

## Transition from Chaotic to Nonchaotic Behavior in Randomly Driven Systems

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We discuss the explicit dependence of the final trajectory on initial conditions for randomly driven nonlinear dynamical systems which are stopped and restarted with random velocities at regular intervals (a Brownian-type motion). We find a transition from chaotic behavior for long intervals between stops to nonchaotic behavior for short intervals between stops. For short intervals, the Lyapunov exponent is related to the thermal average square force due to the potential. The consequences for "hybrid molecular-dynamics Monte Carlo" sampling methods are discussed.

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In the study of nonlinear dynamical problems, it is a familiar fact that the trajectory of a particle may show extreme sensitivity to initial conditions, i.e., the system exhibits chaotic behavior [1]. The deterministic evolution of such a system appears to display a random character, and modifying its dynamics by adding truly random forces might be expected to make its behavior "more random." We recently discovered a counterintuitive contradiction of this notion: When an ensemble of particles with *different* initial conditions are driven by an *identical* sequence of random forces designed to simulate Brownian motion, their *trajectories may become identical* at long times. (Here, and in the rest of this paper, when we say that trajectories become identical, we mean that the average distance between them converges exponentially to zero.) It is well known that no matter what the initial position of a particle undergoing Brownian motion in a fixed external potential  $V(x)$ , the statistical distribution of its positions at long times is simply given by the Boltzmann distribution [2], proportional to  $\exp[-V(x)/k_B T]$  for the appropriate temperature  $T$ . Our result entails a much stronger statement than the observation that the *statistical* distributions of Brownian trajectories become independent of initial positions; the ensemble of trajectories becomes point by point identical in time, following a single final trajectory, which is, however, highly erratic and random.

We consider a particle of mass  $m$  which moves according to Newton's equations (without friction) in a potential  $V(x)$ , except that at regular time intervals  $\tau$  it is stopped and the components of its velocity are reset to random values chosen from a Gaussian distribution of variance  $k_B T/m$  (i.e., the velocity is reset at regular intervals from a Maxwell distribution for temperature  $T$ ). This motion is in many respects similar to Brownian motion of the particle at a temperature  $T$ . It can be shown that the distribution of positions of the particle for long times is just the Boltzmann distribution, independent of the value of  $\tau$  chosen [3]. Indeed, this approach is frequently used in Monte Carlo simulations [3,4] to sample

points from a probability distribution  $P(x)$  by choosing the classical potential  $V(x) = -k_B T \ln[P(x)]$ . (In the numerical simulations presented here we will set  $k_B T$  and  $m$  equal to unity [5].)

In typical Monte Carlo applications,  $x$  represents a vector with many components, corresponding to motion of a particle in a high-dimensional space. While the phenomenon we describe was discovered in such a situation, the dimension of the space in which the particle moves does not appear to be crucial. For ease of visualization, we will present in detail here the behavior of a two-dimensional system chosen to be a "bad case" in a sense discussed below. This system has the quartic-plus-sinusoidal potential

$$V(x, y) = \sin(2\pi x)/2\pi x + \sin(2\pi y)/2\pi y + r^4/16\pi,$$

shown in Fig. 1. Shown in Fig. 2 is the mean-square distance  $\langle r_{12}^2 \rangle$  between pairs of identically driven particles in this potential, first for 150 steps with a time between stops of  $\tau = 2.5$ , and then for 150 steps with  $\tau = 1.0$ . (By

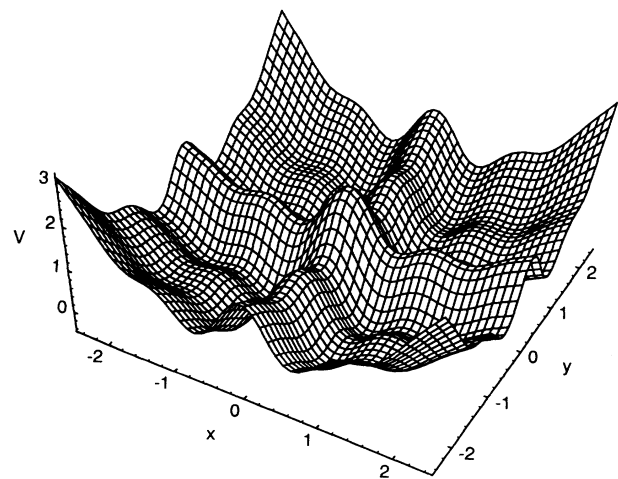


FIG. 1. The potential  $V(x, y) = \sin(2\pi x)/2\pi x + \sin(2\pi y)/2\pi y + r^4/16\pi$ .

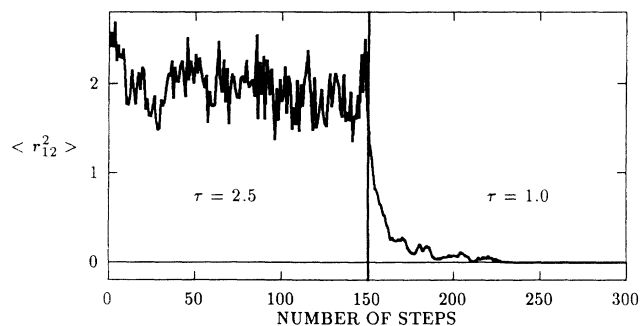


FIG. 2. The mean-square distance  $\langle r_{12}^2 \rangle$  between pairs of identically driven particles vs number of steps, for the potential in Fig. 1. The particle coordinates were initially independently distributed from the Boltzmann distribution. The time  $\tau$  between stops was 2.5 for the first 150 steps and was 1.0 for the second 150 steps. 100 independent simulations were averaged for the curve shown.

“identically driven,” we mean that both particles of each pair were given an identical, randomly chosen velocity [6] at the start of each step of length  $\tau$ .)

The behavior of the particles shown in steps 150–300 of Fig. 2 is an illustration of a phenomenon which may be loosely stated as follows: *If the time interval  $\tau$  between steps is lower than a threshold value  $\tau_c$ , the final trajectory of the particle is entirely independent of the initial conditions to any required level of accuracy.* (For the motion shown in Fig. 2, the threshold  $\tau_c$  is between 1 and 2.5.) When  $\tau < \tau_c$ , if two particles are started at entirely different positions but are “driven” by the same particular choice of velocities, they will (with probability 1) end up traveling along exactly the same trajectory at the same time. The final trajectory depends only on the choice of velocities, not on the initial position of the particle. We have observed this behavior in simulations of a variety of bounded systems (i.e., systems where the Boltzmann distribution effectively confines the particles to a finite region), with as many as 3000 coordinates, as often arise in Monte Carlo applications. We have not yet been able to find a bounded system for which the rule is violated [7]. We will prove the result for bounded one-dimensional systems, by showing that the appropriately defined Lyapunov exponent for the random motion is negative when  $\tau$  is sufficiently short and is simply related to the thermal average of the square of the acceleration due to  $V$ .

Thus, although the trajectory of the particles is highly erratic, the system is *not* chaotic when  $\tau < \tau_c$ , because the final path (though random) is independent of the initial conditions. The threshold value  $\tau_c$  and the rate of convergence of the trajectories for any given value of  $\tau$  depend on the potential energy function  $V(x)$  as well as on the variance  $k_B T/m$  of the velocity components. If the time interval  $\tau$  is greater than  $\tau_c$ , the motion of initially uncorrelated particles subjected to an identical choice of

driving velocities is correlated at large times (as in the first 150 steps of Fig. 2) but never becomes identical. Indeed, particles that started out very close together will not exhibit any greater correlation in their motion at large times than particles that started far apart. In this regime, the system is chaotic in the usual sense of extreme sensitivity to initial conditions.

Among unbounded systems, an obvious counterexample to the result is for a potential  $V(x)$  which is constant everywhere. In a periodic potential, the statement can only be true modulo a period of the potential. For example, in simulations of the two-dimensional periodic system with

$$V(x, y) = \{\cos(2\pi x) + \cos(2\pi y) + \cos^2[2\pi(x - y)]\}/2\pi,$$

we observe that particles started at random positions but driven by the same set of velocities end up following exactly identical motion except for a constant shift of a random number of complete periods of the potential in the  $x$  and  $y$  directions. In general, we suspect that the original statement will only be true for systems where the particle is confined to a finite region, either by the potential or by the geometry of the problem (e.g., by folding a periodic potential onto a torus).

For bounded linear systems, where  $V(x)$  has a quadratic form, the final motion is independent of the initial motion for all values of  $\tau$ ; i.e., the value of  $\tau_c$  is infinite. The action of regularly stopping and restarting the particle can be thought of as an infinite damping force “turned on” for an infinitesimal time at intervals  $\tau$  apart, followed by a driving force with the appropriate impulse also applied at intervals of  $\tau$ . Because harmonic oscillators obey linear superposition, we see that after the damping term causes the initial conditions to decay, the final motion depends only on the velocities chosen to drive the particle. The damping analogy can be used for nonlinear systems also, but linear superposition is not obeyed, and the effects of initial conditions need not vanish at large times.

We now show analytically that for any one-dimensional potential  $V$  which confines particles to a finite region, and for short enough intervals  $\tau$  between stops, the average rate of contraction  $\gamma$  of the distance between two particles initially close together (i.e., the negative of the Lyapunov exponent) is given by  $\gamma = \gamma_0 + O(\tau^2)$ , where

$$\gamma_0 = \tau \langle (\partial V / \partial x)^2 \rangle / 2mk_B T. \quad (1)$$

The angle brackets denote the thermal average (with respect to the Boltzmann distribution). To prove this, consider two particles initially at points  $x_0$  and  $x'_0$  close together. Let the two particles be started with equal velocity  $\dot{x}$ . For short times, the positions of the particles are given by  $x(t) = x_0 + \dot{x}t + \ddot{x}t^2/2 + \dots$  and  $x'(t) = x'_0 + \dot{x}t + \ddot{x}'t^2/2 + \dots$ . The contraction of the distance between the particles at the end of one interval  $\tau$  is then given by

$$\frac{x'(\tau) - x(\tau)}{x'_0 - x_0} \approx 1 + \frac{\tau^2}{2} \frac{\ddot{x}' - \ddot{x}}{x'_0 - x_0} \approx 1 - \frac{\tau^2}{2m} \frac{\partial^2 V}{\partial x^2},$$

since  $m\ddot{x} = -\partial V/\partial x$ . If the curvature of the potential  $\partial^2 V/\partial x^2$  is greater than zero, the particles move closer together, and if it is less than zero, they move farther apart during the motion. So in general the particles do *not* always move closer together in each individual step. However, the probability that a particle is at a position  $x$  during its motion is proportional to  $\exp[-V(x)/k_B T]$ . Thus, the *average* contraction of the distance between identically driven particles in one step of length  $\tau$  is given by

$$1 - \frac{\tau^2}{2Zm} \int \frac{\partial^2 V}{\partial x^2} \exp[-V(x)/k_B T] dx,$$

where  $Z$  is the normalization factor for the Boltzmann distribution. The average rate of contraction over many such steps is then

$$\gamma_0 = \frac{\tau}{2Zm} \int \frac{\partial^2 V}{\partial x^2} \exp[-V(x)/k_B T] dx.$$

Integration by parts (with the assumption that boundary terms vanish) gives the result  $\gamma_0 = \tau \langle (\partial V/\partial x)^2 \rangle / 2mk_B T$ . It is clear how this result breaks down for larger values of  $\tau$ ; the proof relies on the expansion of the trajectories to second order in  $\tau$ , which is not valid for large values of  $\tau$ .

Intuitively, we may consider that the harmonic-oscillator argument above applies when the particle makes a sufficient number of stops within a region of positive curvature. Since positive curvature occurs near minima, and negative curvature near maxima of the potential, the Boltzmann weight favors the former regions. The potential in Fig. 1 was chosen to have a number of accessible regions of negative curvature so that it would clearly illustrate this point.

Although the proof in one dimension does not extend in an obvious way to higher-dimensional systems [8], the numerical evidence suggests that the qualitative nature of the result is true for bounded systems of arbitrary dimension. In fact, for most of the potentials we have investigated, the generalization of Eq. (1) to higher dimensions gives a reasonable estimate (within an order of magnitude) of the average rate of contraction of the distance between pairs of identically driven points in the limit of small  $\tau$ , as shown in Fig. 3 [9]. Note that Fig. 3 shows the *asymptotic* contraction rate  $\gamma$ . For  $\tau < \tau_c$ ,  $-\gamma$  is the Lyapunov exponent, but for  $\tau > \tau_c$  it is identically zero (because the particles are confined to a finite region) and is different from the Lyapunov exponent, which is positive. It is intriguing to find that the value of  $\tau_c$  is similar for both systems shown in Fig. 3. However, we do not clearly understand at this stage the factors which determine  $\tau_c$ . Moreover, although  $\gamma_0$  gives the *average* rate of convergence of two close trajectories, fluctuations in the rate are an important aspect of the behavior of the system, especially near threshold  $\tau_c$ .

Apart from its intrinsic interest, this result has some important consequences for Monte Carlo applications us-

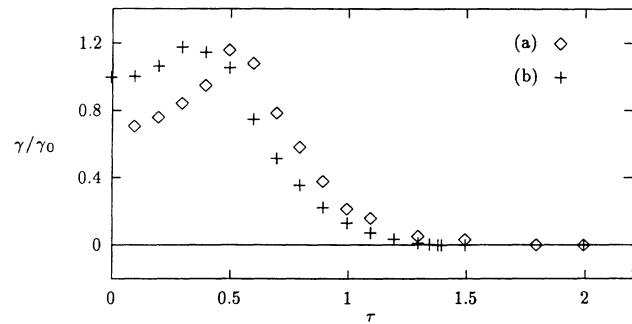


FIG. 3. Asymptotic average contraction rate  $\gamma$ , scaled by  $\gamma_0$  from Eq. (1), vs  $\tau$  for (a) the potential shown in Fig. 1 and (b) the one-dimensional Duffing potential,  $V(x) = x^4 - x^2$ .

ing the sampling idea described above. In many such applications, one must be concerned that measurements of a quantity at nearby times in the simulation will be strongly correlated with one another, substantially reducing the rate at which “effectively independent” samples are generated [4]. The phenomenon of critical slowing down is associated with such correlations becoming very long ranged. However, the autocorrelation time (the time required to generate “effectively” uncorrelated samples [10] from the Boltzmann distribution) depends on the quantity being measured. For example, near a phase transition, measurements of the order parameter relevant to the transition tend to have very long autocorrelation times, whereas the measurements of other quantities may be relatively well behaved [10]. It is clear that the present result (when applicable) ensures that the time required for trajectories to become identical is an absolute upper bound on the autocorrelation time for measurements of *all* quantities. Thus, it may be used to test for critical slowing down, even when the nature of the transition and the associated order parameter are unknown. However, we emphasize that this result provides no *solution* to such critical slowing down.

We have empirically observed the independence of initial conditions to occur in other, less natural, forms of driven motion for which the particles do not have a Boltzmann distribution. For example, independence of initial conditions also occurs for short time steps if some of the coordinates  $x_i$  (instead of the corresponding components  $\dot{x}_i$  of the velocity) are reset at random from a Gaussian distribution at the end of each step. This seems to suggest that something other than the Boltzmann distribution explicitly used in the derivation of Eq. (1) may be at the heart of the behavior.

It is possible to modify the stop-start motion in other ways and still observe the independence of the final trajectory on initial conditions. For a fixed value of  $\tau$  one may mix in some of the “old” velocity  $\mathbf{v}_{\text{old}}$  with the random velocity  $\mathbf{v}_{\text{ran}}$  to get a new starting velocity,  $\mathbf{v}_{\text{new}} = a\mathbf{v}_{\text{old}} + \beta\mathbf{v}_{\text{ran}}$ , where  $a^2 + \beta^2 = 1$ . As  $a$  increases from 0 to 1, the motion changes gradually from the stop-start

kind already discussed to an uninterrupted conservative motion. A threshold value of  $\alpha = \alpha_c$  separates nonchaotic behavior of the motion (for  $\alpha < \alpha_c$ ) from chaotic behavior (for  $\alpha > \alpha_c$ ). The value of  $\alpha_c$  depends on  $\tau$ . Simulations of motion in the periodic potential given above under Gaussian random driving forces applied at regular intervals with the addition of a constant damping proportional to velocity (but without stopping the particle at regular intervals) reveal a similar transition from nonchaotic behavior for large damping to chaotic behavior for small damping.

Finally, we note that the nature of this result (i.e., the exponential convergence of trajectories, with a well-defined Lyapunov exponent) ensures that it is insensitive to round-off and truncation errors in the numerical simulations. Of course, at what point the machine representations of two trajectories become truly identical depends on the machine precision.

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- [1] See, for example, G. L. Baker and J. P. Gollub, *Chaotic Dynamics: An Introduction* (Cambridge Univ. Press, Cambridge, 1990); also, *Noise and Chaos in Nonlinear Dynamical Systems*, edited by F. Moss, L. A. Lugiato, and W. Schleich (Cambridge Univ. Press, Cambridge, 1990).
  - [2] See, for example, R. Balescu, *Equilibrium and Non-Equilibrium Statistical Mechanics* (Wiley, New York, 1975).
  - [3] S. Duane, A. D. Kennedy, B. J. Pendleton, and D. Roweth, Phys. Lett. B **195**, 216 (1987), and references therein.
  - [4] R. T. Scalettar, D. J. Scalapino, and R. L. Sugar, Phys.

Rev. B **34**, 7911 (1986); S. R. White and J. W. Wilkins, Phys. Rev. B **37**, 5024 (1989); D. R. Hamann and S. Fahy, Phys. Rev. B **41**, 11 352 (1990).

- [5] Usually in Monte Carlo simulations there is an "accept-reject" part of each step also (see Ref. [3]), to allow for inexact energy conservation in integrating the equations of motion. This does not alter our results, and we have removed it in the simulations shown here, having verified that our results are insensitive to the step length used in numerical integration.
- [6] We have verified, using various subtractive and linear congruential pseudorandom number generators in choosing velocities, that our results do not depend on the details of the generator used.
- [7] There is no reason for the usual considerations limiting passage through energy barriers large compared to the temperature to be circumvented in the present problem [see S. Chandrasekar, Rev. Mod. Phys. **15**, 1 (1943)]. Presumably, for particles started in different regions, separated by large potential barriers, the time for them to "find" each other must be at least as great as the typical barrier penetration time.
- [8] The argument breaks down because pairs of particles entering a region tend to align themselves to some extent along the most slowly contracting direction in that region. Thus, the naive formal extension of the one-dimensional result to higher dimensions gives only an upper bound on the contraction rate as  $\tau \rightarrow 0$  and does not rule out an average dilation.
- [9] The only potential we investigated for which Eq. (1) did not give a reasonable estimate was the quartic-plus-quadratic potential  $V(x,y) = x^2y^2 + (x^2 + y^2)/n$  for large values of  $n$ . As  $n \rightarrow \infty$ , this potential becomes nonbounding along the  $x$  and  $y$  axes, and the observed contraction rate tends to zero.
- [10] See, for example, K. Binder and D. W. Heermann, *Monte Carlo Simulation in Statistical Physics* (Springer, Berlin, 1988).