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Ergodic time-reversible chaos for Gibbs' canonical oscillator

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ABSTRACT

Nosé's pioneering 1984 work inspired a variety of time-reversible deterministic thermostats. Though several groups have developed successful *doubly*-thermostated models, single-thermostat models have failed to generate Gibbs' canonical distribution for the one-dimensional harmonic oscillator. A 2001 doubly-thermostated model, claimed to be ergodic, has a singly-thermostated version. Though neither of these models *is* ergodic this work has suggested a successful route toward singly-thermostated ergodicity. We illustrate both ergodicity and its lack for these models using phase-space cross sections and Lyapunov instability as diagnostic tools.

1. Single-variable thermostats and Gaussian ergodicity

In 1984 Hoover explored the application of the Nosé–Hoover version [1] of Nosé's canonical motion equations [2,3] to a harmonic oscillator at thermal equilibrium with coordinate q, momentum p, temperature T, and thermostat variable ζ:

$$\{ \dot{q} = p \; ; \; \dot{p} = -q - \zeta p \; ; \; \dot{\zeta} = [\, p^2 - T \,]/\tau^2 \,\} \; [\, \mathrm{NH} \,] \, .$$

Posch, Hoover, and Vesely found that this model partitions the (q, p, ζ) phase space into many separate toroidal regions embedded in a chaotic sea [4]. The complexity and the stiffness of the solutions increase rapidly as the thermostat response time τ is reduced. In addition to equilibrium applications analogous motion equations can be used to thermostat irreversible nonequilibrium simulations such as steady shear and heat flows. The harmonic oscillator can generate steady-state heat flow problems if the temperature varies in space [5,6]:

$$1 - \epsilon < T = T(q) = 1 + \epsilon \tanh(q) < 1 + \epsilon \, .$$

Here ϵ is the maximum value of the temperature gradient, (dT/dq), to which the oscillator is exposed. It can be viewed as the strength of nonlinearity, and depending on its value, one can move from the equilibrium regime (where $\epsilon = 0$) to the nonequilibrium regime (where $\epsilon > 0$).

Somewhat paradoxically, the Nosé–Hoover motion equations as well as all the others we consider here are *time-reversible*, even away from equilibrium. That is, any time-ordered sequence of (q, p, ζ) points can be reversed either [1] by changing the sign of dt in the integrator, or [2] by changing the signs of the (p, ζ) variables. The harmonic oscillator equations also have mirror symmetry. Changing the signs $(+q, +p) \longleftrightarrow (-q, -p)$ gives an additional pairing of solutions.

Apart from being time-reversible, a good thermostat must result in *ergodic* dynamics. Ergodicity of the dynamics connects dynamical averages with corresponding Boltzmann–Gibbs phase averages. In describing the results of the present work, we have used Ehrenfests' idea of "quasiergodicity", where the dynamics eventually comes arbitrarily close to each feasible point, interchangeably with "ergodicity".

For the equilibrium Nosé–Hoover harmonic oscillator, the Gaussian distribution is the stationary solution of the Liouville's phase-space continuity equation:

$$v \;=\; \dot{r} = (\dot{q}, \dot{p}, \dot{\zeta}) \longrightarrow (\partial f/\partial t) = -\nabla_r \cdot (f v) \equiv 0$$
$$\longrightarrow f(q, p, \zeta) \propto e^{-q^2/2T} e^{-p^2/2T} e^{-\zeta^2 \tau^2/2T} \, .$$

On the other hand, numerical work gives two kinds of solutions, either quasi-periodic tori, with all Lyapunov exponents being zero or a single chaotic, Lyapunov-unstable sea. The global dynamics, therefore, either remains confined within the tori, or occupies the chaotic sea separated from the tori, depending upon the initial conditions, the temperature T, and the response time τ. In other words the presence of two sets of global maximal Lyapunov

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exponents – one positive and another zero, indicates that a trajectory starting from an arbitrary initial condition is unable to explore the neighborhood of the entire feasible phase-space. As a result, the phase-space gets partitioned into at least two noncommunicating regions, violating the metric indecomposibility of the phase space – the necessary and sufficient condition for ergodic dynamics according to Birkhoff's theorem. Thus the singly-thermostated oscillator equations are not "ergodic", so that Gibbs' statistical mechanics is unable to describe the oscillator's properties. For the next 15 years, which included many failed attempts, no singly-thermostated oscillator models were found to be ergodic.

This letter announces our recent achievements toward the long-standing goal of ergodic singly-thermostated oscillator models. We have carried out a comprehensive exploration of a previous model claimed to be ergodic, and found that it is not. As a result of those investigations we have found a path leading to a singly-thermostated and physically motivated ergodic model for the harmonic oscillator. We lay out the details of these discoveries in what follows and encourage the reader to help explore the new areas opened up by our work.

2. Ergodicity is typically absent in the SF model

In 2001 Sergi and Ferrario [SF] announced that they had found an ergodic thermostated oscillator model [7]. In addition to the oscillator coordinate, momentum, and thermostat variable (q, p, ζ) their model includes a parameter ν which can be either positive or negative:

$$\dot{q} = p(1+\zeta\nu)\ ;\ \dot{p} = -q - \zeta p\ ;\ \dot{\zeta} = [\ p^2 - T - qp\nu\ ]/\tau^2\ ;\ \dot{\eta} = \zeta .$$

Here, and in what follows, we will ignore the fact that SF actually solve the above *four* equations, not just the three shown below:

$$\{\ \dot{q} = p(1+\zeta\nu)\ ;\ \dot{p} = -q - \zeta p\ ;\ \dot{\zeta} = p^2 - T - qp\nu\ \}\ [\text{ SF }].$$

This is because their work was based on a Hamiltonian with two degrees of freedom. Consider a particular initial condition $(q,\ p,\ \zeta)$ that evolves in some time t to a unique $(q',\ p',\ \zeta')$. The latter variables do not depend on the initial value of η, which could be given or not, arbitrarily. The fourth equation, for the evolution of a variable which is the time integral of ζ, plays no role at all in the dynamics of $(qp\zeta)$ and can so be ignored, which we do throughout. This extraneous variable obscured the fact that SF implicitly claimed ergodicity for a *singly*-thermostated oscillator. As a result, this desirable feature of their relatively widely-cited paper has been previously ignored. However, as a consequence of removing $\dot{\eta}$, the symplecticity of the dynamics disappears.

Like the NH model the SF oscillator has mirror symmetry $(+q, +p) \longleftrightarrow (-q, -p)$. In addition the time reversibility of the Sergi–Ferrario equations requires that the functions p and ζ, *as well as the parameter* ν, all change sign in the reversed motion with the coordinate values unchanged. For clarity we have replaced Sergi and Ferrario's parameter "τ" by ν throughout the present work. This change emphasizes that an increase in $|\nu|$ reduces the response time of the thermostat terms.

For the remainder of this study, we choose to keep $\tau = 1$. Usually τ, which represents the relaxation time of the dynamics, is chosen according to the relation [12]: $\tau^2 = kT/\omega^2$, where ω is the angular frequency of the system. In our present case, since the system comprises a single harmonic oscillator with unit mass and spring constant, $\omega = 1$. Additionally, most of the work ascertaining the ergodicity of thermostatted dynamics has taken the relaxation time to be unity. We wish to highlight the fact that if the relaxation time is chosen too large, it will have no effect on the system dynamics, while if τ is chosen too small, the equations become too stiff.

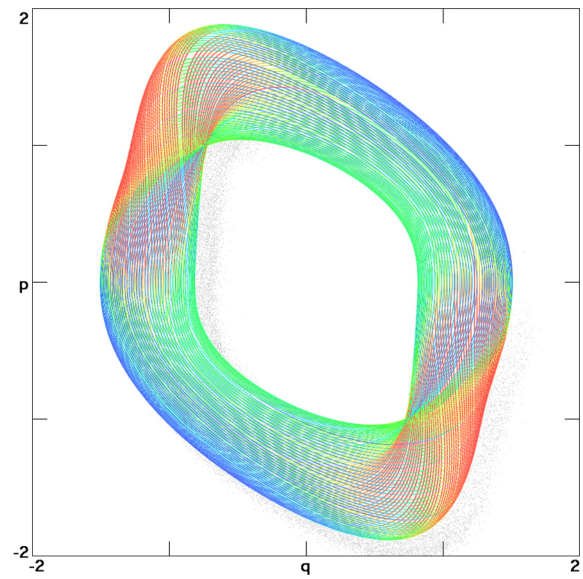

Fig. 1. The torus shown here results from the initial conditions $(q, p, \zeta) = (1, 1, 1)$ using Sergi and Ferrario's original equations with $\nu = +1$. The local values of the largest Lyapunov exponent on the torus are indicated by color: -1.06 (blue) $< \lambda_1(t) < 1.89$ (red). Its time-averaged mean value, $\lambda_1 = \langle\lambda_1(t)\rangle$ is zero. The temperature is unity. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Sergi and Ferrario claimed that their four [but actually only three, for the reason just cited] oscillator equations [7] were ergodic (filling out the entire three-dimensional Gaussian distribution) for $\nu > 0.5$. That surprising claim sparked the present work. To begin our exploration of their model we carried out a simulation of the SF equations with the temperature T and parameter ν both equal to unity and with the initial conditions $(q, p, \zeta) = (1, 1, 1)$. Fig. 1 shows the resulting torus, colored according to the local flow instability. Evidently this special case of the SF model is definitely *not* ergodic.

The difficulty in isolating a small embedded torus by looking at the global dynamics [13] prompted us to investigate the Poincaré section at $\zeta = 0$. In fact, any other *typical* Poincaré section would have served our purpose. Recall that Gibbs' probability density is Gaussian in both q and p. Accordingly sections in q and p (as well as in ζ) that are far from origin are atypical, and may not give any useful results. So long as the section chosen is a typical one, the dynamics within it can be studied to understand ergodicity.

Rather than abandoning the SF approach we also looked for modifications that might be ergodic. Changing the parameter ν from 1 to 2 or 3 or 4 or 5 or 6 and applying due diligence led in each case to the discovery of nested tori. Typically the tori penetrate the plane $\zeta = 0$ in four widely-separated distinct places. Fig. 2 illustrates these "period-four" equilibrium points for the SF equations. Just as in the other figures the online version is colored according to the local value of the largest of the three Lyapunov exponents, $\lambda_1(t)$. We denote the long-time average value of this exponent by $\lambda_1 \equiv \langle\lambda_1(t)\rangle$.

Holes in the chaotic sea are most easily found visually. Then, zooming in on such a hole the central point corresponding to a periodic orbit can be found. By first looking at cross sections decorated by a million penetration points and then zooming in on the holes we can obtain precise six-figure estimates for the $(q, p, 0)$ points that lie at the center of each hole, on the central periodic orbit. Viewed in the $(q, p, 0)$ plane, diligent searches showed that the six choices of ν shown in Fig. 2, *all* include simple tori centered on a periodic orbit and embedded in a chaotic sea. Looking at the figure, the relatively small but clearly visible holes can be seen for $\nu = 2, 4, 5$, and 6. The large irregular holes for $\nu = 1$ form