The Nosé-Hoover, Dettmann, and Hoover-Holian Oscillators

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(Dated: August 13, 2019)

Abstract

To follow up recent work of Xiao-Song Yang[1] on the Nosé-Hoover oscillator[2–5] we consider Dettmann's harmonic oscillator[6,7], which relates Yang's ideas directly to Hamiltonian mechanics. We also use the Hoover-Holian oscillator[8] to relate our mechanical studies to Gibbs' statistical mechanics. All three oscillators are described by a coordinate q and a momentum p. Additional control variables (ζ, ξ) vary the energy. Dettmann's description includes a time-scaling variable s, as does Nosé's original work[2,3]. Time scaling controls the rates at which the (q, p, ζ) variables change. The ergodic Hoover-Holian oscillator provides the stationary Gibbsian probability density for the time-scaling variable s. Yang considered *qualitative* features of Nosé-Hoover dynamics. He showed that longtime Nosé-Hoover trajectories change energy, repeatedly crossing the $\zeta = 0$ plane. We use moments of the motion equations to give two new, different, and brief proofs of Yang's long-time limiting result.

Keywords: Nosé-Hoover Oscillator, Dettmann Oscillator, Hoover-Holian Oscillator, Nonlinear Dynamics

I. BACKGROUND

Nosé-Hoover dynamics was developed in 1984 as a side benefit of a Centre Européen de Calcul Atomique et Moléculaire ("CECAM") Workshop on Constrained Dynamics organized by Carl Moser. The workshop was held at Orsay, about 20 miles southwest of Paris. Shuichi Nosé and Bill Hoover met by chance at the Orly airport a few days prior to the Orsay meeting and were able to spend several hours together near the Notre Dame cathedral, discussing Nosé's recent work on the thermal control of molecular dynamics simulations[2,3].

Seeking better to understand Nosé's innovative work Hoover applied Nosé's ideas to the one-dimensional harmonic oscillator problem[4–12]. He generated hundreds of solutions of the set of three ordinary differential equations using the fourth-order Runge-Kutta algorithm. The time-dependent variables (q, p, ζ) are respectively the oscillator coordinate, momentum, and friction coefficient. Here are the three equations :

$$\{ \ \dot{q} = p \ ; \ \dot{p} = -q - \zeta p \ ; \ \dot{\zeta} = [\ p^2 - 1 \ ]/\tau^2 \ \} \ [\text{ Nosé} - \text{Hoover }].$$

Provided that the mean value of the friction coefficient ζ is finite (so that the longtime average of its time derivative, $\langle \ \dot{\zeta} \ \rangle$, vanishes) the last equation implies that the mean oscillator temperature $\langle \ p^2 \ \rangle$ is unity for long times. Thus ζ acts as a "thermostat". Posch, Hoover, and Vesely explored the detailed nature of the oscillator solutions[5] for a variety of response times τ. Wang and Yang extended this work[9,10] and found, in addition to the known periodic, toroidal, and fat-fractal chaotic trajectories, additional periodic trajectories, and tori, in the form of knots ! The types of solutions found vary with τ and with the initial values of (q, p, ζ). In the present work we choose $\tau = 1$.

II. CONSEQUENCES OF TIME SCALING

In the Summer of 1996 Carl Dettmann discovered a *vanishing* Hamiltonian which precisely reproduces the time-dependence of the Nosé-Hoover flow where the Nosé-Hoover momentum becomes (p/s)[6,7].

$$\mathcal{H}_D(q, p, s, \zeta) \equiv (s/2)[\ q^2 + (p/s)^2 + \ln(s^2) + \zeta^2 \ ] \equiv 0 \rightarrow$$

$$s^2 = e^{-(q^2+(p/s)^2+\zeta^2)} \ .$$

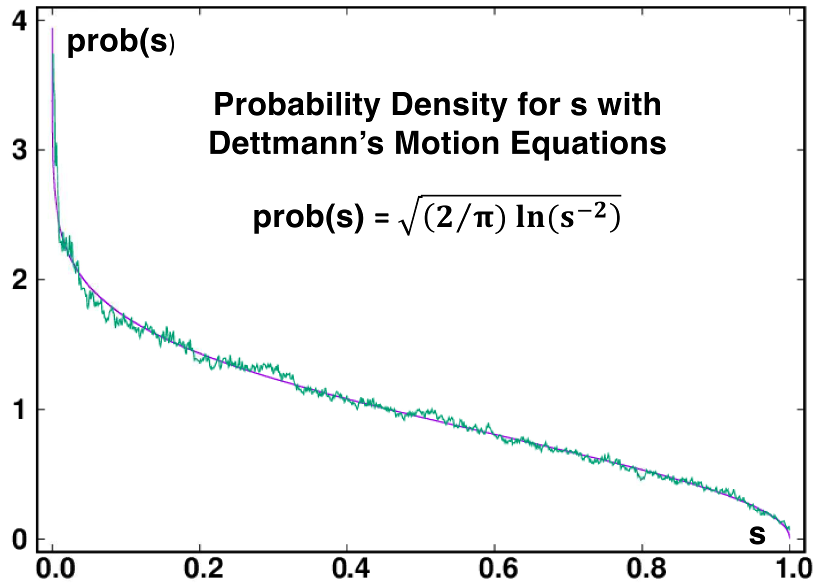

FIG. 1: Analytic and numerical probability densities for the time-scaling variable s. Both are based on the three-dimensional Gaussian distribution with numerical values from the Hoover-Holian model.

The "time-scaling variable" s has the conjugate momentum $p_s = \zeta$. $|s|$ must be less than unity for $\mathcal{H}_D$ to vanish. We select positive values, $0 < s < 1$, in our numerical work. The various resulting flows can occupy one-, two-, or three-dimensional subspaces of the full stationary solution, the Gaussian function :

$$(2\pi)^{-3/2}\exp[\ -(q^2 + (p/s)^2 + \zeta^2)/2\ ]\ .$$

With this Gaussian distribution known the normalized probability density for s follows easily,

$$\sqrt{(2/\pi)\ln(s^{-2})}\ .$$

Figure 1 compares this analytic distribution to a thousand-point histogram from a fourth-order Runge-Kutta solution of the (ergodic) Hoover-Holian oscillator equations[8] :

$$\{\ \dot{q} = p\ ;\ \dot{p} = -q - \zeta p - \xi p^3\ ;\ \dot{\zeta} = p^2 - 1\ ;\ \dot{\xi} = p^4 - 3p^2\ \}\ .$$

For the Figure q and p were initially unity and the two control variables were zero. Ten million timesteps, $dt = 0.001$, were used. The stationary distribution for the Hoover-Holian equations is the four-dimensional Gaussian $(2\pi)^{-2}\exp[\ (-q^2 - p^2 - \zeta^2 - \xi^2)/2\ ]$. Because the model is ergodic, covering the entire four-dimensional Gaussian[8], we were able to use the three-dimensional Hoover-Holian subset (q^2, p^2, ζ^2) data as a model for the stationary Dettmann distribution ($q^2, (p/s)^2, \zeta^2$) with s determined from the condition $\mathcal{H}_D \equiv 0$. These numerical data, confirming our analytic work, are shown in Figure 1.

Following up his earlier investigations of oscillator trajectories (including knots[9,10] !) Professor Xiao-Song Yang has recently proved that the oscillator motion, independent of the chosen initial conditions, must nearly always cross the $\zeta = 0$ plane[1]. Yang considered the Nosé-Hoover equations, which follow from Dettmann's Hamiltonian with the replacement $(p/s) \rightarrow p$:

$$\{ \ \dot{q} = p \ ; \ \dot{p} = -q - \zeta p \ ; \ \dot{\zeta} = p^2 - 1 \ \} \ .$$

The only situation in which the $\zeta = 0$ plane is not crossed repeatedly is an unstable straight-line portion of the ζ axis :

$$q(t) = q(0) = 0 \ ; \ p(t) = p(0) = 0 \ ; \ \zeta(t) = \zeta(0) - t \ .$$

In the present work we first consider oscillator trajectories from the standpoint of the continuity equation in (q, p, ζ) space. Because the Nosé-Hoover equations are not strictly Hamiltonian, except in the $\mathcal{H}_D \equiv 0$ case discovered by Dettmann, the Nosé-Hoover flow is compressible – the three-dimensional divergence is locally nonzero, responding linearly to the control variable ζ :

$$(\partial \dot{q}/\partial q) + (\partial \dot{p}/\partial p) + (\partial \dot{\zeta}/\partial \zeta) = 0 - \zeta + 0 \ [\ \mathrm{Dettmann} = \mathrm{Nosé} - \mathrm{Hoover} \ ] \ .$$

Consider a longtime trajectory. Evidently a *positive* longtime average of ζ would correspond to a *vanishing of the comoving volume* and a dimensionality loss. A negative average would correspond to divergence, a numerical instability. In fact, the continuity equation has been used to explain the fractal nature of chaotic flows with positive friction[12].

In (q, p, ζ) space the continuity equation shows that the comoving volume element $\otimes$ vanishes and can become fractal if the longtime-averaged control variable is positive. The volume diverges, and the simulation stops, if that averaged variable is negative. The motion equations for the oscillator, in either (q, p, ζ) space or $(q, p, s, p_s = \zeta)$ space, can also be used to prove Professor Yang's zero-crossing result. We turn to that next.

III. PROOFS OF PROFESSOR YANG'S $\zeta = 0$ PLANE RESULT

Yang's recent contribution[1] considers the three-variable Nosé-Hoover oscillator and shows algebraically that any longtime trajectory – other than the special constant $(q, p, \dot{\zeta})$ unstable straight line – must repeatedly cross the $\zeta = 0$ plane. This is a handy result as the Poincaré sections at that plane are commonly used to diagnose the fractal character of nonlinear flows. Yang's proof-of-crossing is relatively long, thirty pages, mainly algebra. Let us provide two simpler demonstrations of his result. Multiply the three motion equations by q, p, and ζ respectively and compute their longtime ($t \to \infty$) averages $\langle \ \dots \ \rangle$ in the usual way :

$$\langle \ f[q, p, \zeta] \ \rangle = (1/t) \int_0^{t \to \infty} f[\ q(t'), p(t'), \zeta(t') \ ] dt' \ .$$

Assume also that $\langle \ q^2, p^2, \zeta^2 \ \rangle$ are finite (so that their time derivatives average to zero). The three Nosé-Hoover differential equations then give three identities:

$$\{ \ \langle \ qp \ \rangle = 0 \ ; \ \langle \ qp \ \rangle = \langle \ -\zeta p^2 \ \rangle \ ; \langle \ \zeta \ \rangle = \langle \ \zeta p^2 \ \rangle \ \ \} \ .$$

Combining the three shows that the mean value of ζ vanishes, equivalent to Professor Yang's result.

An even simpler demonstration follows from Nosé's original Hamiltonian[2,3], $\mathcal{H}_N \equiv (1/s)\mathcal{H}_D$, which gives a simple evolution equation for s : $\dot{s} = p_s$. Because p_s and ζ are identical, as shown by Dettmann, the time-average of the $\dot{s}$ equation shows directly (assuming numerical convergence of the motion) that the control variable ζ has mean value zero, again implying Yang's result.

IV. AN AFTERWORD FOR YOUNG RESEARCHERS

Lingering geometric and topological questions remain where the chaotic sea is concerned. The sea is an enduring paradoxical concept. Is it a set of three-dimensional points? Is it a continuum with holes here and there? Is it just a single chaotic trajectory? Is it an ill-defined limit? These questions remain at the research frontier. Let us have a look at the chaotic sea for the Nosé-Hoover oscillator.

Figure 2 shows cross-sections of the three-dimensional oscillator's (q, p, ζ) phase space showing about ten million crossings of the three planes where each of the variables vanishes. The fourfold symmetry of these sections reflects the time-reversibility of the motion equations

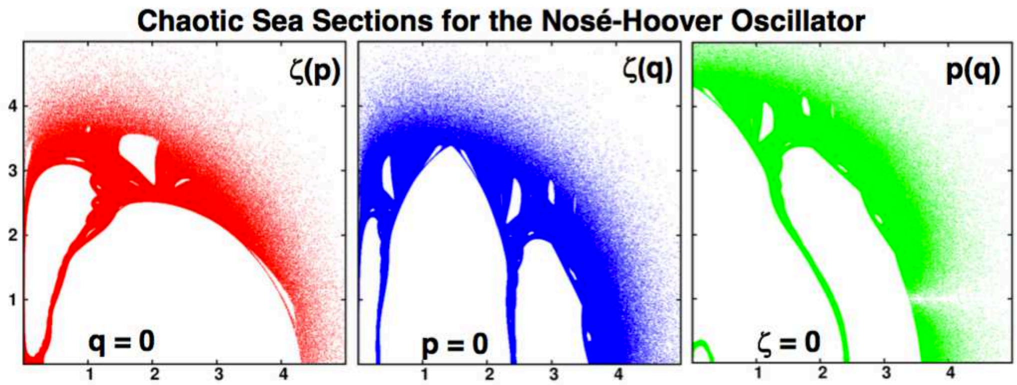

FIG. 2: Sections of the Nosé-Hoover Chaotic Sea where q or p or ζ vanishes. Only one quadrant is shown here as each of the Sections has fourfold symmetry.

as well as the fact that any solution $\{ +q, +p, +\zeta \}_t$ implies the existence of a mirror-image solution $\{ -q, -p, +\zeta \}_t$, as well as $\{ +q, -p, -\zeta \}_t$.

For $\tau = 1$ about six percent of the Gaussian distribution[13] $e^{-(q^2+p^2+\zeta^2)/2}$ appears to be a cohesive connected sea, penetrated by infinitely many regular orbits with zero Lyapunov exponents $\{ \lambda \}$. These exponents describe the longtime average growth or decay rates of small perturbations. The boundary between points with a positive λ, charateristic of the sea, and points with all zero Lyapunov exponents is evidently murky and uncertain. The boundary region is likely fractal in the sense that in the neighborhood of any chaotic point in the sea there must be other points only a small distance away, located on periodic orbits of great length, well beyond our capacity to compute in any meaningful way.

The mathematics of such sets of points is confused through concepts related to Hilbert's Hotel and the Banach-Tarski Theorem. Hilbert's Hotel, with positive integer room numbers, is alway full (with $\aleph_0$ guests) but with always an available room (by moving customers from n to n+1). Similar mappings of points in two or three (or many) dimensional spaces enable the disection of a sphere into a finite number of pieces which can then be reassembled to make two spheres. This is an active field of mathematics at the moment. For a nicely illustrated description of the Banach-Tarski paradox see Reference 14.

V. ACKNOWLEDGEMENT

We thank Professor Xiao-Song Yang for useful email communications and the anonymous referee for several useful suggestions which have improved this manuscript.

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