CMST 24(3) 169–176 (2018) DOI:10.12921/cmst.2018.0000042

Ergodicity of One-dimensional Oscillators with a Signum Thermostat

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Received: 29 August 2018; accepted: 25 September 2018; published online: 28 September 2018

Abstract: Gibbs' canonical ensemble describes the exponential equilibrium distribution $f(q,p,T) \propto e^{-\mathcal{H}(q,p)/kT}$ for an ergodic Hamiltonian system interacting with a 'heat bath' at temperature T. The simplest deterministic heat bath can be represented by a single 'thermostat variable' ζ. Ideally, this thermostat controls the kinetic energy so as to give the canonical distribution of the coordinates and momenta $\{q,p\}$. The most elegant thermostats are time-reversible and include the extra variable(s) needed to extract or inject energy. This paper describes a single-variable 'signum thermostat.' It is a limiting case of a recently proposed 'logistic thermostat.' It has a single adjustable parameter and can access all of Gibbs' microstates for a wide variety of one-dimensional oscillators.

Key words: signum thermostat, ergodicity, Gibbs' ensemble, Nosé-Hoover system

I. INTRODUCTION

J. Willard Gibbs [1] showed that an oscillator with Hamiltonian $\mathcal{H}$ in thermal equilibrium with a source of heat (a 'heat bath') at temperature T will have an energy that fluctuates in time but with a canonical distribution proportional to $e^{-\mathcal{H}/kT}$, where k is Boltzmann's constant, hereafter taken as unity. The simplest such example is a harmonic oscillator such as a mass m suspended by an ideal spring with spring constant κ whose kinetic energy is $\frac{1}{2}mv^2 = \frac{1}{2m}p^2$ and whose potential energy is $V(q) = \frac{1}{2}\kappa q^2$. For simplicity, we take m and κ equal to unity. The corresponding Hamiltonian is $\mathcal{H}(q,p) = q^2/2 + p^2/2$, leading to the equations of motion $\dot{q} = \partial\mathcal{H}/\partial q = p$ and $\dot{p} = -\partial\mathcal{H}/\partial p = -q$. Hamiltonian systems conserve the total energy and are thus *isoenergetic*.

For most of the 19^{th} and 20^{th} centuries, physicists imagined controlling the energy of an oscillator using a heat bath at an average temperature T in contact with the oscillator. The number of degrees of freedom in the heat bath was assumed large enough so that the heat flow to or from the oscillator is negligible relative to the whole. In 1984 Shuichi Nosé proposed a method for replacing the heat bath with a single additional degree of freedom added to the oscillator equations of motion [2, 3]. Since his original proposal, several models have been developed that are consistent with Gibbs' canonical distribution for the oscillator, the simplest of which is the Nosé–Hoover system [4],

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

If ζ were a positive constant, this system would be a damped harmonic oscillator. However, by allowing ζ to change in time, being alternately positive and negative, energy is added to the oscillator when its energy is too low and removed from it when its energy is too high. The $\dot{\zeta}$ equation thus acts like a 'thermostat.' As a result, the long-time average energy is kept constant at $\langle p^2 \rangle = T$ but with large fluctuations about the average. Equation (1) is sometimes written with different or additional parameters, but it is inherently a one-parameter system through an appropriate transformation of the variables, and so the use of T as the parameter is somewhat arbitrary.

The resulting system shares many of the properties of a Hamiltonian system except that the energy is allowed to fluctuate in time rather than being rigidly fixed. Such systems are said to be *isothermal* rather than isoenergetic and to be *nonuniformly conservative* [5]. As with other conservative systems, Eq. (1) is time-reversible since the transformation $(q,p,\zeta,t) \rightarrow (q,-p,-\zeta,-t)$ leaves the equations unchanged. This three-dimensional modification of the simple harmonic oscillator has chaotic solutions as required for the orbit to visit all points in (q,p) phase space as expected for a physical oscillator in contact with a real heat bath.

However, Eq. (1) fails to generate the entire canonical distribution, $f(q,p,\zeta) = f(q)f(p)f(\zeta) = e^{-q^2/2T}e^{-p^2/2T}e^{-\zeta^2/2T}/(2\pi T)^{3/2}$, but traces out only a small part of it depending on the initial values of (q,p,ζ). For initial conditions chosen randomly from Gibbs' Gaussian measure, 94% of the orbits are quasiperiodic and lie on two-dimensional tori that surround an infinite number of stable one-dimensional periodic orbits. The remaining 6% of the initial conditions lie in a surrounding three-dimensional chaotic sea [6]. In theory, trajectories within the sea come arbitrarily close to any point within it.

Nosé left us with the problem of finding an ergodic dynamics, one accessing all of phase space starting from almost any initial condition. Over the past thirty years, a variety of motion equations designed to improve on Nosé's approach were developed [7-15]. The goal was a simple, deterministic, time-reversible dynamics accessing every (q,p,ζ) state for any initial condition.

II. LOGISTIC THERMOSTAT OSCILLATOR

In response to the 2016 Ian Snook prize challenge [15], Diego Tapias, Alessandro Bravetti, and David P. Sanders [16] proposed a variant of the Nosé–Hoover oscillator using what they call a 'logistic thermostat' given by

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -q - \left(\frac{T}{Q}\right)\tanh\left(\frac{\zeta}{2Q}\right)p \\ \dot{\zeta} &= p^2 - T. \end{aligned} \tag{2}$$

For Q sufficiently small, they show that the resulting system is ergodic as confirmed through (1) inspection of the Poincaré sections for lack of holes, (2) independence of the Lyapunov exponents on the initial conditions, (3) comparison of the time-averaged dynamical moments of q, p, and ζ with the analytic moments for their respective ergodic Gibbs' distributions, and (4) convergence of the global joint distribution to $f(q,p,\zeta) = e^{-q^2/2T}e^{-p^2/2T}\mathrm{sech}^2(\zeta/2Q)/8\pi QT$, as measured by the Hellinger distance.

For example, $Q = 0.1, T = 1$ gives the flow whose $\zeta = 0$ cross section is shown in Fig. 1. (We do not call this a 'Poincaré section' because crossings in both directions are plotted.) In this and the similar plots to follow, the value of the local largest Lyapunov exponent is shown with a continuum of colors from blue for the most negative to red for the most positive with green indicating values near zero. The horizontal stripes at $p = \pm\sqrt{T}$ are the ζ-nullclines where $\dot{\zeta} = 0$ and the orbit is locally tangent to the $\zeta = 0$ plane. Despite the intricate and unexplained structure in the local Lyapunov exponent, the phase-space distribution $f(q,p,0)$ is featureless without evident regions of quasiperiodicity. The global Lyapunov exponents for all initial conditions are $(0.2804, 0, -0.2804)$, and the system is nonuniformly conservative and time-reversible with a chaotic sea that fills all of space. The authors also show similar ergodic behavior for the cubic and two-well Duffing oscillators, corresponding to quartic and 'Mexican-hat' potentials, respectively, but using $Q = 0.02$ for the latter case.

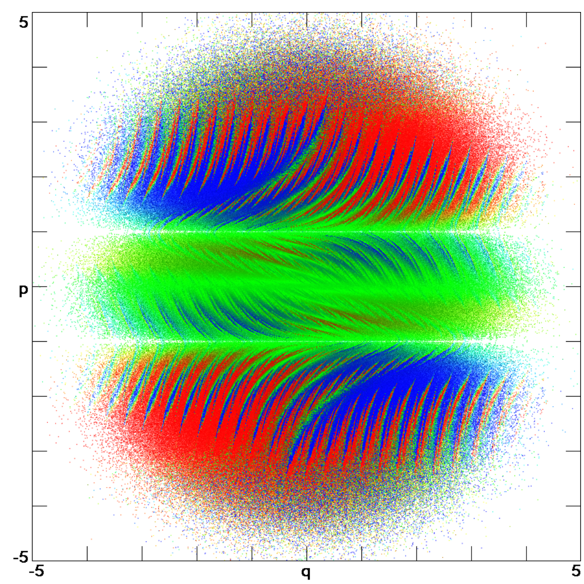

Fig. 1. Cross section of the flow for the logistic thermostat oscillator in Eq. (2) with $Q = 0.1$ and $T = 1$ in the $\zeta = 0$ plane showing that the chaotic sea fills all of space without quasiperiodic 'holes.' The colors indicate the value of the local largest Lyapunov exponent (red positive and blue negative)

III. SIGNUM THERMOSTATTED LINEAR OSCILLATOR

Since $\lim_{Q\to 0}\tanh(\zeta/2Q) = \mathrm{sgn}(\zeta)$, Eq. (2) suggests taking the limit $Q, T \rightarrow 0$ but with $\alpha = T/Q$ constant giving

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -q - \alpha\mathrm{sgn}(\zeta)p \\ \dot{\zeta} &= p^2 - T. \end{aligned} \tag{3}$$

This *bang-bang controller* is arguably a better model for a real thermostat where the furnace abruptly turns on full when the temperature drops below a set point and the air conditioner turns on full when the temperature rises above that point. However, the signum function limits the rate at which heat can be delivered to or extracted from the oscillator, unlike the *proportional controller* in Eq. (1), and that rate is governed by the parameter α. In this sense, the oscillator is more weakly coupled to the heat bath than in the Nosé–Hoover case but with a faster response.

Although Eq. (3) corresponds to the logistic thermostat only in the zero-temperature ($T \to 0$) limit, the solution is apparently ergodic for α greater than about 1.8 for *all* values of T. For example, $\alpha = 2, T = 1$ gives the flow whose $\zeta = 0$ cross section is shown in Fig. 2. The Lyapunov exponents are $(0.3032, 0, -0.3032)$, and the system is nonuniformly conservative and time-reversible with a chaotic sea that fills all of space.

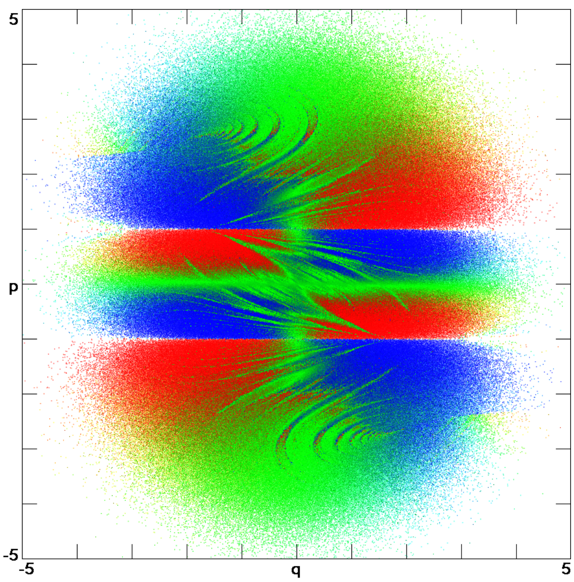

Fig. 2. Cross section of the flow for the signum thermostatted linear oscillator in Eq. (3) with $\alpha = 2$ and $T = 1$ in the $\zeta = 0$ plane

Furthermore, the probability distribution of q and p is canonical, $f(q,p) = e^{-q^2/2T}e^{-p^2/2T}/2\pi T$, while the probability $f(\zeta)$ is governed by $Tf'(\zeta) = -\alpha f(\zeta)\mathrm{sgn}(\zeta)$, whose normalized solution is $f(\zeta) = (\alpha/2T)e^{-\alpha|\zeta|/T}$. Thus the numerically calculated distributions shown in Fig. 3 for $\alpha = 2$ and $T = 1$ provide additional evidence of ergodicity. The thin black line at the edge of the red region is the theoretical distribution. The measured even moments agree to within statistical fluctuations with the theoretical (ergodic) predictions of $f(q)$ and $f(p)$ given by $\langle q^m \rangle = \langle p^m \rangle = (m-1)!! = \{0, 1, 3, 15, 105, 945, 10395, ...\}$, and $f(\zeta)$ given by $\langle \zeta^m \rangle = m!/\alpha^m = \{0, 0.5, 1.5, 11.25, 157.5, 3543.75, 116943.75, ...\}$ for $\alpha = 2$.

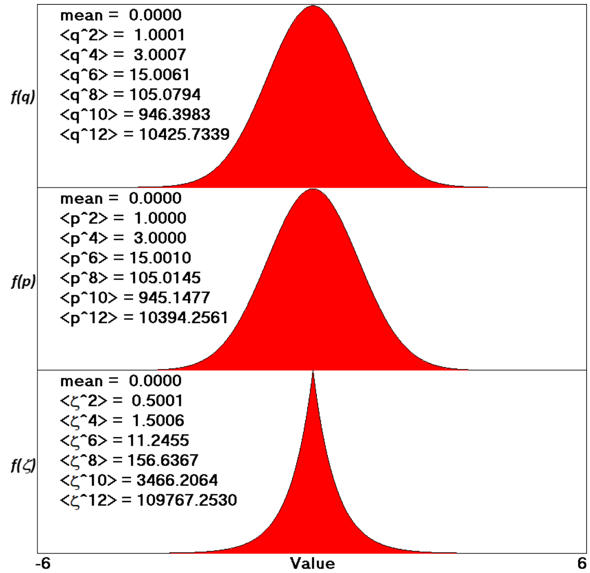

Fig. 3. Probability distributions and their even moments for the three variables of the signum thermostatted linear oscillator in Eq. (3) with $\alpha = 2$ and $T = 1$. The expected distributions are shown as black lines

Finally, Eq. (3) has the nice property that the $\dot{q}$ and $\dot{p}$ equations are linear except at $\zeta = 0$, and so the dynamics is independent of the amplitude of the oscillation. Said differently, T is an *amplitude parameter* that only affects the magnitude of the variables and thus can be taken as unity without loss of generality. If the system is ergodic for *any* temperature, it is ergodic for *ever*y temperature, and it has only a single bifurcation parameter α, which facilitates analysis of the system, especially since the system is two-dimensional and linear for $\zeta \neq 0$.

The dependence of the Lyapunov exponents and the *kurtosis* $K_p = \langle p^4 \rangle / \langle p^2 \rangle^2 - 3$ (which is zero for a Gaussian) on the parameter α is shown in Fig. 4. For each of the 500 values of α, initial conditions are chosen randomly from the canonical distribution so that the instances and prevalence of quasiperiodic solutions (where the Lyapunov exponents are zero) are evident. A wider range of initial conditions would allow a better estimate of the value of α at the onset of ergodicity but at considerable computational cost. A much longer calculation at $\alpha = 2$ with a million randomly chosen initial conditions did not reveal any quasiperiodic solutions, and so the evidence is strong that the system is ergodic with the canonical phase-space distribution.

These calculations are crucially dependent on using a good adaptive integrator with stringent error control because of the discontinuity in the signum function at $\zeta = 0$. This causes no difficulty in calculating orbits and Poincaré sections because the flow is continuous, but the singularity in the Jacobian matrix can render Lyapunov exponent calculations unreliable. However, the error in the calculated Lyapunov exponent is found to be proportional to the integration step size

Δt, and four-digit accuracy requires $\Delta t \approx 10^{-12}$ in the vicinity of $\zeta = 0$ when using a fourth-order adaptive Runge–Kutta integrator patterned after the one in Press, et al. [17].

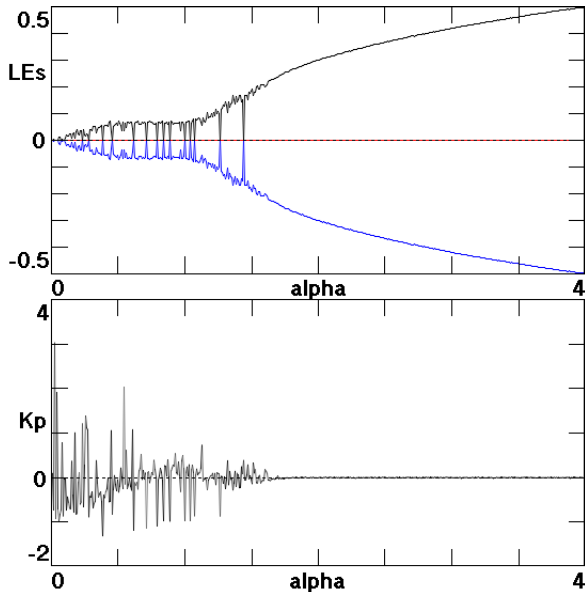

Fig. 4. Variation of the Lyapunov exponents (LEs) and the kurtosis of p (Kp) as a function of the bifurcation parameter α for the signum thermostatted linear oscillator in Eq. (3) with $T = 1$ showing the ergodic region for $\alpha > 1.8$

There are two methods to verify the correctness of the calculation. One method avoids integrating over the singularity, but calculates the contribution of the singularity analytically [18]. The other replaces $\mathrm{sgn}(\zeta)$ with $\tanh(N\zeta)$ and demonstrates convergence as $N \to \infty$ [19]. The second method was used here, where a value of $N = 500$ approaches four-digit accuracy. Even so, the least significant digit of the quoted Lyapunov exponents is only an estimate. Precise values are not essential for distinguishing chaos from quasiperiodicity and for testing ergodicity.

IV. SIGNUM THERMOSTATTED NONLINEAR OSCILLATOR

Just as with the logistic thermostat, the signum thermostat can give ergodic solutions for nonlinear oscillators. An example is given by

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -q^n - \alpha \mathrm{sgn}(\zeta) p \\ \dot{\zeta} &= p^2 - T, \end{aligned} \tag{4}$$

where n is a positive odd integer, corresponding to a symmetric potential $V(q) = q^{n+1}/(n+1)$. Using values of $n = 3, \alpha = 3$, and $T = 1$ gives the cross section at $\zeta = 0$ shown in Fig. 5. The absence of quasiperiodic holes suggests that the dynamics is ergodic, and this is confirmed by calculation of the distribution functions. Similar results occur for higher odd powers of n.

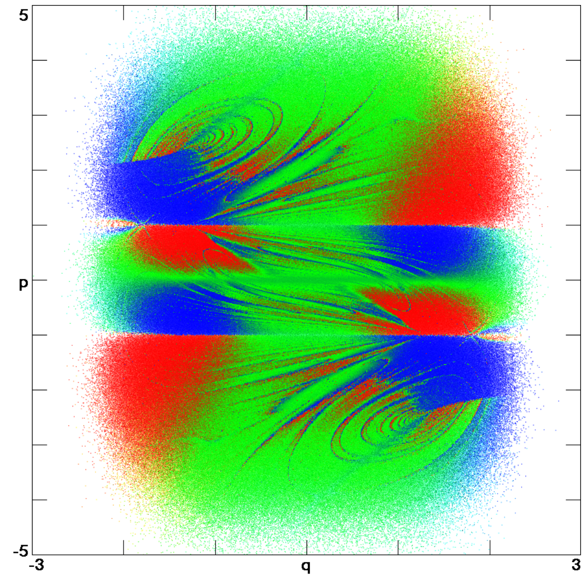

Fig. 5. Cross section of the flow for the signum thermostatted nonlinear oscillator in Eq. (4) with $n = 3, \alpha = 3$, and $T = 1$ in the $\zeta = 0$ plane

The corresponding Hamiltonian is given by $\mathcal{H}(q,p) = q^{n+1}/(n+1) + p^2/2$, and thus the probability distribution function is $f(q,p) = e^{-q^4/4} e^{-p^2/2}/6.4262...$ for $n = 3$ and $T = 1$. The Lyapunov exponents are $(0.4077, 0, -0.4077)$, and the system is time-reversible and nonuniformly conservative.

Note that since the oscillator is nonlinear, T is no longer an amplitude parameter. However, making the linear transformation $(q,p,\zeta,t) \to (T^{\frac{1}{n+1}} q, T^{\frac{1}{2}} p, T^{\frac{n+3}{2n+2}} \zeta, T^{\frac{1-n}{2n+2}} t)$ eliminates the T in the $\dot{\zeta}$ equation and replaces α in the $\dot{p}$ equation with $\alpha T^{\frac{1-n}{2n+2}}$. Thus Eq. (4) is still a single-parameter system. This result also follows from the fact that Eq. (4) has only five terms, four of whose coefficients can be set to unity through a linear rescaling of the four variables (q,p,ζ,t). If the system is ergodic with $\alpha = 3$ and $T = 1$ for a given n as appears to be the case, there is a value of $\alpha = 3T^{\frac{1-n}{2n+2}}$ that makes it ergodic for any value of T with that choice of n.

V. SIGNUM THERMOSTATTED DUFFING OSCILLATOR

The signum thermostat also gives ergodic solutions for the two-well Duffing oscillator given by

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= q - q^3 - \alpha \mathrm{sgn}(\zeta) p \\ \dot{\zeta} &= p^2 - T. \end{aligned} \tag{5}$$

The corresponding potential is $V(q) = -q^2/2 + q^4/4$ and is called a 'Mexican hat' because of its shape in the two-dimensional case. Using values of $\alpha = 5$ and $T = 1$ gives the cross section at $\zeta = 0$ shown in Fig. 6. The absence of quasiperiodic holes suggests that the dynamics is ergodic.

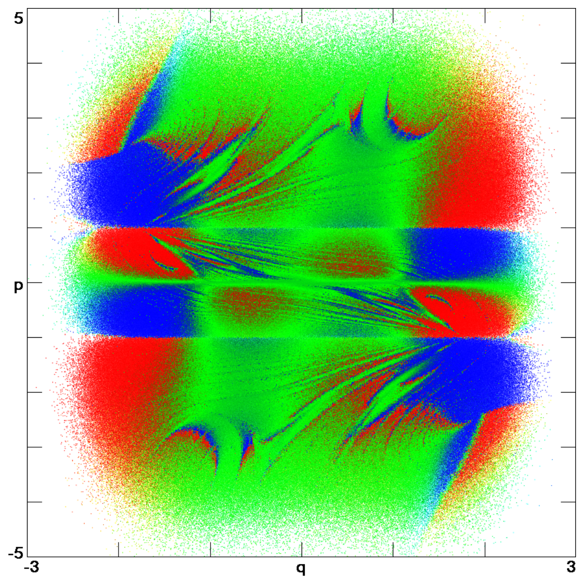

Fig. 6. Cross section of the flow for the signum thermostatted two-well Duffing oscillator in Eq. (5) with $\alpha = 5$ and $T = 1$ in the $\zeta = 0$ plane

The Hamiltonian is given by $\mathcal{H}(q, p) = -q^2/2 + q^4/4 + p^2/2$, and thus the probability distribution function for $T = 1$ is $f(q, p) = e^{q^2/2 - q^4/4} e^{-p^2/2}/9.7887\ldots$. The Lyapunov exponents are $(0.5012, 0, -0.5012)$, and the system is time-reversible and nonuniformly conservative.

As with the previous nonlinear oscillator, T is not an amplitude parameter, but in this case there is not a linear transformation of variables that preserves the form of the equations, and so it is a two-parameter system. This follows from the fact that Eq. (5) has six terms, only four of whose coefficients can be set to unity through a transformation of the variables. A complete examination of the two-parameter space would be a worthy project.

VI. SIGNUM THERMOSTATTED PENDULUM

A more challenging problem is to use the signum thermostat to obtain ergodic solutions for the simple pendulum. It appears that no combination of α and T suffice for the simple signum thermostat, but there is a solution for the system given by

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\sin(q) - \alpha(\zeta - \mathrm{sgn}(\zeta))p \\ \dot{\zeta} &= p^2 - T, \end{aligned} \tag{6}$$

which can be viewed as a superposition of the Nosé–Hoover thermostat and the signum thermostat (but with a sign reversal in the latter). For $T = 1$, there is a range of approximately $1.6 < \alpha < 2.0$ where the solution appears ergodic as shown in Fig. 7.

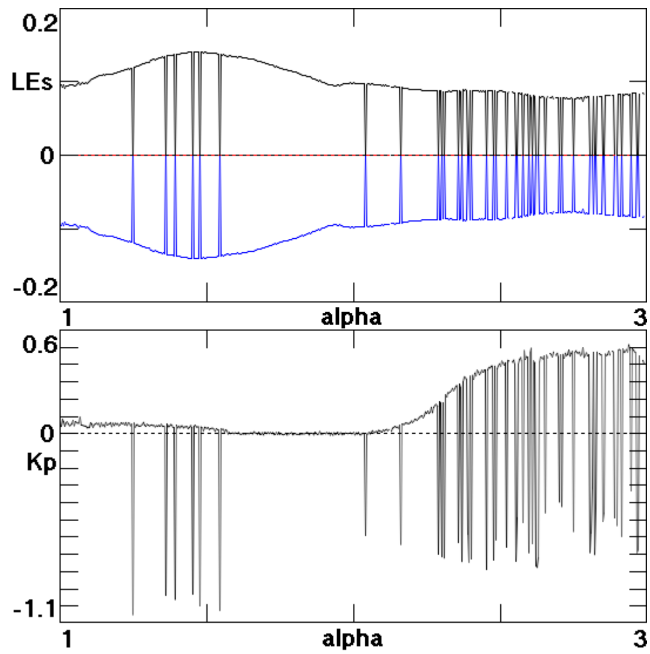

Fig. 7. Variation of the Lyapunov exponents (LEs) and the kurtosis of p (Kp) as a function of the bifurcation parameter α for the signum thermostatted pendulum in Eq. (6) with $T = 1$ showing the ergodic region for $1.6 < \alpha < 2.0$

Fig. 8 shows a cross section at $\zeta = 0$ for $\alpha = 1.8$ and $T = 1$. No quasiperiodic holes are evident. Since the solution is periodic in q with a wavelength of 2π, only a single wavelength of the orbit is shown for $-\pi < q < \pi$ with periodic boundary conditions.

The Hamiltonian is given by $\mathcal{H}(q, p) = 1 - \cos q + p^2/2$ with a corresponding probability distribution function for $T = 1$ of $f(q, p) = e^{-1+\cos q} e^{-p^2/2}/7.3355\ldots$ and $f(\zeta) = e^{1.8(|\zeta| - \zeta^2/2)}/8.3648\ldots$. The Lyapunov exponents are $(0.1079, 0, -0.1079)$, and the system is time-reversible and nonuniformly conservative.

As with the other nonlinear oscillators, T is not an amplitude parameter, and it cannot be transformed away. In fact, the system has three parameters because there are six terms, one of which ($\sin q$) is specified by two parameters, an amplitude and a wavelength. Conveniently, ergodicity occurs when two of the parameters are taken as unity making the system especially elegant. Exploration of the full three-dimensional parameter space would be a challenging study and could reveal regions where the ordinary signum thermostat produces ergodicity.

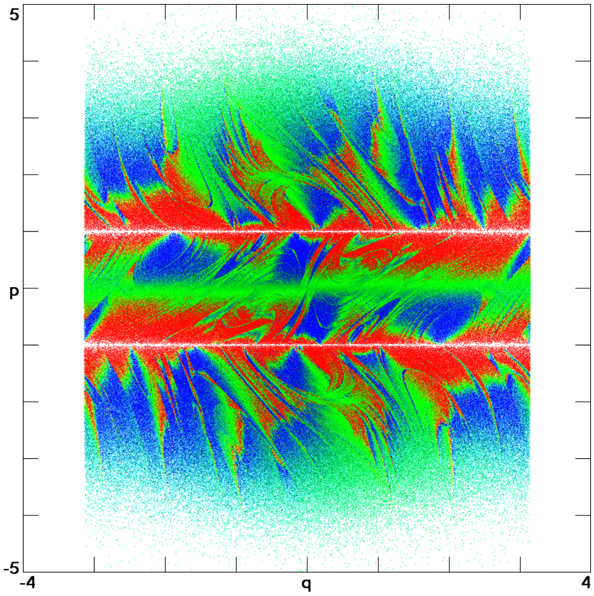

Fig. 8. Cross section of the flow for the signum thermostatted pendulum in Eq. (6) with $\alpha = 1.8$ and $T = 1$ in the $\zeta = 0$ plane

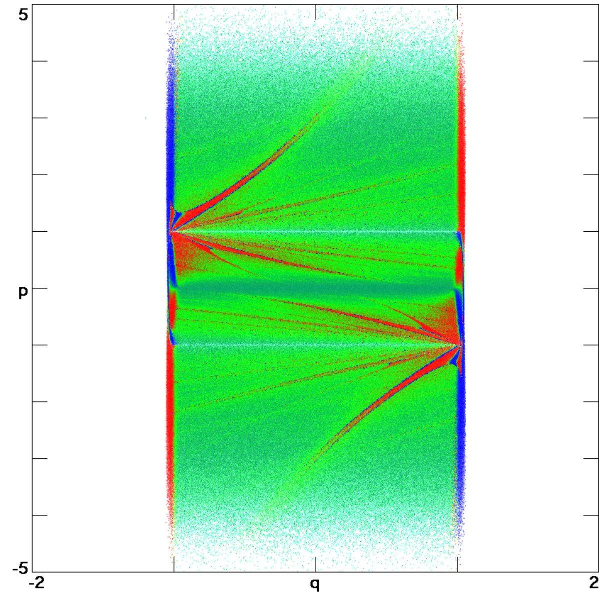

Fig. 9. Cross section of the flow for the signum thermostatted nonlinear oscillator in Eq. (4) with $n = 99, \alpha = 3$, and $T = 1$ in the $\zeta = 0$ plane. This system closely approximates an infinite square-well potential

VII. SIGNUM THERMOSTATTED SQUARE-WELL OSCILLATOR

The final example is the infinite square-well oscillator in which $V(q) = 0$ for $-1 < q < 1$ and $V(q) = \infty$ for $q = \pm 1$. The equations of motion are

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\alpha \mathrm{sgn}(\zeta) p \\ \dot{\zeta} &= p^2 - T, \end{aligned} \tag{7}$$

but with reflecting boundaries at $q = \pm 1$. The reflection is accomplished by applying the transformation $(q, p) \to (2\mathrm{sgn}(q) - q, -p)$ whenever $|q| > 1$. However, it appears that this system does not have chaotic solutions for any choice of α and initial conditions. In fact, with only four terms, Eq. (7) has no adjustable parameters, and so α can be set to 1.0 without loss of generality through a linear transformation of the variables.

To reconcile the absence of chaos in Eq. (7) with the observation that Eq. (4) has chaotic solutions that can be made ergodic for arbitrarily large n, where the limit $n \to \infty$ represents a perfect square well, consider Eq. (4) with $n = 99$, corresponding to a very deep but flat potential well given by $V(q) = q^{100}/100$. Values of $\alpha = 3$, and $T = 1$ give the cross section at $\zeta = 0$ shown in Fig. 9. Evidently, the dynamics is chaotic and ergodic. The Lyapunov exponents are $(0.3068, 0, -0.3068)$, and the system is time-reversible and nonuniformly conservative.

The corresponding Hamiltonian is given by $\mathcal{H}(q, p) = q^{100}/100 + p^2/2$, and thus the probability distribution function is $f(q, p) = e^{-q^{100}/100} e^{-p^2/2}/5.21728\ldots$. Fig. 10 shows good agreement between the expected and calculated distributions. The expected even moments of $f(q)$ are $\langle q^m \rangle = \{0, 0.3615, 0.2354, 0.1826, 0.1543, 0.1372, 0.1263\ldots\}$, in good agreement with the calculated values.

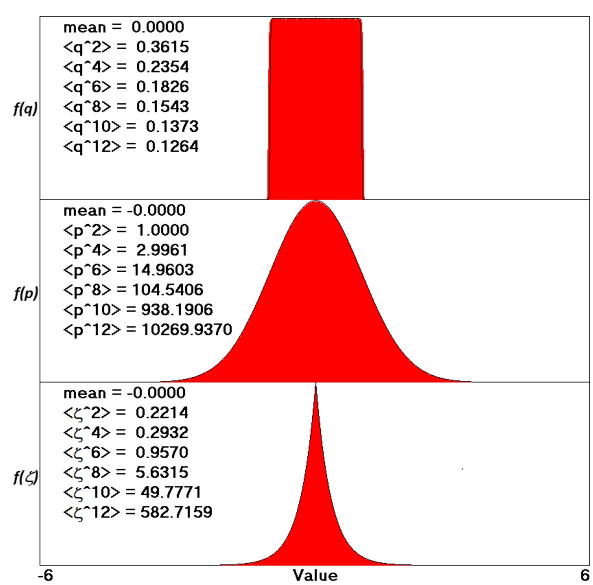

Fig. 10. Probability distributions and their even moments for the three variables of the signum thermostatted nonlinear oscillator in Eq. (4) with $n = 99, \alpha = 3$ and $T = 1$. The expected distributions are shown as black lines

Not evident in the figure is the fact that $f(p)$ converges very slowly to the expected value of $1/\sqrt{2\pi T}$ in the vicinity of $p = 0$. The reason is that if p is very small, it remains small for a long time since the restoring force $-q^{99}$ is tiny except near $q = \pm 1$. The frequency of oscillation approaches zero as $|p| \to 0$. Furthermore, unlike the linear thermostat in Eq. (1) where ζp can increase indefinitely, the signum thermostat is limited to αp. Thus the thermostat continues to turn up the furnace (increasing $-\zeta$), but the heat delivered to the oscillator is throttled by the signum function. Since p remains near zero for a long time, it can only acquire the canonical distribution by seldom visiting that region of phase space, thus accounting for the slow convergence. The more closely the nonlinear oscillator approaches the square-well limit, the longer it takes for the oscillator to reach thermal equilibrium with the heat bath and fill out the canonical distribution of momentum and kinetic energy.

VIII. SUMMARY AND CONCLUSIONS

The signum thermostat in Eq. (3) with $\alpha = 2$ is probably the simplest paradigm for an oscillator in thermal equilibrium with a heat bath. It has a number of advantages over the many alternatives that have been proposed during the past thirty years. It has an elegant simplicity, with a simple form and a single parameter, thereby simplifying analysis. For many one-dimensional oscillators, it can be rigorously shown that if the system is ergodic for *any* temperature, then it is ergodic for *every* temperature. The signum thermostat provides a wide range of one-dimensional ergodic oscillators with the canonical phase-space distribution predicted by Gibbs.

In addition to the several cases described in detail here, the signum thermostat has been successfully tested with oscillators having a variety of other restoring forces including $-\tan(q), -\sinh(q), -\arctan(q), q^2 - q^3, q^2 - q^5$, and $q^4 - q^5$, all with $\alpha = 3$ and $T = 1$. In fact, the only case for which it is known to fail is the square-well potential, and even there it fails only in the limit of a perfect square well.

A logical next step would be to apply the signum thermostat to systems with (many) more degrees of freedom. Preliminary tests indicate that the orthogonal components of the linear oscillator synchronize, with the system behaving like a one-dimensional oscillator rotated in space according to the initial conditions, while the nonlinear oscillators are more nearly ergodic for all the thermostats. It will be left as a challenge for the mathematicians to calculate the conditions for which the signum thermostat is guaranteed to exhibit ergodicity with the canonical distribution or to find other conditions where it fails to do so.

Acknowledgments

I am grateful to Bill and Carol Hoover for extensive discussions, confirmation of some of the calculations, and a careful reading of the manuscript.

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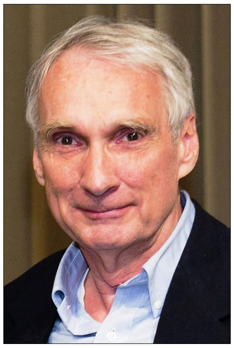

Julien Clinton Sprott received his PhD in physics from the University of Wisconsin in 1969 and joined the faculty there in 1973. After a 25-year career in experimental plasma physics, he became interested in computational nonlinear dynamics and chaos in 1988. He has authored or coauthored hundreds of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

DOI:10.12921/cmst.2018.0000042