collision number NC required to observe all $4n$ velocity-pairs versus the allowed velocity number $4n$. The data for Fig. 1 were gathered using the same position-velocity initial conditions $(x_{10}, x_{20}, w_{10}, w_{20})$ to generate a single system trajectory for each θ-value in the $\theta = 2\pi/n$ sequence. The curve shown in Fig. 1 changes its shape dramatically upon varying the initial state $(x_{10}, x_{20}, w_{10}, w_{20})$. By varying the initial state for fixed θ, we found that the collision number NC varies from its minimum of $4n$ to greater than 500,000, our longest run. Now, it is straightforward to show that at least a few periodic trajectories exist (for any θ) along which not all allowed velocity-pairs actually occur; clearly, for these trajectories NC is infinity. The surprise to us was the relative paucity of trajectories yielding an NC-value very near the minimum of $4n$. Before closing this paragraph, it is perhaps worth noting that replacing (w_{10}, w_{20}) by $(\lambda w_{10}, \lambda w_{20})$ for λ real and positive scales all subsequent velocity-pairs by the factor λ and changes the collision rate, but does not alter the collision sequence; consequently there is, in effect, only one energy surface for each θ-value.

To provide supporting evidence for ergodicity on the full energy surface, we computed a surface of section plot for each rational θ-value listed in the preceding paragraph. In Fig. 2, we present a typical case, that for $\theta = 2\pi/11$. The points in Fig. 2 were obtained by numerically integrating a single trajectory and plotting the set of position-velocity points (x_1, w_1) of particle one for which particle two was instantaneously at the right wall $(x_2 = 10)$ with positive velocity $(w_2 \geqslant 0)$. In all our calculations, the left wall lay at $x = 0$ and the right wall at $x = 10$. For the sake of graphical clarity in Fig. 2, we chose to plot only the upper half plane of (x_1, w_1)-points for which $w_1 \geqslant 0$ and $10 \geqslant x_1 \geqslant 0$; the lower half plane is, of course, merely the mirror image of the upper. In Fig. 2, we note that the

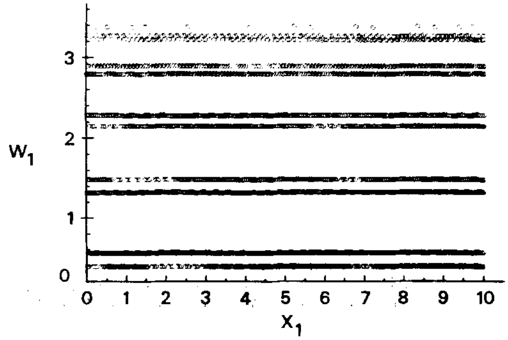

FIG. 2. A surface of section for $\theta = 2\pi/11$ after 14,000 collisions along a single trajectory. Only the upper half plane is shown.

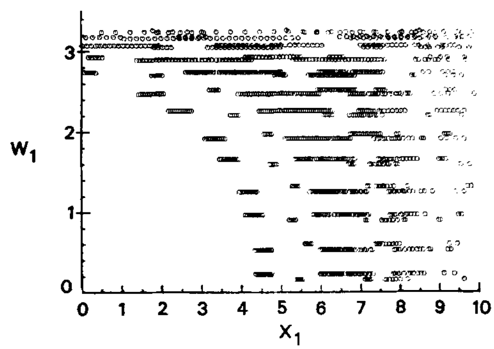

FIG. 3. A surface of section for $\theta = 2\pi/27$ after about 7000 collisions along a single trajectory.

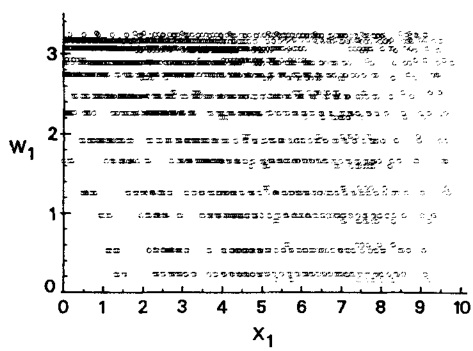

FIG. 4. A surface of section for $\theta = 2\pi/27$ after about 32,000 collisions along the same trajectory as used for Fig. 3. A trend toward uniformity is apparent.

observed points rather uniformly cover the 11 velocity lines allowed by $\theta = 2\pi/11$, $w_1 \geqslant 0$, and $w_2 \geqslant 0$. Approximately 14,000 collisions (wall plus particle–particle) were required to obtain this rather uniform distribution; however, again for clarity, not all the computed (x_1, w_1)-points were graphed.

In Fig. 3, we graph a surface of section for $\theta = 2\pi/27$ obtained by integrating a single trajectory for only about 7000 collisions while Fig. 4 shows the same surface of section obtained by integrating the given trajectory for 32,000 collisions. Even after 32,000 collisions, the distribution of (x_1, w_1)-points is not completely uniform over the 27 allowed velocity lines, although a comparison of Figs. 3 and 4 indicates that uniformity is being approached. Figures 2–4 are typical of the results obtained for all the rational θ-values studied; these results support the view that irrational θ-values yield ergodic behavior over the full energy surface.

Figure 5 presents a full surface of section ($w_1 \gtrless 0$) showing the mixing behavior observed for a $\theta = 2\pi/11$ system. Initially, 110 points in the (x_1, w_1)-plane were selected as initial points for generating 110 trajectories. These initial (x_1, w_1)-points were spaced uniformly between $x_1 = 5$ and $x_1 = 9$ on the uppermost velocity line for which $w_1 = 1.353$. In Fig. 5, we show the locations of these 110 points after about 70,000 collisions along each trajectory; the initial points

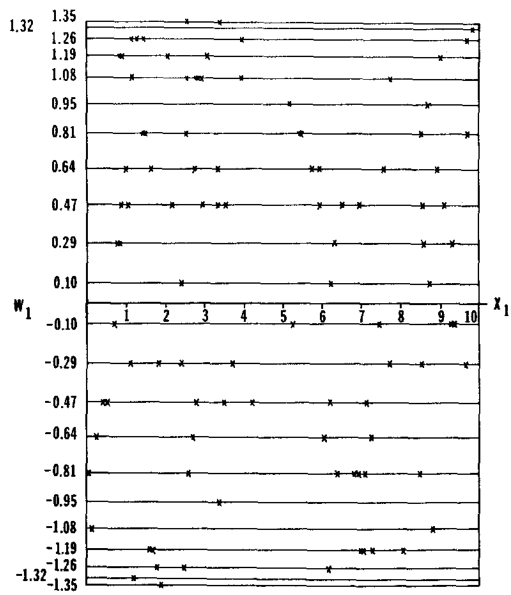

FIG. 5. A full surface of section for $\theta = 2\pi/11$ showing mixing behavior for a set of 110 initially close trajectories. Each trajectory was initiated with the same (w_1, w_2) velocity-pair. In this figure, only the distribution of the 110 points at the end of about 70,000 collisions for each trajectory is shown.

have scattered over all 22 allowed velocity lines. Were the mixing perfectly uniform, Fig. 5 would show five points evenly spread over each velocity line. This is not the case in Fig. 5, primarily because of expected statistical fluctuations from perfect uniformity; however, in addition here, about 10 of the 110 final points are unseparated in horizontal position, at least to the graphical accuracy used. This occurs because all 110 initial points for Fig. 5 had the same velocity w_1 (and, therefore, the same w_2 also). In this situation, the associated trajectories do not initially separate with time. Indeed, the points approximately maintain their initial closely spaced configuration until the velocity sequences along the various trajectories become different; in Fig. 5, even after 70,000 collisions, about 10 of the initial points have very nearly maintained their initial separation from a closest neighbor. Nonetheless, Fig. 5 indicates that mixing does slowly occur on the specified, two-dimensional invariant integral surface. To illustrate the more rapid mixing, which occurs when the initial velocities are not all equal, Fig. 6 presents a full surface of section for $\theta = 2\pi/11$ using 400 initial points uniformly spread over an initial rectangle in the surface of section plane. The positions of these points initially lay between $x_1 = 5$ and $x_1 = 6$, while the velocities w_1 of the points lay between $w_1 = 1.25$ and $w_1 = 1.35$. Figure 6 shows the distribution of these points after about 12,000 collisions. One notes here, as expected,

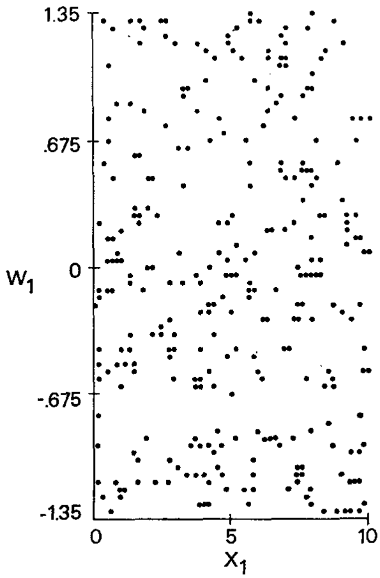

FIG. 6. A full surface of section for $\theta = 2\pi/11$ showing the mixing behavior when not all initially close trajectories have the same initial (w_1, w_2) velocity-pair. The distribution of points at the end of about 12,000 collisions (for each trajectory) is shown for a set of 400 trajectories.

that a somewhat uniform distribution has been achieved much quicker than for Fig. 5. Only about 300 points appear in Fig. 6 with the remaining 100 points being unresolved from some close neighbor. Initially, 20 points were uniformly distributed along 20 velocity lines in the initial rectangle; the 100 unresolved points are all close to some neighbor having the same initial velocity. Figure 6 is a computer generated typewriter plot; a more precise plot might move each point slightly, but would not alter the figure significantly. As a further test of mixing, we integrated 36 trajectories (using $\theta = 2\pi/27$) that were initially very close together on the energy surface, and then we plotted the positions of the time evolved points in (x_1, x_2)-space and separately, on the velocity circle. Figures 7 and 8 show the

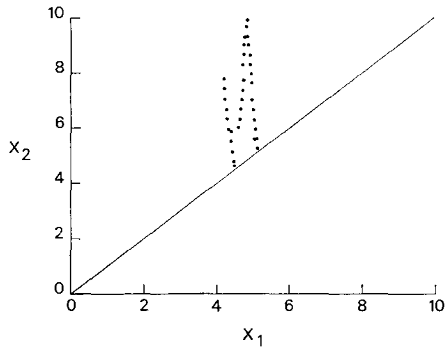

FIG. 7. A graph of the position points (x_1, x_2) for 36 initially close trajectories after 60 collisions. Here $\theta = 2\pi/27$.

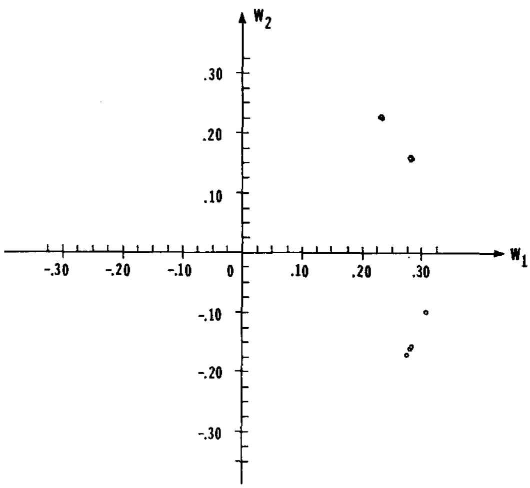

FIG. 8. A graph of the velocity points (w_1, w_2) for 36 initially close trajectories after 60 collisions. Here $\theta = 2\pi/27$.

distribution of the 36 points after about 60 collisions while Figs. 9 and 10 show a somewhat uniform distribution after about 60,000 collisions. In Figs. 7 and 9, the 36 points always lie above the line $x_1 = x_2$ since the hard points cannot pass through each other. In Figs. 8 and 10, since here, $\theta = 2\pi/27$ for 36 distinct initial velocity-pairs, there are $4 \times 27 \times 36 = 3888$ distinct, allowed final velocity-pairs. Figures 5–10, which are typical of many such calculations we have made, certainly make it highly plausible that the hard point gas is mixing as well as ergodic when θ is an irrational multiple of π.

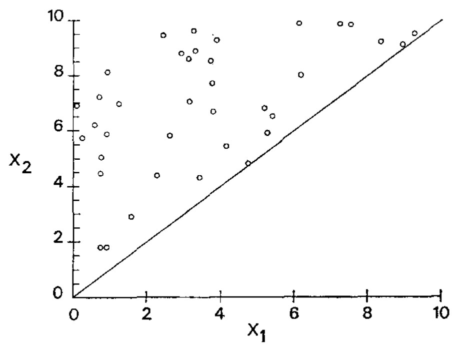

FIG. 9. A graph of the 36 position points (x_1, x_2) shown in Fig. 7 after about 60,000 collisions.

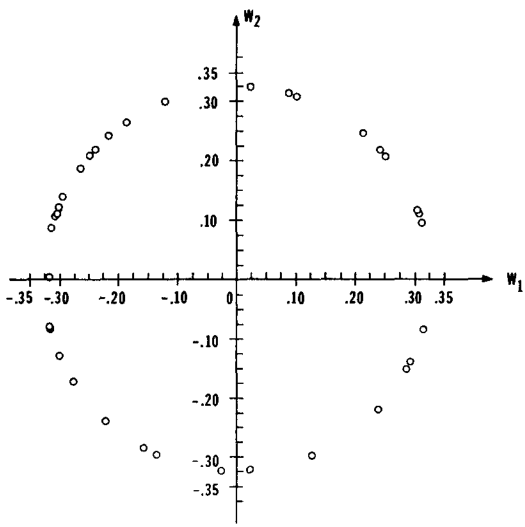

FIG. 10. A graph of the 36 velocity points (w_1, w_2) shown in Fig. 8 after about 60,000 collisions.

Finally, in Fig. 11, we show computer verification of a linear, rather than an exponential, growth of separation distance between the members of an initially close trajectory-pair. The two trajectories were initiated at the same positions $(x_1', x_2') = (x_1, x_2)$, but at distinct velocities $(w_1', w_2') \neq (w_2, w_2)$. Thus, D_x, the distance between the two trajectories in position space is initially zero; D_w, the distance between the trajectories in velocity space, was initially chosen to be 10^{-6} velocity units. Now, since the matrices L, R, and C each leave the quadratic form $(dw_1^2 + dw_2^2)$ invariant, where dw_1 and dw_2 are differentials of w_1 and w_2,

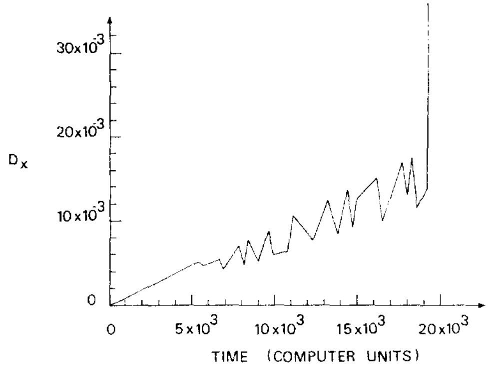

FIG. 11. A plot of $D_x(t)$, the position space distance between an initially close trajectory-pair, versus time (in arbitrary units). Here one notes, as expected, that $D_x(t)$ shows a short-term linear growth with time.

D_w does not change with time as long as the velocity sequence along each trajectory is the same, except for brief spikes away from 10^{-6}, quickly followed by a return, during the time interval when one trajectory has undergone m collisions while the other has undergone only $(m - 1)$. Because $D_w(t)$ thus is essentially a constant for a considerable period, the growth in distance between trajectories is due almost solely to the growth of $D_x(t)$. As a consequence, in Fig. 11, we chose to graph $D_x(t)$ versus time. In this figure, as long as the collision sequence is the same for both trajectories, one expects $D_x(t) \approx \alpha t$, where α is some constant, since $D_w(t) \approx 10^{-6}$. Indeed, this is precisely what is observed in Fig. 11 from $t \cong 0$ to $t \cong 5{,}000$ (approximately 600 collisions). At $t \cong 5000$, the spikes in the velocity distance $D_w(t)$ become broad enough to cause the increasing oscillation in $D_x(t)$ seen from $t \cong 5000$ to $t \cong 19{,}000$ (approximately 2200 collisions). Nonetheless, the average growth in $D_x(t)$ remains linear. At $t \cong 19{,}000$, however, there is a large jump in $D_w(t)$ (with no return) and consequently a very rapid rise in $D_x(t)$. We have verified that this behavior at $t = 19{,}000$ occurs because the collision sequences along the two trajectories first become different at that instant.

4. Discussion of Results

In this paper, we have presented various types of computer evidence indicating that the two-particle hard point gas is, under suitable circumstances, ergodic and mixing. However, we have seen that this system is ergodic and mixing or not as θ is an irrational multiple of π or not. Thus, one naturally asks how a computer can decide such a delicate issue using only the arithmetic of finite rational numbers. Here, we have attempted to circumvent this problem by investigating sequences of rational θ that indicate the results to be expected for irrational θ.

For rational θ, we know quite rigorously that only a finite number of velocity-pairs are allowed to occur. For the calculations resulting in Fig. 1, we thus need only be accurate enough to ensure that none of the rigorously allowed velocity-pairs that were observed in the integration process appeared due to computational error. For the more detailed calculations of Figs. 2–6, we need only sufficient accuracy to ensure that the relatively uniform covering of the allowed velocity lines is not due to computational error. To ensure that our computations were indeed accurate enough to meet these requirements, we reversed particle velocities at the end of several long trajectory integrations (about 500,000 collisions) and, in each case, regained the initial state to at least six- or seven-digit accuracy. In addition, Fig. 11 shows that an initial trajectory "error" of 10^{-6} grows linearly to approximately 10^{-2} during about 10^3 collisions. All our calculations were performed on a UNIVAC 1108 using 16-digit double precision arithmetic. Thus, if one grossly overestimates our initial error at 10^{-14}, the final error in a trajectory integration involving 500,000 collisions would be no more than about 10^{-7}. Finally, then, in regard to the distinction between rational and irrational θ, a noticeable difference (greater than 10^{-7}, say) between the trajectories of extremely close (less than 10^{-14}, say) rational and irrational θ-values would appear only after 500,000 collisions. It is thus quite clear that Figs. 1–11, which use at most three-digit accuracy and involve at most 100,000 collisions, would be strictly unchanged had we performed our integrations using infinite mathematical precision for irrational θ-values differing infinitesimally from the rational values quoted in these figures.

Nonetheless, even though accurate in themselves, the computer results presented here certainly do not constitute a mathematical proof of ergodicity and mixing. Our results provide, at best, strong evidence in support of these properties and, pending the discovery of a rigorous proof, the creditability of our evidence must be determined by each reader. Should this system indeed prove to be mixing, it is quite interesting to note that this mixing results from a linear rather than an exponential separation of initially close trajectory-pairs. Moreover, for this system, mixing would arise from two sources. First, there is the short-term linear separation of trajectories shown in Fig. 11, and second, there is a long-term "linear" separation of trajectories due to differing collision sequences for initially close trajectories. Indeed, in Fig. 5, where all initial velocities are the same, there is no short-term linear separation and mixing results solely from differing collision sequences. This system is thus mathematically quite interesting; however, since exponential separation (C-system behavior) is expected [9] for physically realistic systems, the hard point gas would not appear to possess as much appeal to physicists as to mathematicians.

As a concluding note, let us mention that for most initial conditions, the time averaged, single particle kinetic energies approached equipartition of energy independent of mass ratio. In particular, equipartition was observed even for the integrable, equal-mass, hard point gas. Thus, equipartition of energy is not always, as has been supposed in the past, an adequate test for ergodic or mixing behavior.

Acknowledgment

The empirical tests for ergodicity and mixing described in this paper parallel quite closely an unpublished mathematical investigation of the unequal-mass hard point gas conducted by Professor Arthur Hobson of the University of Arkansas. The present authors are indebted to Professor Hobson for allowing them to read a preprint of his manuscript and for exchanging with them much useful correspondence. This research was sponsored by the Air Force Office of Scientific Research under Grant No. AFOSR-73-2453.

References

1. Ja. G. Sinai, *Russian Math. Surveys* **25** (1970), 137.
2. V. I. Arnold and A. Avez, "Ergodic Problems of Classical Mechanics," Appendix 26, Benjamin, New York, 1968.
3. A. Hobson and B. K. Cheng, Exact nonequilibrium analysis of N hard rods in a finite box, Preprint.
4. J. L. Lebowitz, Hamiltonian flows and rigorous results in nonequilibrium statistical mechanics, *in* "Statistical Mechanics: Proceedings I.U.P.A.P. Conference, Chicago, 1971," (S. A. Rice, K. F. Freed, and J. L. Light, Eds.), University of Chicago Press, Chicago, 1972.
5. V. I. Arnold and A. Avez, "Ergodic Problems of Classical Mechanics," Appendix 1, Benjamin, New York, 1968.
6. V. I. Arnold and A. Avez, "Ergodic Problems of Classical Mechanics," Appendix 31, Benjamin, New York, 1968.
7. V. I. Arnold and A. Avez, "Ergodic Problems of Classical Mechanics," p. 20. Benjamin, New York, 1968.
8. V. I. Arnold and A. Avez, "Ergodic Problems of Classical Mechanics," Chap. 3, Benjamin, New York, 1968.
9. J. Ford, *Adv. Chem. Phys.* **24** (1973), 155.