

Comment on
“Logarithmic Oscillators: Ideal Hamiltonian Thermostats”

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Abstract

Campisi, Zhan, Talkner and Hänggi have recently proposed a novel Hamiltonian thermostat which they claim may be used both in simulations and experiments. We show, however, that this is not possible due to the length and time scales involved, which depend *exponentially* on the total energy of the system. The implementation suggested by Campisi *et alii* implies equilibration times greater than the age of the universe for systems with more than a few dozen particles.

Campisi, Zhan, Talkner and Hänggi have recently proposed the use of the logarithmic oscillator as a novel Hamiltonian thermostat [1] and have claimed that “it may be implemented not only in a computer but also with real-world experiments”. Unfortunately, this is not possible in most practical applications, because of the length and time scales involved, which depend *exponentially* on the total energy of the system (which in turn should be set to a large value, according to [1]).

Consider the implementations suggested in [1]: an ion in a two-dimensional Coulomb potential generated by a thin oppositely charged wire (or a laser beam) that interacts through short ranged forces with a gas of neutral atoms confined in a box. The size L of the box is chosen according to $L = 2\sigma\sqrt{e^{2\beta E_{\text{tot}}} - 1}$, which guarantees that the ion never leaves the box. In addition, the energy E_{tot} should be “large” in order to reduce the effect of an approximation introduced in the logarithmic potential (for 2 and 3 particles, the values chosen in [1] were $5k_B T$ and $8k_B T$, respectively). Furthermore, Campisi *et alii* estimate that, if the number N of atoms increases, then E_{tot} should increase accordingly, with $E_{\text{tot}} \propto 3Nk_B T/2$. For a system of just 26 atoms this means that the length L of the box is larger than the diameter of planet Earth (setting $\sigma = 10^{-10}$ m). But, apart from the obvious problems that such a setup would imply, the system formed by the ion plus 26 atoms would take extraordinarily long to equilibrate. A crude estimate of the mean free time for the logarithmic oscillator gives

$$\tau \sim \sqrt{\frac{m}{k_B T}} \frac{L^2 \sigma}{4\pi N \sigma^2} \sim 10^{19} \text{ s},$$

($m = 1$ amu, $T = 1$ K), exceeding the age of the universe.

The same problems arise in computational simulations. Even in simulations with only two or three particles, the number of time steps necessary to sample the theoretical canonical distribution is of the order of 10^9 steps if one wishes a reasonable reproduction of the results presented in [1].

Campisi *et alii* have also suggested that the logarithmic oscillator can be used in other settings as, for example, “to study the response of a system to a varying temperature”. Following this suggestion, we have explored the behaviour of *two* logarithmic oscillators at different temperatures brought into contact by means of two 9-atom ϕ^4 chains [2] with periodic boundary conditions. No tendency towards the theoretical linear temperature gradient was observed.

The logarithmic oscillator Hamiltonian presented by Campisi *et alii* is undoubtedly the simplest example for which Gibbs’s statistical mechanics implies the canonical distribution in phase space, but although log-thermostats have excellent pedagogical values, they are not useful in most practical applications, whether simulations or experiments.

ADDENDUM OF 17 JUNE 2012 (*REVISED 18 JULY 2012*)

ϕ^4 Chains with Two Log-Thermostat Particles

The comprehensive investigation of the “ ϕ^4 ” atomistic model for heat flow carried out by Aoki and Kusnezov [2–4] showed that this model behaves “normally”, even in one space dimension. Heat flows through a chain of ϕ^4 particles according to Fourier’s Law [5], $Q_x = -\kappa(dT/dx)$. Thus this model can provide good test cases for the logarithmic oscillator thermostat. The model we investigate here is a periodic chain of 20 one-dimensional particles. Two are “log-thermostat” particles, characterized by their individual specified “thermostat temperatures” $\{T\}$, and interacting with their lattice sites $\{q_0\}$ with a logarithmic potential:

$$\phi_{\log} = (T/2) \ln(\delta q^2 + 0.1) ; \delta q = q - q_0 .$$

The remaining eighteen are ϕ^4 particles, tethered to their lattice sites $\{q_0\}$ with a *quartic* potential :

$$\phi_{\text{tether}} = (1/4)(q - q_0)^4 .$$

In addition to these two types of lattice-site potentials all 20 nearest-neighbor pairs interact with a Hooke’s-Law potential,

$$\phi(q_i, q_{i+1}) = (\kappa/2)(|q_i - q_{i+1}| - 1)^2 ; \kappa = 1.00 \text{ or } 0.10 .$$

Because the log-thermostat model is imagined to be “weakly coupled” to the chain we considered a model with a much smaller force constant $\kappa = 0.1$ linking the two thermostat particles to their four neighbors in the chain. Experiments with $\kappa = 0.01$ showed no tendency at all towards equilibration with simulations of 10^9 time steps. With initial velocities ± 1 alternating along the chain the longtime averaged temperatures along the chain reflect the initial conditions rather than the thermostat temperatures, ending up with all the time-

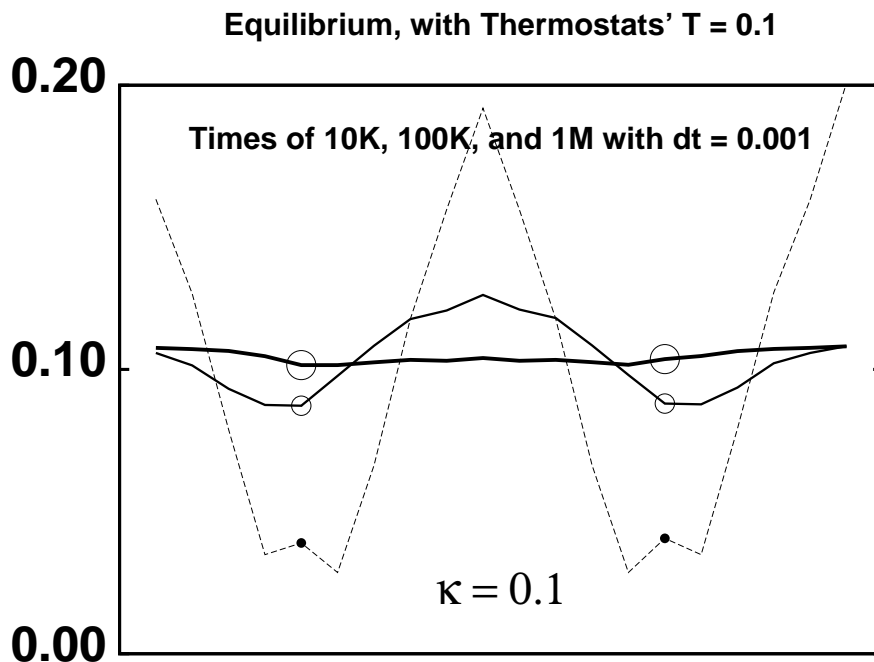


FIG. 1. Equilibrium temperature profiles for a 20-particle periodic chain.

averaged kinetic temperatures near $\langle p^2 \rangle = 0.5$. The log-thermostats are apparently unable to absorb much energy in a reasonable time [6].

Equilibrium simulations with alternating initial velocities $\pm\sqrt{0.2}$ along the chain and with both specified thermostat temperatures equal to 0.10 were more nearly successful. Figure 1 shows that the time-averaged kinetic temperatures along the chain are within 8% of the specified temperature 0.10 after a simulation of 10^9 time steps, corresponding to a time of one million in reduced units. Evidently, under propitious conditions log-thermostat temperature control *can* approach equilibrium on a sufficiently long timescale.

We next carried out a similar, but *nonequilibrium* simulation, with the same initial conditions but with different specified thermostat temperatures: 0.05 for thermostat Particle 5 and 0.15 for thermostat Particle 15. The temperature profile which resulted (again with 10^9 fourth-order Runge-Kutta time steps) was scarcely different to the equilibrium one (see figure 2). The log-thermostats were *unable* to provide a nonequilibrium temperature profile.

But why do logarithmic thermostats fail? Apart from the large time intervals mentioned above [6], there is another more fundamental reason for their failure in *nonequilibrium* problems, traceable to their Hamiltonian heritage [7]: Deterministic nonequilibrium heat-flow problems generate *fractal* phase-space distributions, with a vanishing phase volume. A

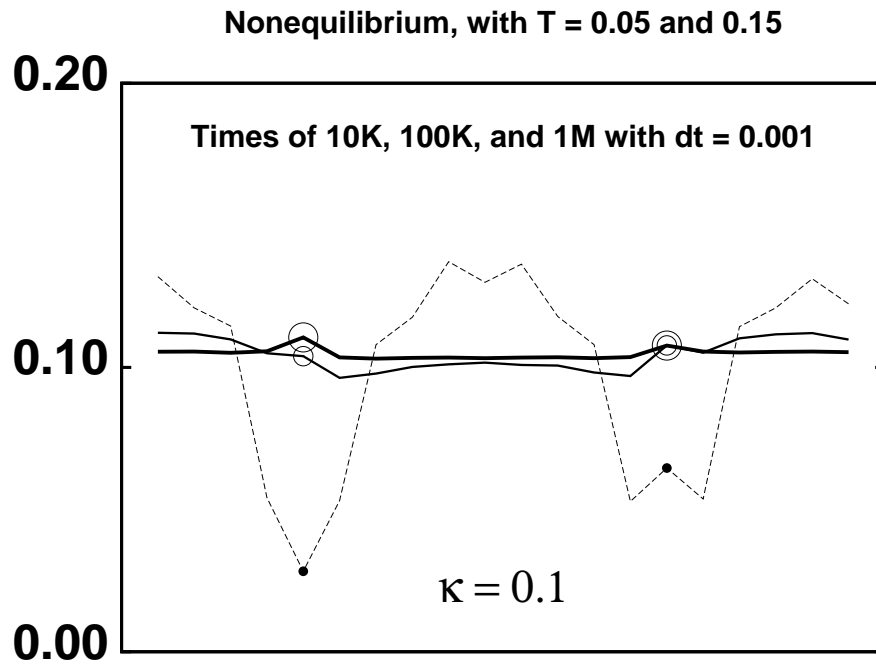


FIG. 2. “Nonequilibrium” temperature profiles for a 20-particle chain.

Hamiltonian system obeying Liouville’s Theorem in phase space, $df(q, p)/dt \equiv 0$, simply *cannot* produce a fractal.

Aoki and Kusnezov showed that heat flow through a ϕ^4 chain generates fractal phase-space distributions, with a dimensionality reduced from the equilibrium Gibbs’ distribution [2–4]. Hoover *et alii* [8] showed that similar fractals result using seven different thermostat types (none of which obeys the equilibrium version of Liouville’s Theorem).

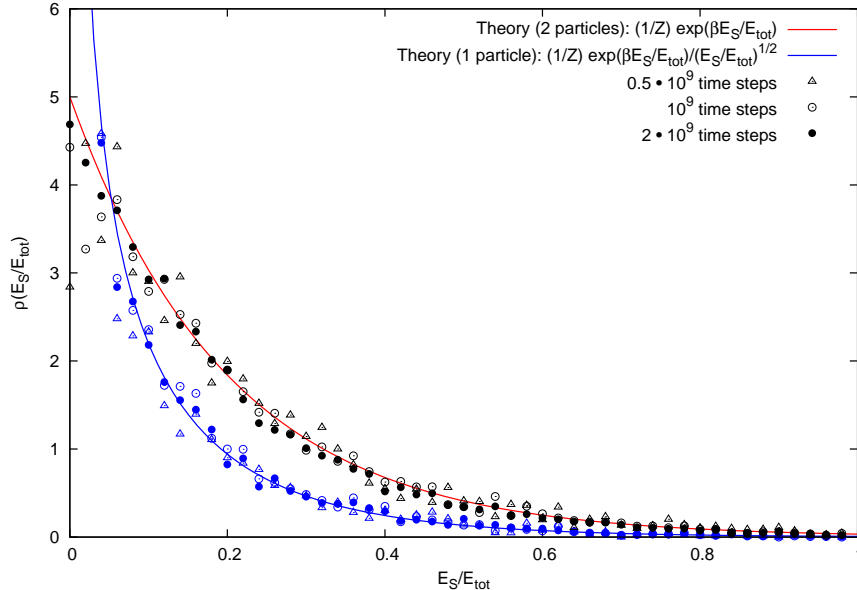


FIG. 3. Probability distribution for E_S/E_{tot} in the original numerical experiment proposed by Campisi *et alii* in [1]. E_S is the energy of a system interacting with the logarithmic oscillator. The theoretical prediction follows the solid line (red for two particles and blue for only one). The black points correspond to the numerical results for $t = 0.5 \cdot 10^6, 10^6$ and $2 \cdot 10^6$ for a system of two particles, as in the original article (the time step was set to $\Delta t = 0.001$). The blue points correspond to a system of only one thermostated particle, which also takes about the same time to converge to the prediction.

Lennard-Jones Potentials

Even the original one-dimensional simulations proposed by Campisi *et alii* for a couple of particles turn out to imply very long simulation times. We carried out simulations with one and two particles setting the mass of the logarithmic oscillator equal to ten particle masses. A classic fourth-order Runge-Kutta integrator took $2 \cdot 10^9$ time steps to generate a reasonable reproduction of the energy histogram presented in [1] (see figure 3).

In their discussion of a three-dimensional simulation, Campisi *et alii* pointed out that an increase in the number of particles led to a very significant departure from the predicted velocity distribution. The solution suggested was simply to increase the total energy of the system by $\Delta E \propto 3Nk_B T/2$. This solution, however, leads to the exponential increase in the typical lengths and times for the logarithmic oscillator that we have already explained above.

Our investigations reveal that unless the initial conditions and the problem are carefully “tuned” the thermostat is ineffective at equilibrium, even for extraordinarily long simulation times. The situation away from equilibrium is worse yet, as the thermostat fails to act rapidly enough to affect change. We conclude that log-thermostats are not useful in most practical applications, whether simulations or experiments.

We would like to thank Campisi *et alii* for correcting a mistake in the previous version of this article [9].

ADDENDUM 29 JANUARY 2013

Our comment was published in Physical Review Letters on the 11th January 2013 [10], followed by a reply [11] where Campisi and his colleagues proposed a new experimental arrangement for the logarithmic oscillator, without the unreasonable time or length scales that we had described. The number of degrees of freedom in the original experiment was reduced to one third by forcing the neutral atoms and logarithmic oscillator ion to move along a single dimension. Table I, taken from the reply, illustrates the exponential growth of mean free times τ and box lengths L as the required precision H_{KS} or the number of particles N increase.

Campisi *et alii* claimed that this version of the experiment could be implemented with present day cold-atom technology [12]. Having no prior experience with cold-atom physics, we contacted Prof. I. Bloch, who kindly lent us some of his time and confirmed that such a precise one-dimensional setup, though “challenging”, should be feasible in principle. We are grateful for his helpful comments.

Although the magnitudes shown in the table are correct, they are slightly misleading because they assume that the system of interest begins at (or very near) the “thermostat temperature”. However, if we assume that the initial temperature is off by ΔT degrees, then the logarithmic oscillator will have to absorb at least $\Delta E = Nk_B\Delta T/2$ units of energy. For $N = 20$ and $\Delta T = 5\text{K}$, for example, the energy absorbed must be about $\Delta E = 50k_B$. Compare this value to those in the table, where the total energy of system plus oscillator never exceeds $30k_B$.

Logarithmic oscillators indeed “possess an infinite heat capacity”, but this statement is easily misunderstood. The logarithmic oscillator’s mean kinetic temperature is not a function

TABLE I. Total energy, box lengths and mean free times for the logarithmic oscillator experiment as a function of the number of degrees of freedom, N , and the required precision, H_{KS} , measured as a Kolmogorov-Smirnov distance (from Campisi *et alii* [11]).

N	H_{KS}	E_{tot}/k_B	L [m]	τ [s]
20	0.005	16.45	3×10^{-1}	1×10^{-3}
20	0.01	14.8	5×10^{-2}	3×10^{-4}
20	0.02	13.1	9×10^{-3}	5×10^{-5}
30	0.02	18.1	1×10^0	5×10^{-3}
40	0.02	23.1	2×10^2	5×10^{-1}
50	0.02	28	3×10^4	6×10^1

of its energy (if one considers time averages with intervals that are very large compared to the period of oscillation). In practice, though, a logarithmic oscillator *cannot* absorb an arbitrary amount of heat because any physical potential will lack a singularity at the origin and the size of the experiment, L , will limit the amount of energy that the oscillator may absorb, so that

$$\Delta E_{max.} = \frac{1}{2} k_B T \ln \left(\frac{L^2 + b^2}{b^2} \right),$$

which is an extremely slowly growing function of L .

Our comment pointed out that applying *two* logarithmic oscillators, with different temperatures, to a chaotic Hamiltonian system failed to create the expected linear temperature gradient. In their Reply, Campisi *et alii* disregarded this observation, arguing that their Letter suggested temperatures that varied in time and not in space, so that our simulations were not relevant to their work. This conclusion strikes us as ill-conceived. Unless they can somehow explain how to change a system's temperature *homogeneously*, one would expect to find that a *time*-varying temperature would necessarily create gradients in *space*.

Consequently we stand by our claim that the logarithmic oscillator cannot be used as an effective thermostat in practical applications.

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