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Ergodicity of a singly-thermostated harmonic oscillator

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ABSTRACT

Although Nosé's thermostated mechanics is formally consistent with Gibbs' canonical ensemble, the thermostated Nosé–Hoover (harmonic) oscillator, with its mean kinetic temperature controlled, is far from ergodic. Much of its phase space is occupied by regular conservative tori. Oscillator ergodicity has previously been achieved by controlling two oscillator moments with *two* thermostat variables. Here we use computerized searches in conjunction with visualization to find *singly*-thermostated motion equations for the oscillator which are consistent with Gibbs' canonical distribution. Such models are the simplest able to bridge the gap between Gibbs' statistical ensembles and Newtonian single-particle dynamics.

1. Ergodicity of the equations of motion

Gibbs' statistical mechanics is based on summing contributions from ensembles of similar systems. His *microcanonical* ensemble includes all the states of a given system which have the same energy. These energy states are accessible to a single "ergodic" system obeying Newtonian mechanics [1]. A periodic hard-disk or hard-sphere fluid is the usual example. Comparisons of Monte Carlo microcanonical-ensemble averages with molecular dynamics dynamical averages have confirmed this equivalence, even for small systems of just a few particles [2].

Certainly Boltzmann and Gibbs both realized that *all* states need to be accessible to the dynamics in order for the dynamical and phase averages to correspond. The Ehrenfests had a practical definition of "quasiergodicity". They used the word to indicate that the dynamics eventually comes "arbitrarily close" to all states. Their idea expresses very well our own view of what we call "ergodicity" in the present work.

Gibbs' *canonical* ensemble sums Boltzmann-weighted contributions from *all* energy states. The underlying idea is that the system of interest is weakly coupled to a heat reservoir with an ideal-gas density of states characteristic of a fixed kinetic temperature T. Nosé [3,4] developed a dynamics consistent with the canonical distribution by including a "time-scaling" variable s and its conjugate momentum p_s in the equations of motion. The new momentum p_s acts as a thermostat variable capable of exchanging energy between the system and a heat reservoir at temperature T.

Hoover showed that a harmonic oscillator thermostated in this way is not at all ergodic [5]. That is, there is no initial condition from which the oscillator is able to access *all* of its phase-space states. Instead, this thermostated oscillator has a nonergodic highly-complicated multi-part phase-space structure [6]. There are infinitely-many regular nonchaotic orbits embedded in a

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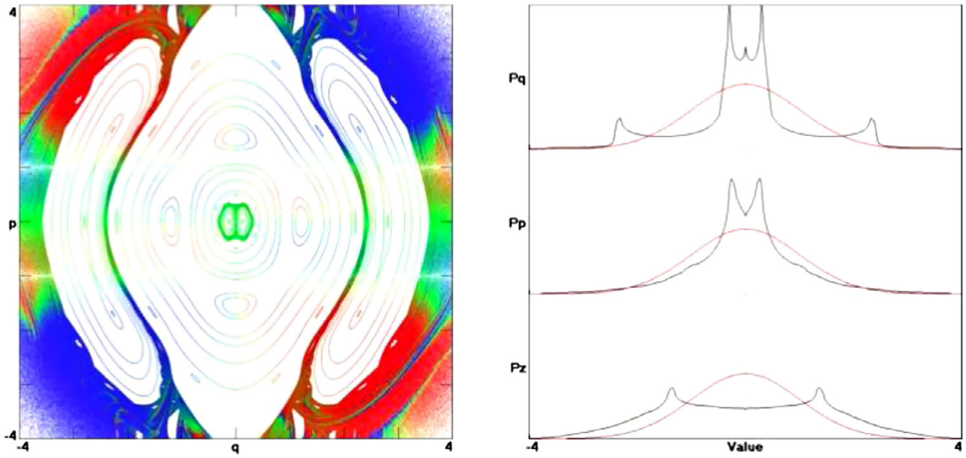

Fig. 1. This Nosé–Hoover oscillator phase-space section corresponds to the plane $\zeta = 0$. The coloring reflects the local value of the instantaneous Lyapunov exponent at each $(q, p, 0)$ point, with red least stable and blue most. The distributions of $\{q, p, \zeta\}$ in the chaotic sea are compared to Gibbs' Gaussian distributions at the right. The white space indicates nonchaotic regions filled with regular nested tori, some of which are shown. In the chaotic sea $\lambda_1 = \langle\lambda_1(t)\rangle = 0.0139$. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article).

single chaotic sea. Where "chaos" controls the motion two closeby points, $r_1(t)$ and $r_2(t)$, tend to separate from one another exponentially fast, either forward or backward in time. Such a motion is said to be "Lyapunov unstable". The averaged separation rate is described by the largest Lyapunov exponent, λ_1:

$$\delta \equiv |r_2 - r_1| \simeq e^{\lambda_1 t};\ \lambda_1 \equiv \langle\lambda_1(t)\rangle.$$

The time-averaged Lyapunov exponent λ_1 is computed as an average of the instantaneous local Lyapunov exponent, $\lambda_1(t)$. The local value is only rarely zero, even on conservative tori, where the long-time averages vanish. We illustrate $\lambda_1(t)$ for the Nosé–Hoover oscillator in Fig. 1. We choose the simplest equations of motion,

$$\{\dot{q} = p;\ \dot{p} = -q - \zeta p;\ \dot{\zeta} = p^2 - 1\}\ [\text{NH}].$$

They are time-reversible: any time-ordered sequence $\{+q, +p, +\zeta\}$ satisfying the motion equations has a time-reversed backward twin, $\{+q, -p, -\zeta\}$ satisfying the same equations. The Nosé–Hoover oscillator in $\{q, p, \zeta\}$ space is an improved and simplified version of Nosé's dynamics, which occupies a four-dimensional $\{q, p, s, p_s\}$ space [5,6].

For this Nosé–Hoover oscillator we have computed the local Lyapunov exponent on a grid of about a million points by the simple expedient of integrating backward in time and then forward, for a time of 100 in both directions. The "reversed" trajectory going forward in time can be compared to a nearby constrained "satellite" trajectory. We compute the instantaneous value of the time-dependent Lyapunov exponent just as the $\zeta = 0$ plane is crossed. In the figure red corresponds to the most positive exponent value and blue to the most negative. Within the chaotic sea the largest (time-averaged) Lyapunov exponent is 0.013_9. See Reference 6 for details.

Outside the chaotic sea lie an infinite number of regular orbits. All have a largest time-averaged Lyapunov exponent (and also a smallest) of zero. Because the oscillator is prototypical of systems with smooth minima in their energy surfaces a considerable effort has been made to find motion equations providing Gibbs' canonical distribution for it [7–18].

2. Feedback control of oscillator moments

For simplicity we choose units of force, mass, time, and temperature corresponding to choosing the oscillator force constant, mass, angular velocity, and Boltzmann's constant all equal to unity. In these units and without any thermostating the oscillator motion equation is $\ddot{q} = \dot{p} = -q$. Because distribution functions for the oscillator's displacement and momentum can be described in terms of their moments $\langle q^{2m}p^{2n}\rangle$, it was natural to control oscillator force and velocity moments with feedback variables such as ζ and ξ:

$$\{\dot{q} = p - \xi q;\ \dot{p} = -q - \zeta p\}.$$

The time dependence of the friction coefficients $\zeta(t)$ and $\xi(t)$ can be arranged so as to control one or more of the oscillator moments:

$$\dot{\zeta} = (p^2/T) - 1 \rightarrow \langle p^2\rangle \equiv T;\ \dot{\xi} = (q^4/T^2) - 3(q^2/T) \rightarrow \langle q^4\rangle \equiv 3T\langle q^2\rangle\ \ldots.$$

Bulgac and Kusnezov, along with their coworkers Bauer and Ju [15,16], considered a variety of simple systems and concluded that *cubic* contributions to the control equations, such as those in the [HH] and [JB] equations below, were especially useful in promoting chaos and ergodicity.