How Efficiently Do Three Pointlike Particles Sample Phase Space?

S. G. Cox and G. J. Ackland
Department of Physics and Astronomy, The University of Edinburgh, Edinburgh, EH9 3JZ, Scotland, United Kingdom
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We show that the continuous phase space of a hard particle system can be mapped onto a discrete but infinite phase space. For three pointlike particles confined to a ring, the evolution of the system maps onto a chaotic walk on a hexagonal lattice. This facilitates direct measurement of the departure of the system from its original configuration. In special cases of mass ratios the phase space becomes closed and finite (nonergodic). There are qualitative differences between this chaotic walk and a random walk, in particular a more rapid sampling of phase space.

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Statistical mechanics holds a central position in the physicist's armory, and its demonstrable successes make it easy to overlook the validity of its central assumption, namely that a physical system samples a representative region of its theoretical phase space.

An essential ingredient in computational investigation of an ensemble is to perform such sampling—e.g., in a good Monte Carlo simulation significant effort is invested in *eliminating correlations* introduced by the sampling method or random number generator. However, for the physical system the sampling of the phase space is *perfectly correlated*, in that the system itself is completely deterministic (assuming classical dynamics in the microcanonical ensemble).

A simple reconciliation of these apparently opposite viewpoints leads to the ergodic hypothesis: namely that all microstates are sampled with equal likelihood (in the microcanonical ensemble). It is far from clear that a deterministic system will in fact access all microstates [1]: indeed there are many classical systems in which a periodic orbit through phase space is observed. Even if such a periodic orbit is achieved only for special initial conditions, while more general conditions lead to chaotic behavior, the microstates of the periodic orbit remain inaccessible to the general case, which therefore also violates ergodicity.

It is thus of interest to study the phase space sampling behavior of simple systems to determine how closely deterministic systems approach ergodicity [2], and how rapidly they explore their phase space.

A practical problem arises from the definition of the phase space. Within a finite phase space Poincaré recurrence means that states arbitrarily close to the initial state will occur, thus a measure of how far the system has departed from its initial microstate in terms of a distance in the phase space will ultimately tend to zero.

In this paper we avoid the Poincaré problem by mapping a finite, continuous phase space onto an infinite, discrete phase space. This enables us to make a well-defined measurement of the rate of departure of the system from its initial state [3].

The system we investigate is that of three hard point particles colliding elastically on a closed, 1D ring. This has recently been shown to be equivalent to the classic problem of a billiard in a triangular stadium [4,5]. The natural phase space for this system is six dimensional, axes consisting of the three positions and three momenta of the particles. Introducing conservation of energy and momentum constraints reduce the accessible phase space to a four dimensional hypersurface in this space. Along a typical trajectory, the position variables vary continuously, while the momenta remain constant between collisions and then jump discontinuously. In the remainder of the paper we consider only the projection of the trajectory onto the momentum surface.

The change of velocity on collision between two hard particles can be simply represented by multiplying the phase space vector by a matrix. Until the next collision occurs the system remains in the same momentum microstate. The $(N + M)$th momentum microstate visited can be written in terms of the Nth $\mathbf{p}(N) = (p_1(N), p_2(N), p_3(N))$ thus

$$\mathbf{p}(N + M) = \Pi_{i=1}^{M} \mathbf{A}_i \mathbf{p}(N) . \tag{1}$$

Each matrix $\mathbf{A}_i$ can take one of three possible values, which we label A, B, and C, corresponding to collisions between particles 1 and 2, 2 and 3, or 3 and 1, respectively. The most transparent representation is in terms of 3-vectors $\mathbf{p}(N)$ and 3×3 matrices of the following form:

$$\begin{bmatrix} \alpha & 1+\alpha & 0 \\ 1-\alpha & -\alpha & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \beta & 1+\beta \\ 0 & 1-\beta & -\beta \end{bmatrix} \begin{bmatrix} \delta & 0 & 1+\delta \\ 0 & 1 & 0 \\ 1-\delta & 0 & -\delta \end{bmatrix}, \tag{2}$$

$$\alpha = \frac{m_1 - m_2}{m_1 + m_2}; \quad \beta = \frac{m_2 - m_3}{m_2 + m_3}; \quad \delta = \frac{m_3 - m_1}{m_3 + m_1} . \tag{3}$$

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A more compact representation in terms of 2×2 matrices and 2-vectors of generalized momenta can be obtained by incorporating the conservation laws [6]. Time reversal symmetry means that the matrices are unitary, and it can be easily verified that for all choices of the masses the identity $ABCABC = I$ holds [7]. The evolution of the system in the momentum space can be represented by a sequence of these collision matrices. This allows us to introduce a discrete geometric representation of the phase space: each state is connected to three others only, corresponding to the states accessible via a single collision. In this representation adjacent states are actually accessible from one another, in contrast to the continuous phase space where there is no way for the system to get directly from one point to another infinitesimally close.

The relationship $ABCABC = I$ means that the topology of the discrete phase space is that of a hexagonal (honeycomb) lattice. Since the spectrum of possible momenta is continuous, there are an infinite number of states and this two-dimensional lattice extends infinitely [8] (see Fig. 1). Evolution of the system can be represented as a chaotic walk [9] on this lattice—hence we can directly measure the efficiency of sampling the phase space by studying the properties of this walk.

The sequence of matrices obtained from a particular set of initial collisions was obtained from computer simulation. In the spatial part of the phase space, it was observed

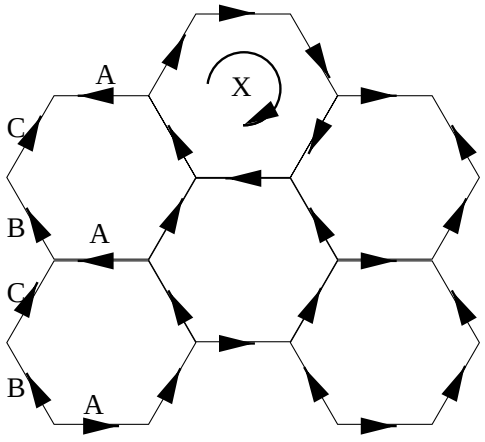

FIG. 1. Discrete geometric representation of the momentum phase space: nodes correspond to realizable states while arrows show possible subsequent states, and are labeled *A*, *B*, or *C* to correspond to the collision matrices. Whether there are one or two arrows leaving a node is determined by whether one or two pairs of particles are approaching one another: in a loop it is obviously impossible for all three pairs of particles to be moving away from each other, or for all three to move towards one another. Similarly, the arrow *A* points from a node in which particles 1 and 2 are approaching one another to a node in which they are moving apart. The loop around *X* shows a case for which the particles can recover their original momenta, although in general their positions will be different allowing the system to subsequently escape from the loop. Periodic collision sequences of repeat length 6 (*ABCABC*), 10 (*ABCABABCAB*), and higher even numbers arise from closed loops on this lattice: similarly, there are no odd period repeats.

that each particle covered the entire ring with a triangular probability distribution, going to zero at the points where a triple collision occurs. The centers of mass (not the peaks) of these distributions were found to be equispaced around the ring irrespective of the particle mass. This is consistent with maximizing the free volume (length) entropy which is independent of the masses [10]. The momenta have a distribution of the form

$$P(p_i) = [(p_i^{\max})^2 - p_i^2]^{-1/2}, \tag{4}$$

where $p_i^{\max}$ is the largest possible value of p_i consistent with the conservation laws. This distribution is the projection of an ellipse onto one axis in the 3D momentum phase space—an ellipse being the region of phase space satisfying conservation of energy and momentum. The mean energy of each particle is thus

$$E_i = \int \frac{p_i^2}{2m_i} P(p_i)\, dp_i = \frac{M - m_i}{2M} E_{\text{tot}}, \tag{5}$$

i.e., proportional to the mass of the other two. This generalized form of equipartition arises because center of mass motion is suppressed by the conservation of momentum: the simulation is in the so-called molecular dynamics ensemble rather than the microcanonical [6,11].

It is interesting to note that cases involving negative masses can be treated straightforwardly in the simulation. Moreover, analytic solutions for a series of collision matrices being equal to the identity are solved only if one negative mass is considered and hence are apparently not physically realizable, although we note that it has been shown that the negative mass cases correspond to a billiard in an obtuse triangle [4].

The walk on the hexagonal lattice was sampled via a series of calculations with different initial conditions for the same set of mass ratios. We calculate the distance traveled by the walk after every 1000 collisions for a run of 100 000 collisions, creating a graph of 100 data points. For each set of mass ratios 1000 such graphs were calculated, and an average graph found. These averaged graphs were found to be well approximated by a power law: (distance traveled) $\propto$ (number of collisions)^n.

By repeating the calculations for the same mass ratios and starting conditions we found that the errors in our calculated exponents are about 0.02. The various mass ratios showed a range of exponents, which are represented in Fig. 2. A number of features are immediately obvious from this graph: For the majority of mass ratios, the exponent is close to 0.5. This is not unexpected, since it is well known that a random walk has $n = \frac{1}{2}$.

For the case where two of the masses are identical the exponent is around 0.88. For a series of masses satisfying

$$\frac{m_1}{m_3} = \frac{m_2 + m_3}{m_2 - m_3} \quad \text{or} \quad \frac{m_1}{m_3} = 3\,\frac{m_2 + m_3}{m_2 - 3m_3} \tag{6}$$

the exponents are 0.22 ± 0.02 and 0.35 ± 0.04, respectively.

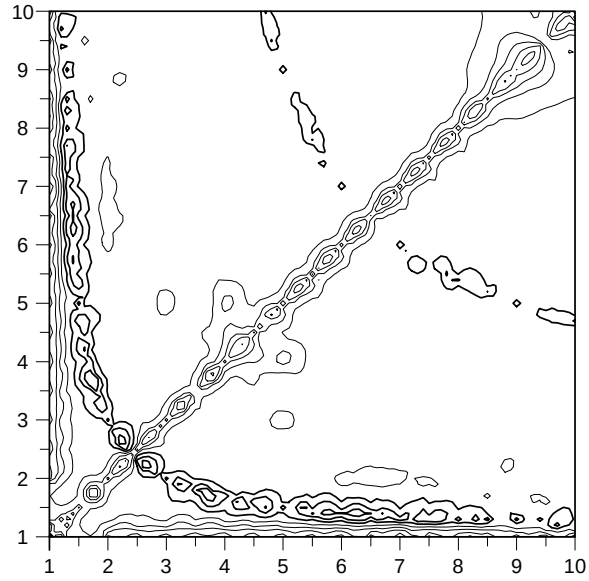

FIG. 2. Contour plot of exponent n as calculated from 10^8 collisions for various sets of mass ratios. Axes correspond to ratios m_1/m_3 and m_2/m_3 and run from 1 to 10. The data are collected from an initial grid of 1600 points with an additional 2000 data points collected close to the special cases. The majority of the graph has $n = 0.5$. The thicker contour lines surround regions with $n < 0.5$—notably the two approximately hyperbolic regions corresponding to Eqs. (6) and (7). The finer contours surround regions of $n > 0.5$—notably along the axes and the $m_1 = m_2$ diagonal. The contour interval is 0.1. The plot is created using a linear interpolation scheme between 3638 separate mass ratios, and the combination of this and the finite sampling length broadens the regions around the special case lines [Eqs. (6) and (7)].

The $n > 0.5$ cases are easily understood: collisions between identical mass particles simply exchange momenta. Thus the system is similar to the two particle case where the same sequence (*ABABAB*) repeats indefinitely. Very repeated long segments make the walk more similar to a "Newtonian" case, in which the moving body (phase space point) continues to move in the same direction and the distance traveled is simply proportional to the time.

The "sub random" cases are more curious. They correspond to mass ratios which produce matrices which satisfy relations $ABAB = -I$, or $ABABAB = -I$. When these sequences occur they have the effect of causing the walk to reverse, running backwards along its previous trajectory. Consequently, these walks escape more slowly from the origin than do random ones.

Figure 2 suggests other special cases corresponding to longer combinations of collision matrices producing $\pm I$. It appears that the longer such a special sequence needs to be, the closer the exponent is to 0.5.

If, e.g., $ABAB = -I$, two hexagonal lattice sites may correspond to the *same* point in p_1, p_2, p_3 space. To obtain a one-to-one correspondence with the continuous phase space the hexagonal lattice should be folded onto an infinite cylinder (like a "buckytube"). Where two of these lines (in Fig. 2) of special cases intercept there are two such closures, and hence the walk will be confined to a finite region in the discrete space, corresponding to a discrete set of states in the p_1, p_2, p_3 space [12]. Even in these cases the averaged integrated quantities take the values given in Eq. (5).

For the majority of mass ratios, the exponent of the chaotic walk is 0.5, and so we examine whether these walks can be distinguished from a random walk. Figure 3 depicts typical trajectories corresponding to random, nonreturning random, and chaotic walks. The difference is that whereas each step in the random walk is independent of its predecessor, the chaotic walk has long strongly correlated sections. This is clearly the origin of the recently reported long-time tails in the autocorrelation function of the triangular Lorentz gas [13]. One effect is that the chaotic walk covers the phase space more rapidly than the random walk: one might think of the correlated sections as being individual steps at many different length scales and the walk corresponding to Levy rather than Brownian dynamics [14]. The agreement between the simulation and analytic phase space integration provides strong evidence that the chaotic walk gives an equivalent phase space sampling to a random process, and the fact that it diverges faster from its initial condition suggests possible applications in Monte Carlo simulation: in particular, the technique of a molecular dynamics/Monte Carlo hybrid which combines long ordered sections with occasional random moves.

The walk does not depend simply on the number of *A*, *B*, and *C* collisions which occur. The number of occurrences of each collision (N_A, say) is simply related to the mean velocity of each particle: using Eq. (5) we obtain, for example,

$$N_A \propto \sqrt{m_3/(m_1 + m_2)}\,. \tag{7}$$

However, it is clear from Fig. 1 that the steps of the walk on the hexagonal lattice corresponding to *A* may be in either the forward or backward direction, and that the final position depends on the difference between numbers of "*A*"s in even and odd positions in the collision sequence [15], not the total.

Lyapunov exponents [16,17] are not useful for this system. Similar initial positions and momenta lead to *identical* walks on the lattice until the sequence of collisions differs. After this the walks are totally different. Thus there is a discrete point at which the trajectories bifurcate, rather than a continuous drift apart.

In summary, we have introduced a method for studying the divergence in phase space of a system from its initial conditions: transposing the finite, continuous phase space of conventional statistical mechanics onto an infinite, discrete space. For a prototypical chaotic system, three hard particles on a ring or the triangular billiard, the deterministic walk corresponding to system evolution is shown to diverge faster than does an equivalent random walk, yet the distribution of energies and velocities remain as predicted

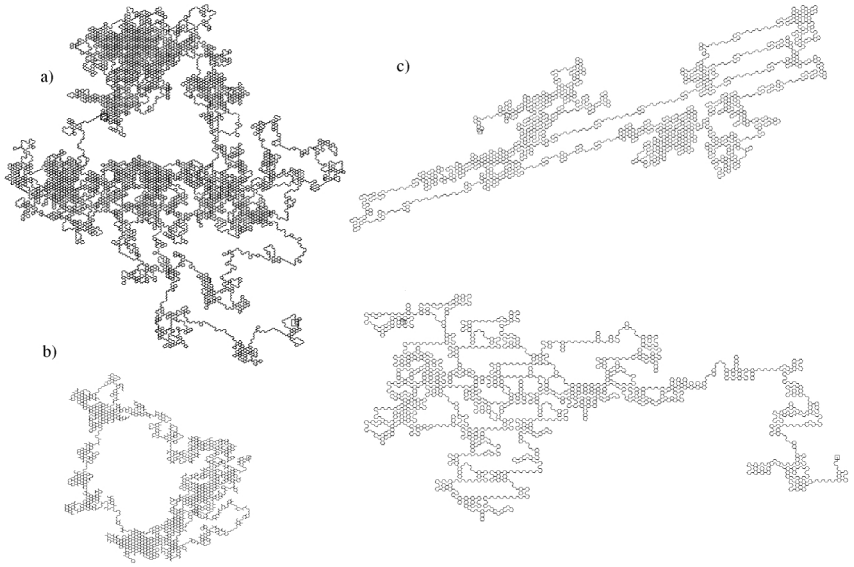

FIG. 3. Typical walks on the hexagonal lattice, illustrating the qualitative difference between (a) a random walk on the hexagonal lattice, (b) the uncorrelated nonreturning random walk, and (c) correlated chaotic walks. Plots are created by joining the vertices visited by the walk. It should be noted that some vertices are revisited in all cases—identical momenta are observed, although the positions are different. The frequency of such revisits is not shown explicitly.

by phase space integration and converge faster than with the random walk.

Further, the more rapid sampling of the phase space is related to the structure of the walk, with long correlated sections. In some special cases the lattice representation wraps back on itself. A single such fold leads to anomalously slow departure from the initial state, while two such folds close the phase space and lead to nonergodic behavior—only a finite number of discrete momentum states are accessible although the orbit remains aperiodic.

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[1] P. B. M. Vranas, Philos. Sci. **65**, 688 (1998).
[2] Z. G. Zheng, G. Hu, and J. Y. Zhang, Phys. Rev. E **53**, 3246 (1996).
[3] This measure is not the Lyapunov exponent, which is poorly defined for a system with singular interactions in 1D where curvature cannot be invoked; see C. Dellago and H. A. Posch, Phys. Rev. E **52**, 2401 (1995).
[4] S. L. Glashow and L. Mittag, J. Stat. Phys. **87**, 937 (1997).
[5] E. Gutkin, J. Stat. Phys. **81**, 7 (1996).
[6] G. J. Ackland, Phys. Rev. E **47**, 3268 (1993).
[7] This arises from momentum conservation, and underlies the well-known feature that periodic orbits of order 6 exist in all triangular billiard problems: it is straightforward to find relations between the four initial positions and momenta which satisfy the two constraints that the positions also exactly recur. Similar relations exist for higher dimensions/larger numbers of particles.
[8] Technically, the continuous phase space contains an uncountably infinite number of microstates while the hexagonal lattice contains only a countably infinite number. Since the actual sequence of collisions produces a countable sequence of microstates, this does not present any practical difficulty.
[9] A chaotic walk is one in which each step is determined by the results of a deterministic nonlinear system—here the next collision of the three particles on a ring.
[10] This statistical approach is the most fundamental definition of the entropy: there is no continuous function of the generalized coordinates and momenta themselves which increases monotonically in time; see E. T. Olsen, Found. Phys. Lett. **6**, 327 (1993).
[11] F. L. Roman, J. A. White, and S. Velasco, Phys. Rev. E **51**, 6271 (1995).
[12] These special relations of matrices also mean that for particular mass ratios the phase space breaks into disjoint regions, and the system cannot move between them. In spite of this evident violation of ergodicity the equipartition result [Eq. (5)] still holds. Ergodicity is a sufficient condition for Eq. (5), but not a necessary one.
[13] H. Matsuoka and R. F. Martin, J. Stat. Phys. **88**, 81 (1997).
[14] G. Zaslavsky, U. Frisch, and M. Shlesinger, *Lecture Notes in Physics* (Springer, New York, 1995), p. 450; C. Tsallis, S. V. F. Levy, A. M. C. Souza, and R. Maynard, Phys. Rev. Lett. **75**, 3589 (1995).
[15] The nodes of the lattice can be regarded a representation of a non-Abelian group of collision sequences for which *A*, *B*, and *C* act as generators. The hexagonal lattice is not a 2D-Bravais lattice, and the existence of two distinct types of node in the crystallographic basis, one visited after even numbers of collisions and one after odd, gives rise to two "types" of *A* collision which cancel in the overall distance traveled in phase space.
[16] P. L. Garrido, J. Stat. Phys. **88**, 807 (1997).
[17] H. Lamba and C. J. Budd, Phys. Rev. E **50**, 84 (1994).