Another Hamiltonian "Thermostat" – Comments on arXiv 1203.5968, 1204.4412, 1205.3478, and 1206.0188

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Abstract

Campisi, Zhan, Talkner, and Hänggi state, in promoting a new logarithmic computational thermostat [arXiv 1203.5968 and 1204.4412] , that (thermostated) Nosé-Hoover mechanics is not Hamiltonian. First I point out that Dettmann clearly showed the Hamiltonian nature of Nosé-Hoover mechanics. The trajectories $\{ q(t) \}$ generated by Dettmann's Hamiltonian are *identical* to those generated by Nosé-Hoover mechanics. I also observe that when the (Hamiltonian) Campisi thermostat is applied to "nonequilibrium" heat transfer problems some very interesting, and somewhat paradoxical, phase portraits result. See too Marc Meléndez' nice arXiv 1205.3478 as well as our joint work arXiv 1206.0188.

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In 1984 Shuichi Nosé discovered a deterministic, time-reversible, logarithmic thermostat[1]. This computational thermostat imposes a time-averaged kinetic temperature $kT \equiv m\langle\ v^2\ \rangle$ through a thermostated Hamiltonian. His Hamiltonian includes a "time-scaling variable", s, along with its conjugate momentum p_s. Consider the simplest interesting example. For a single harmonic oscillator (with mass m, force constant κ, relaxation time τ and Boltzmann's constant k all set equal to unity) Nosé's thermostated Hamiltonian is :

$$2\mathcal{H}_{\text{Nosé}} = [\ (p/s)^2 + q^2 + p_s^2 + T\ln(s^2)\ ]\ .$$

The equations of motion which follow from Nosé's Hamiltonian ,

$$\dot{q} = (p/s^2)\ ;\ \dot{p} = -q\ ;\ \dot{s} = p_s\ ;\ \dot{p}_s = (p^2/s^3) - (T/s)\ ,$$

are somewhat "stiff" because s can become arbitrarily small. "Scaling the time" in these equations of motion, by a factor of s, gives a *new*, and better behaved, set :

$$\dot{q} = (p/s)\ ;\ \dot{p} = -sq\ ;\ \dot{s} = sp_s\ ;\ \dot{p}_s = (p/s)^2 - T\ .$$

Then, to convert to the simpler "Nosé-Hoover" form: introduce $v = (p/s)$ and $\zeta = p_s$:

$$\dot{q} = v\ ;\ \ddot{q} = \dot{v} = -q - \zeta\dot{q} = -q - \zeta v\ ;\ \dot{\zeta} = [\ \dot{q}^2 - T\ ] = [\ v^2 - T\ ]\ .$$

The time scaling used to obtain the Nosé-Hoover equations suggests (wrongly, it turns out) that they are "non-Hamiltonian". Though well-behaved, these Nosé-Hoover motion equations are not ergodic. For the harmonic oscillator they have a wide variety of periodic, nearly-periodic, and chaotic, solutions[2].

On the other hand, in July 1996, Carl Dettmann discovered that a *different*, but closely related, Hamiltonian ,

$$2\mathcal{H}_{\text{Dettmann}} \equiv s\mathcal{H}_{\text{Nosé}} = (p^2/s) + s[\ q^2 + p_s^2 + T\ln(s^2)\ ] \equiv 0\ ,$$

gives directly the Nosé-Hoover motion equations but *without any time scaling*[3–5]. The equations of motion from Dettmann's Hamiltonian are as follows :

$$\dot{q} = (p/s)\ ;\ \dot{p} = -sq\ ;\ \dot{s} = sp_s\ ;\ \dot{p}_s = (1/2)(p/s)^2 - [\ (1/2)q^2 + (1/2)p_s^2 + T\ln s\ ] - T\ .$$

Because Dettmann's Hamiltonian is identically equal to zero, the combination in square brackets is equal to $-(1/2)(p/s)^2$:

$$[\ (1/2)q^2 + (1/2)(p_s^2 + T\ln s\ ] \equiv -(1/2)(p/s)^2\ .$$

Introducing $v = (p/s)$ and $\zeta = p_s$ *again* produces the Nosé-Hoover equations, but this time *without the need for any time scaling* :

$$\dot{q} = v \ ; \ \ddot{q} = \dot{v} = -q - \zeta \dot{q} = -q - \zeta v \ ; \ \dot{\zeta} = [\ \dot{q}^2 - T \ ] = [\ v^2 - T \ ] \ .$$

A year later Dettmann and Gary Morriss published yet *another* Hamiltonian form[4] :

$$2\mathcal{H}_{\rm DM} \equiv e^{-Q}[\ p^2 + P^2 \ ] + e^{+Q}[\ q^2 + 2TQ \ ] \equiv 0 \ .$$

This Dettmann-Morriss Hamiltonian, though slightly different, leads, in a very similar way, to the same Nosé-Hoover motion equations. This approach was soon rediscovered by Bond, Leimkuhler, and Laird[6], who refer to Dettmann's original Hamiltonian as the Nosé-Poincaré Hamiltonian. All these discoveries make the Hamiltonian nature of the Nosé-Hoover equations quite clear.

Campisi *et alii*[7] cited Klages' book[8] as the source of their "nonHamiltonian" characterization of Nosé-Hoover mechanics. In that book Klages warns the reader: "one should carefully distinguish between traditional Hamiltonian formulations of classical mechanics and the generalized Hamiltonian formalism outlined [in the book]." It seems to me that one can take this warning too seriously. In several helpful and stimulating private communications Campisi, Hänggi, and Klages emphasized the arbitrary value of Dettmann's Hamiltonian, zero, as well as the failure of the (q, v, ζ) Nosé-Hoover equations to follow Liouville's Theorem.

Admittedly, Dettmann's zeroing of the Hamiltonian could be accomplished in several ways. One way is to add a term proportional to s , chosen in conjunction with the initial conditions in order to make the Hamiltonian vanish. This is essentially the "Poincaré" transformation noticed by Bond, Leimkuhler, and Laird. Continuing with the simple harmonic oscillator example, with T additionally chosen equal to unity :

$$\{ \ q, p, s, p_s \ \} = \{ \ 1, 0, 1, 1 \ \} \ \ [\text{ initial conditions }] \ ,$$

the Hamiltonian becomes :

$$\mathcal{H}_{\rm Another} \equiv (s/2)[\ (p/s)^2 + q^2 + p_s^2 \ ] + s \ln(s) - s \ .$$

The corresponding equations of motion that follow from it (and satisfy Liouville's theorem) are :

$$\{ \ \dot{q} = (p/s) \ ; \ \dot{p} = -sq \ ; \ \dot{s} = sp_s \ ; \ \dot{p}_s = (1/2)[\ (p/s)^2 - q^2 - p_s^2 \ ] - \ln s \ \} \ .$$

The solution of these equations is identical to that from the Nosé-Hoover equations,

$$\{ \dot{q} = v \ ; \ \dot{v} = -q - \zeta v \ ; \ \dot{\zeta} = v^2 - 1 \} \ ,$$

where $v = (p/s)$, $\zeta = p_s$, and the initial values are $\{ q, v, \zeta \} = \{ 1, 0, 1 \}$.

There is no obvious way to introduce a second temperature into the Nosé, Dettmann, or Dettmann-Morriss Hamiltonian. Nevertheless multi-temperature problems can be treated easily by generalizing the Nosé-Hoover equations of motion to control sets of velocities through a set of friction coefficients[5]. By sandwiching Newtonian degrees of freedom between two sets of boundary particles (a "hot" set and a "cold" set) it is easy to simulate steady heat flow. It is well-established that such dissipative systems give multifractal strange attractors in the full system+thermostats phase space[5].

Campisi *et alii* claim that their own Hamiltonian ,

$$\mathcal{H}_{\rm Campisi} = \mathcal{H}_{\rm usual} + (kT/2) \ln(\delta^2 + S^2) + (P^2/2M) \ ,$$

plus an unspecified (and crucial) weak coupling between the system variables $\{ q \}$ and the thermostat variable S is an improvement[7]. If their thermostat is more easily matched in laboratory experiments then it is indeed a step forward. But, if a multi-temperature Campisi Hamiltonian, including $\Sigma[\ (kT_i/2) \ln(\delta^2 + S_i^2) \ ]$, *could* impose more than a single temperature on selected degrees of freedom, either Liouville's theorem or the fractal phase-space structures that arise away from equilibrium *would* be casualties. Typically, Hamiltonians don't give fractals.

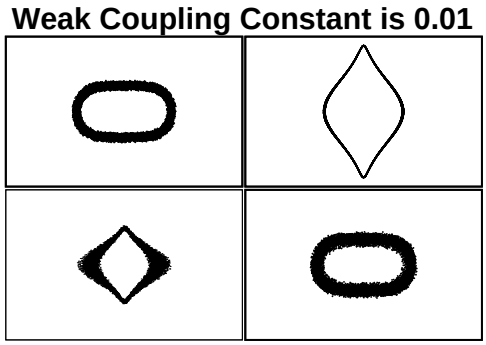

Figure 1: Phase-plane portraits with $\epsilon = 0.01$. The specified boundary temperatures are 0.5 and 1.5 . Actual kinetic temperatures are $\{ 0.46, 0.70, 0.74, 1.40 \}$, left to right, starting at the bottom.

I. ADDENDUM OF 30 APRIL 2012

How can a strictly Hamiltonian thermostat satisfy Liouville's Theorem (incompressible flow in phase space) while simultaneously giving the multifractal structures (on all scales) associated with dissipative systems? These two demands are contradictory, and so merit investigation. After trying several inconclusive modifications of the simple thermostated harmonic oscillator problem I introduced more complexity, considering a short (two-particle) "ϕ^4" chain, with one particle coupled to a "hot" Campisi Thermostat and the other to a "cold" one. The Figures show phase portraits for both the chain and the thermostat particles, for the two choices $\{\epsilon\} = \{ 0.01, 0.10 \}$, using the Hamiltonian :

$$2\mathcal{H} \equiv \sum_{i=1}^{2} [\, T_i \ln(S_i^2 + \epsilon) + P_i^2 \,] + \epsilon [\, (S_1 - x_1)^2 + (S_2 - x_2)^2 \,] + (x_1^4 + x_2^4)/2 + (x_1 - x_2)^2 + p_1^2 + p_2^2 \; .$$

The particle phase-plane $\{ q, p \}$ trajectories are shown in Figures 1 and 2. The two imposed temperatures, nominally 1.5 and 0.5, and the weak-coupling parameter $\epsilon = 0.01$ and 0.10 , provide typical, but quite surprising, results.

The nature of these solutions is at the least "odd", from the standpoint of the Second Law of Thermodynamics. They provide a large temperature gradient, but with nowhere for the heat to flow! There are no energy sources or sinks in these problems. Evidently these Hamiltonian systems cannot be dissipative, *despite* their temperature gradients, and have instead perfectly well-behaved solutions satisfying Liouville's incompressible Theorem, $(df/dt) \equiv 0$.

This odd behavior deserves a more thorough investigation than I can undertake here.

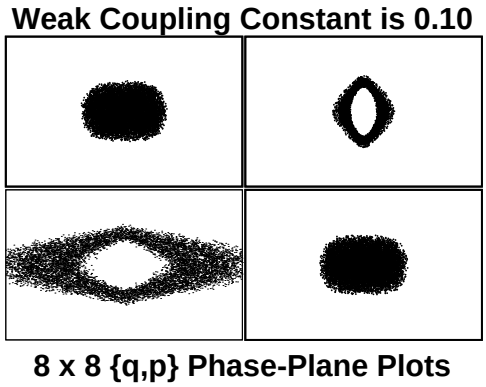

Figure 2: Phase-plane portraits with $\epsilon = 0.10$. The specified boundary temperatures are 0.5 and 1.5 . Actual kinetic temperatures are $\{ 0.71, 0.53, 0.60, 0.97 \}$, left to right, starting at the bottom.

But the broad outlines seem clear. The nature of the Hamiltonian thermostat coupling is crucial. If the coupling is weak then the thermostats oscillate independently of the "system" (here a two-particle chain). If the coupling is strong then the thermostats no longer impose the desired kinetic temperatures on the hot and cold parts of the system. These problems deserve, and will no doubt receive, detailed investigation.

II. ADDENDUM OF 23 MAY 2012

There are two other examples of non-dissipative Hamiltonian thermostats in "Hamiltonian Dynamics of Thermostated Systems: Two-Temperature Heat-Conducting ϕ^4 Chains", published in the Journal of Chemical Physics **126**, 164113 (2007). The "Hoover-Leete Hamiltonian thermostat" keeps the kinetic energy constant through a straightforward application of Lagrangian constraints. The "Landau-Lifshitz Hamiltonian thermostat" keeps the *configurational* temperature constant. *Both these latter thermostats are unable to stimulate heat flow.* The log-thermostat of Campisi *et alii* [Reference 7, which will soon appear in Physical Review Letters] is certainly the simplest example of this anomalous behavior.

I would particularly like to thank Michele Campisi, Peter Hänggi, Rainer Klages, and Marc Meléndez for a series of stimulating and educational emails on this subject. See also Marc's very recent and perceptive [arχiv 1205.3478] contribution of 15 May 2012: "On the Logarithmic Oscillator as a Thermostat".

III. ADDENDUM OF 16 JUNE 2012

More details of the log-thermostats' shortcomings will appear in Marc Meléndez' and my joint work, arXiv 1206.0188 . Another example of Hamiltonian bases for "nonHamiltonian" thermostated equations of motion appears in Wm. G. Hoover, B. Moran, C. G. Hoover, and W. J. Evans' "Irreversibility in the Galton Board *via* Conservative Classical and Quantum Hamiltonian and Gaussian Dynamics", Physics Letters A **133**, 114-120 (1988) .

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