Mixing Rates of Ergodic Algorithms

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Abstract: In response to the 2024 Snook Prize Problem, this paper compares the mixing rates of six simple numerical algorithms that produce an ergodic Gaussian distribution of position and momentum for a one-dimensional harmonic oscillator. A hundred thousand initial conditions spread uniformly over the constant energy surface are used for each of the six systems. The time-dependent kurtosis serves as a measure of the mixing rate. By this criterion, the most rapid mixing occurs for the signum thermostat system with an optimally chosen parameter value.

Key words: Snook prize, ergodicity, Gibbs' canonical distribution, mixing

I. Introduction

By now a number of three- and four-dimensional dynamical systems are known whose chaotic orbit eventually visits every point in their phase space and does so with a Gaussian probability distribution. Such systems are called 'ergodic' and model a one-dimensional harmonic oscillator in thermal equilibrium with a heat bath of constant temperature. In the 2024 Snook Prize Problem, Hoover and Hoover [1] ask "which of these approaches is best" in the sense of converging most rapidly to the Gibbs' canonical distribution [2], which is a Gaussian function for position q and momentum p. All of the systems employ feedback control of the time-averaged momentum squared $\langle p^2 \rangle$, which can be considered as a normalized temperature $T = \langle p^2 \rangle$. Such a feedback mechanism is called a 'thermostat'.

There are many ways to quantify the rate of convergence to a Gaussian distribution $f(p) = e^{-p^2/2T}/\sqrt{2\pi T}$, and similarly for $f(q)$. One of the simplest is the kurtosis $K = \langle p^4 \rangle / \langle p^2 \rangle^2$, which is a dimensionless number equal to 3 for a Gaussian distribution. It is straightforward to calculate $K(t)$ from a running average of p^2 and p^4 for an orbit starting at an arbitrary initial condition (q_0, p_0) and follow its convergence to $K = 3$. Indeed, this is one of several ways to confirm ergodicity.

Since $K(t)$ will in general depend on the initial conditions, it is necessary to average over a large number of orbits, here taken as 10^5 and uniformly distributed over the constant energy surface $q^2 + p^2 = 2T$. One can think of these orbits as a collection of noninteracting particles with a delta function distribution of total (potential plus kinetic) energy chosen to be the same as the average energy of the final thermal distribution. The results are not sensitive to the details of the initial conditions due to Lyapunov instability. Without loss of generality and to facilitate comparison, we hereafter take $T = 1$.

II. Method

To illustrate the method, consider the arguably simplest example of an ergodic system, the harmonic oscillator with a signum thermostat [3] given by

$$\begin{aligned} \dot{q} &= p, \\ \dot{p} &= -q - a\,\mathrm{sgn}(\zeta) p, \\ \dot{\zeta} &= p^2 - 1, \end{aligned} \tag{1}$$

where $\mathrm{sgn}(\zeta) = \zeta/|\zeta|$ is the signum function equal to ± 1 depending on the sign of ζ.

This system is ergodic for $a > 1.7$ and is typically taken as $a = 2$, which corresponds to critical damping ($\dot{p} = -q - 2p$) for $\zeta > 0$ or anti-damping ($\dot{p} = -q + 2p$) for $\zeta < 0$. The signum thermostat is an example of a 'bang-bang controller' since it switches abruptly and fully between two different states, much as does a typical physical thermostat that controls a furnace or air conditioner. In addition, the oscillator dynamics is completely linear except at $p = 0$. Thus the behavior is independent of the temperature.

Initial conditions are given by $q_0 = \sqrt{2}\cos\phi$ and $p_0 = \sqrt{2}\sin\phi$, where ϕ is a phase angle taken uniformly over the range $0 < \phi < 2\pi$. For these initial conditions, the average kurtosis for the delta function of energy $q_0^2 + p_0^2 = 2$ at $t = 0$ is given by $K(0) = \langle\sin^4\phi\rangle/\langle\sin^2\phi\rangle^2 = 1.5$. Thus the asymptotic value of $K = 3$ is approached from below. The initial value of the thermostat variable is taken as $\zeta_0 = 0$.

Time is measured in units of the inverse angular frequency so that $t = 2\pi$ corresponds to one period of the undamped harmonic oscillator. The equations are integrated using the fourth-order Runge-Kutta algorithm with an adaptive step size [4], and the (q, p) values are sampled at intervals of $\Delta t = 0.001$.

III. Results

III. 1. Signum Thermostatted System

The result of the calculation for Eq. (1) with $a = 2$ is shown in Fig. 1. Perhaps not surprisingly, the kurtosis of q as indicated by K_q converges more slowly than does K_p since the latter is more directly controlled by the thermostat. This is a general feature of all the cases that follow, although K_p sometimes overshoots and approaches 3 from above or oscillates about the asymptotic value. As a measure of the convergence time t_c, we arbitrarily take the earliest time at which both K_q and K_p simultaneously fall within 1% of 3.0, which means a value in the range $2.97 < K < 3.03$. The calculated value for the signum thermostatted oscillator is $t_c = 522$. All the times are rounded to an integer and have an uncertainty on the order of 1%.

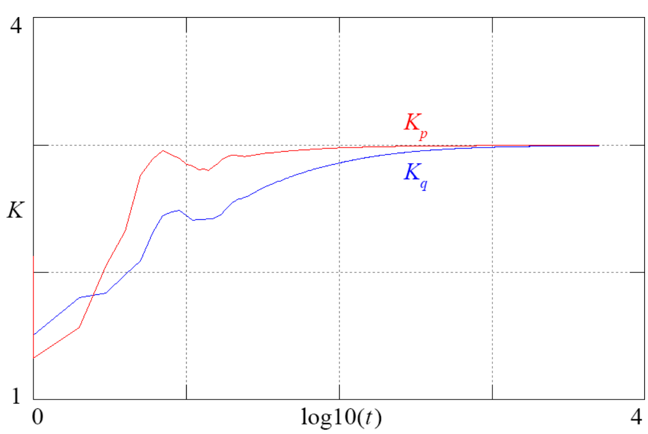

Fig. 1. Kurtosis versus time for the signum thermostatted system in Eq. (1) with $a = 2$

III. 2. 0532 System

An older system with a single thermostat variable but that controls both the second and fourth moments of p is the 0532 system [5] given by

$$\begin{aligned} \dot{q} &= p, \\ \dot{p} &= -q - \zeta(0.05p + 0.32p^3), \\ \dot{\zeta} &= 0.05(p^2 - 1) + 0.32(p^4 - 3p^2). \end{aligned} \tag{2}$$

The result of the calculation for Eq. (2) is shown in Fig. 2. The calculated convergence time is $t_c = 632$ with a small overshoot of K_p that converges slowly from above.

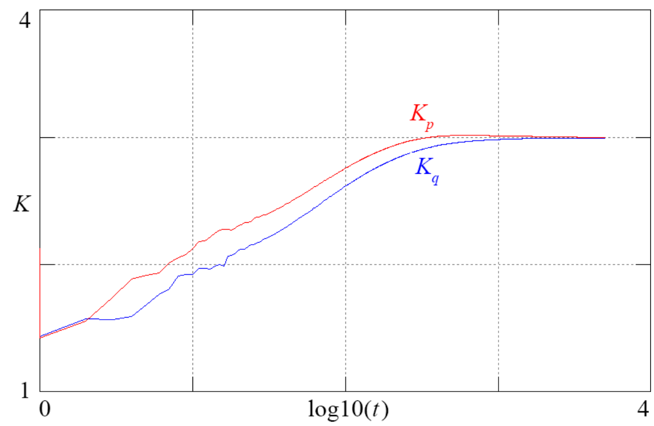

Fig. 2. Kurtosis versus time for the 0532 system in Eq. (2)

III. 3. TBS System

The final system with a single thermostat variable is the one proposed by Tapias, Bravetti, and Sanders (TBS) [6] in response to the 2016 Snook Prize Problem [7]. It can be viewed as a variant of Eq. (1) with a more gradual variation of the damping as given by

$$\begin{aligned} \dot{q} &= p, \\ \dot{p} &= -q - (1/Q)\tanh(\zeta/2Q)p, \\ \dot{\zeta} &= p^2 - 1, \end{aligned} \tag{3}$$

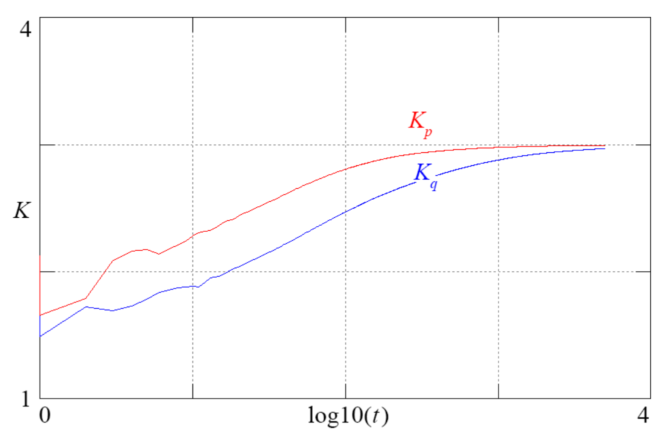

Fig. 3. Kurtosis versus time for the TBS system in Eq. (3) with $Q = 0.1$

with Q small and positive. For example, TBS assumed $Q = 0.1$ which gives the result in Fig. 3. The calculated convergence is relatively slow with $t_c = 4714$.

III. 4. HH System

Ergodic systems are more easily obtained using two thermostat variables to simultaneously control the second and fourth moments. One such example is the Hoover-Holian (HH) system [8] given by

$$\begin{aligned} \dot{q} &= p, \\ \dot{p} &= -q - \zeta p - \xi p^3, \\ \dot{\zeta} &= p^2 - 1, \\ \dot{\xi} &= p^4 - 3p^2. \end{aligned} \tag{4}$$

The result of the calculation for Eq. (4) is shown in Fig. 4. Perhaps not surprisingly, the kurtosis K_p converges rapidly since it is directly controlled by the ξ thermostat variable, although with large oscillations. The calculated convergence time is $t_c = 1309$.

III. 5. BBK System

A minor variant of the HH system was proposed by Bauer, Bulgac, and Kusnezov (BBK) [9, 10] in which the ζp term is replaced by $\zeta^3 p$, which generally improves ergodicity, giving the system

$$\begin{aligned} \dot{q} &= p, \\ \dot{p} &= -q - \zeta^3 p - \xi p^3, \\ \dot{\zeta} &= p^2 - 1, \\ \dot{\xi} &= p^4 - 3p^2. \end{aligned} \tag{5}$$

The result of the calculation for Eq. (5) is shown in Fig. 5. The kurtosis K_p also converges rapidly but with large oscillations. The calculated convergence time is $t_c = 406$.

III. 6. MKT System

An alternate approach is the 'chain thermostat' in which one thermostat controls the temperature of a second one. A simple such case was proposed by Martyna, Klein, and Tuckerman (MKT) [11] as given by

$$\begin{aligned} \dot{q} &= p, \\ \dot{p} &= -q - \zeta p, \\ \dot{\zeta} &= p^2 - 1 - \xi\zeta, \\ \dot{\xi} &= \zeta^2 - 1. \end{aligned} \tag{6}$$

The result of the calculation for Eq. (6) is shown in Fig. 6. The convergence is rapid but with oscillations in both K_p and K_q. The calculated convergence time is $t_c = 162$.

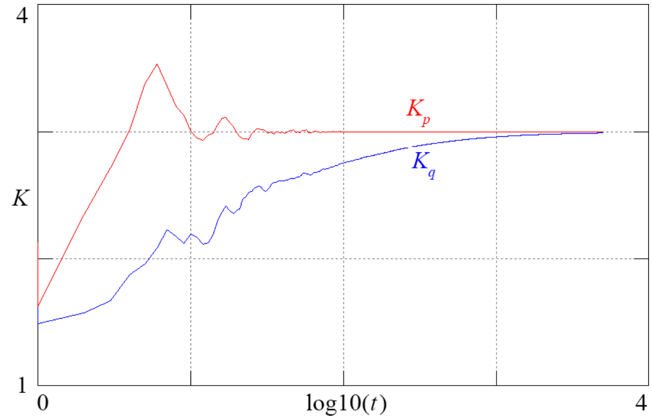

Fig. 4. Kurtosis versus time for the HH system in Eq. (4)

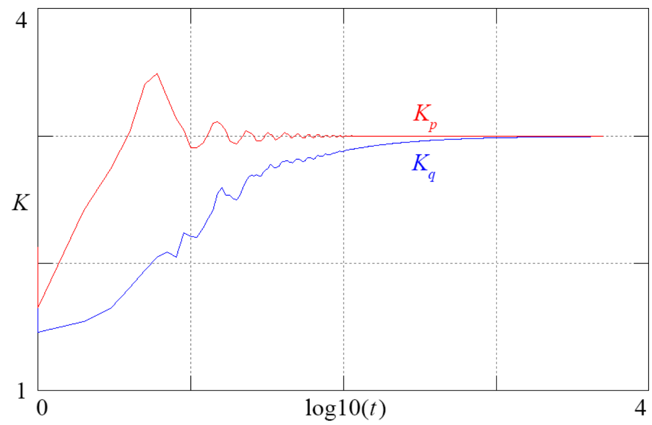

Fig. 5. Kurtosis versus time for the BBK system in Eq. (5)

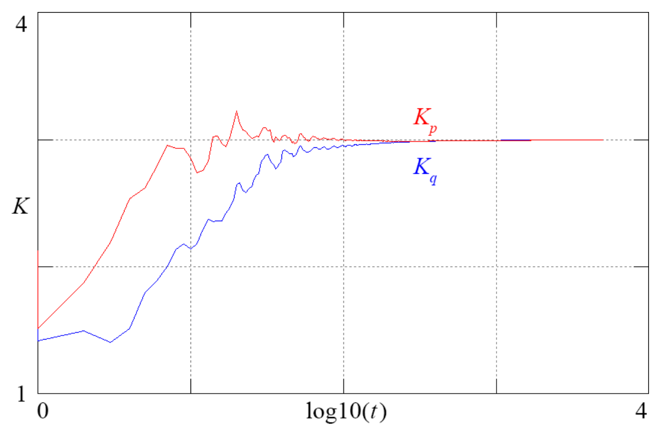

Fig. 6. Kurtosis versus time for the MKT system in Eq. (6)

IV. Optimization

The signum thermostatted system and the TBS system have adjustable parameters that were arbitrarily taken as $a = 2$ and $Q = 0.1$, respectively. It is natural to ask whether t_c can be further reduced by choosing more optimal values of the parameters. Fig. 7 shows that the signum case has a minimum of $t_c = 159$ at $a \approx 4$, and that it is robustly ergodic over a wide range of the parameter in the vicinity of the optimum.

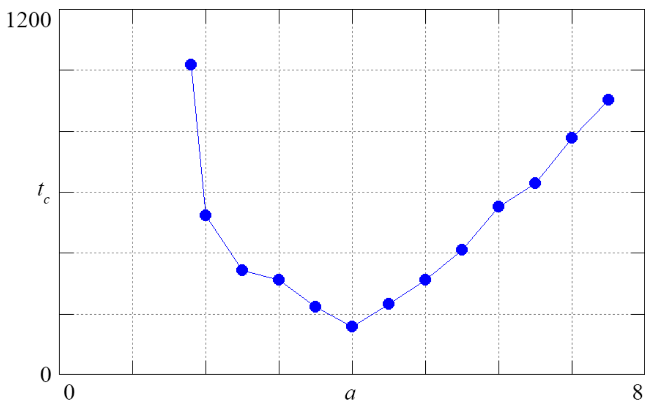

Fig. 7. Convergence time for the signum thermostatted system in Eq. (1) showing a robust minimum of $t_c = 159$ at $a \approx 4$

Fig. 8 shows that the TBS case has a minimum of $t_c = = 1608$ at $Q \approx 0.2$, an order of magnitude worse than the optimized signum case. Ergodicity is lost for slightly larger values of Q where t_c is undefined. This result is confirmed by Poincaré plots at $z = 0$ that show quasiperiodic islands amidst the chaotic sea that become quite large for $Q > 0.22$. Thus the ergodicity is somewhat fragile near the optimum value of t_c.

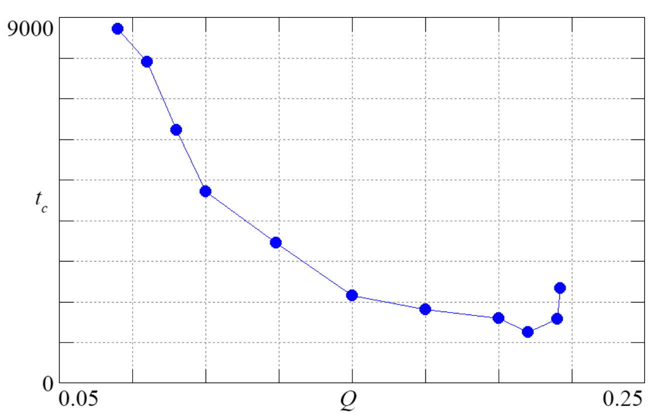

Fig. 8. Convergence time for the TBS system in Eq. (3) showing a fragile minimum of $t_c = 1608$ at $Q \approx 0.2$

V. Summary and Conclusions

The results of the previous calculations are summarized in Tab. 1. Based on the fastest convergence of the kurtosis, the best model (the smallest t_c) is the signum thermostatted system for $a = 4$ with $t_c = 159$. The MKT system is a close second with $t_c = 162$. It seems reasonable that a bang-bang controller would be most effective in rapidly achieving thermal equilibrium since the feedback changes sign abruptly and fully. It might be possible to reduce t_c for some of the other cases by introducing an additional parameter and optimizing its value.

Tab. 1. Summary of results

System	Eq.	t_c	LE
signum ($a = 2$)	(1)	522	0.3032
signum ($a = 4$)	(1)	159	0.5050
0532	(2)	632	0.1440
TBS ($Q = 0.1$)	(3)	4714	0.2804
TBS ($Q = 0.2$)	(3)	1608	0.1446
HH	(4)	1309	0.0680
BBK	(5)	406	0.0796
MKT	(6)	162	0.0665

The table also shows the largest Lyapunov exponent (LE) for each case [12], which does not correlate with t_c in any apparent way. Furthermore, the entropy, defined as the sum of the positive Lyapunov exponents, is identical to the LE since these systems have only one positive Lyapunov exponent.

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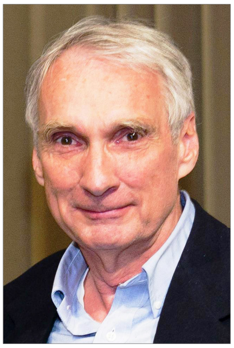

Julien Clinton Sprott received his PhD in physics from the University of Wisconsin in 1969 and joined the faculty there in 1973. After a 25-year career in experimental plasma physics, he became interested in computational nonlinear dynamics and chaos in 1988. He has authored or coauthored hundreds of papers on the subject and a dozen books. He is now Emeritus Professor of Physics at the University of Wisconsin-Madison.