PHYSICAL REVIEW E **73**, 035102(R) (2006)

Fluctuation theorem applied to the Nosé–Hoover thermostated Lorentz gas

Thomas Gilbert*

Center for Nonlinear Phenomena and Complex Systems, Université Libre de Bruxelles, Code Postal 231, Campus Plaine, B-1050 Brussels, Belgium

(Received 7 December 2005; published 10 March 2006)

We present numerical evidence supporting the validity of the Gallavotti–Cohen fluctuation theorem applied to the driven Lorentz gas with Nosé–Hoover thermostating. It is moreover argued that the asymptotic form of the fluctuation formula is independent of the amplitude of the driving force in the limit where it is small.

DOI: 10.1103/PhysRevE.73.035102 PACS number(s): 05.70.Ln, 05.45.−a

Over the past decade, different versions of fluctuation formulas have been the focus of a number of publications in the field of nonequilibrium statistical physics. In particular, dissipative deterministic dynamical systems with time-reversal symmetry have attracted some attention as potential candidates to model externally driven systems with a thermostating mechanism [1–3]. Two distinct results have been proposed, which, in the context of isokinetic thermostats, both characterize the fluctuations of entropy production. One, due to Evans and Searles [2], is usually referred to as *transient fluctuation theorem*, while the other, due to Gallavotti and Cohen [3], is simply known as the *fluctuation theorem*. The former addresses the fluctuations of the work done by the external forcing on the system, and the latter the fluctuations of the phase space contraction rate of nonequilibrium stationary states. It has been rigorously proved in the context of Anosov systems [3].

To be definite, consider the externally driven periodic Lorentz gas with Gaussian thermostating [4]. The trajectory of a particle in between elastic collisions is described by the equation $\dot{\mathbf{p}}=\mathbf{E}-\alpha\mathbf{p}$, where $\alpha=\mathbf{E}\cdot\mathbf{p}/p^2$ is a reversible damping mechanism that acts so as to keep the kinetic-energy constant. α, the phase-space contraction rate for this system is, as seen from its expression, equal to the work done on the particle divided by the constant temperature. Thus the work done on the particle is exactly compensated by the heat dissipation. In other words, work and heat dissipation statistics are identical for this system.

Dolowschiák and Kovács [5] recently made the observation that work and phase-space contraction rate fluctuations behave very differently for the externally driven Lorentz gas with Nosé–Hoover thermostating. On the one hand, the work fluctuations, whether large or small, obey the Evans–Searles formula, in agreement with similar observations made for other systems [6,7]. On the other hand, the authors observed that the phase-space contraction rate fluctuations rapidly saturate. Moreover, no observation of a linear regime of fluctuations in a limited range was reported.

The Nosé-Hoover thermostated Lorentz gas on a periodic lattice has phase-space coordinates $\Gamma=(\mathbf{q},\mathbf{p},\zeta)$. Here $\mathbf{q}$ and $\mathbf{p}$, respectively, denote the position and momentum of the particle, and ζ is the variable associated with the thermal reservoir. Between two elastic collisions, the dynamics is specified by the equations

$$\dot{\mathbf{q}}=\mathbf{p},$$

$$\dot{\mathbf{p}}=\mathbf{E}-\zeta\mathbf{p},$$

$$\dot{\zeta}=\tau_{\text{resp}}^{-2}[p^2/(2T)-1]. \tag{1}$$

Here $\mathbf{E}$ denotes the external field, τ_{resp} the relaxation time of the thermostat, and T the temperature [8].

An essential difference between the Gaussian and Nosé–Hoover thermostated Lorentz gases is that the phase-space of the former is compact. The fluctuation theorem [3] can thus be applied to the Gaussian thermostated Lorentz gas as though it were Anosov [9]. For the Nosé–Hoover thermostated Lorentz gas, the situation is different in that the phase-space contraction rate fluctuations are unbounded. In that case, for large fluctuations, one expects a much larger probability of positive phase-space contraction rate fluctuations.

Nevertheless, an appropriate modification of the fluctuation theorem was given in [10]. Thus consider a time-reversible dissipative system with an average phase-space contraction rate $\langle\sigma(\Gamma)\rangle=\sigma_+>0$ and assume this system verifies the chaotic hypothesis. In a language similar to that used in [5], the statement of the fluctuation theorem for the dimensionless contraction amplitude p is that there exists a finite number $1\leqslant p^*<\infty$, so that

$$\lim_{\tau\to\infty}\frac{1}{\tau}\log\frac{P_\tau(p)}{P_\tau(-p)}=p\sigma_+,\quad |p|<p^*, \tag{2}$$

where $P_\tau(p)$ denotes the probability of observing, over a time interval τ, a fluctuation of the phase-space contraction rate $\langle\sigma\rangle_\tau=p\sigma_+$. In particular, thinking about the external driving parameter in the Lorentz gas, the above result should be independent of its amplitude ($|\mathbf{E}|>0$).

We argue the driven periodic Lorentz gas with Nosé-Hoover thermostating considered in [5] verifies the fluctuation relation Eq. (2); although [5] correctly pointed out the phase-space contraction rate fluctuations are bounded for large fluctuations, their measurements do not point to the violation of Eq. (2). Here we present evidence that the Lorentz gas with Nosé–Hoover thermostating has fluctuations of the phase-space contraction rate which are entirely consistent with the statement above, showing both saturation for large

*Electronic address: thomas.gilbert@ulb.ac.be

RAPID COMMUNICATIONS

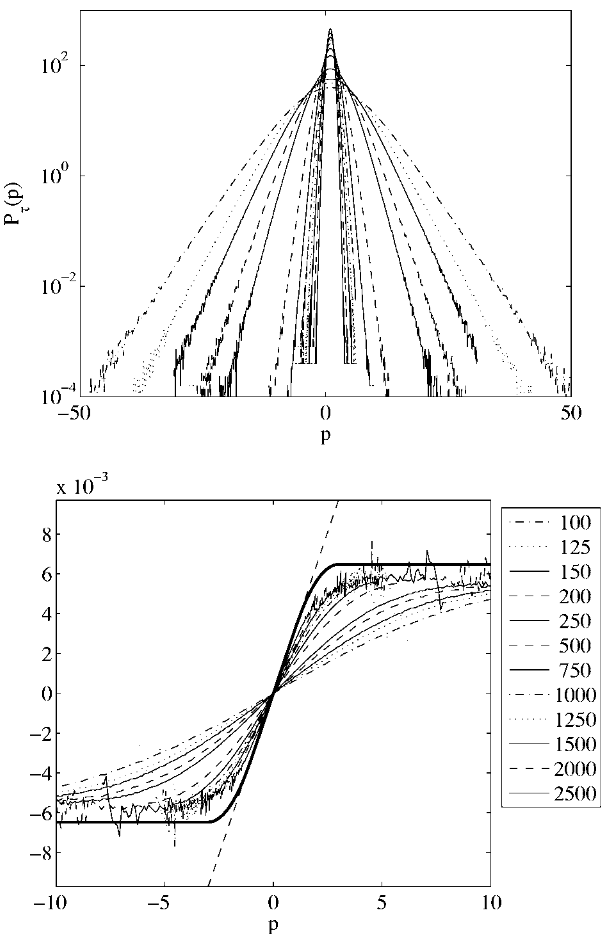

FIG. 1. Probability density function (above) and verification of Eq. (2) (below) for different time averages, as indicated in the legend. The parameters are set to $\mathbf{E}=(0.1,0)$, $T=1/2$, and $\tau_{\rm resp}=1$. The average phase-space contraction rate $\langle 2\zeta\rangle = 3.25\times 10^{-3}$ was measured over a total of $\approx 3\times 10^{8}$ collisions. The thick solid curve corresponds to the prediction in Eqs. (4) and (5).

fluctuations and linear behavior for small fluctuations.

As noted in [10], the phase-space contraction rate for this system has the form

$$\sigma(\Gamma) = \sigma_0(\Gamma) + \frac{1}{T}\frac{d}{dt}H, \tag{3}$$

where $\sigma_0(\Gamma)=\mathbf{E}\cdot\mathbf{p}/T$ is the quantity relevant to the Evans–Searles fluctuation formula. Here $H=p^2/2+T\tau_{\rm resp}^2\zeta^2$. Following the discussion in [10], one can derive the distribution of σ in terms of that of σ_0. This was first done in [11] in the framework of a Brownian particle dragged through water by a moving potential. In that case, σ_0 has Gaussian fluctuations and one can derive the asymptotic form of the right-hand side (RHS) of Eq. (2),

$$\lim_{\tau\to\infty} \frac{1}{\tau} \log \frac{P_\tau(p)}{P_\tau(-p)} = f(p)\sigma_+, \tag{4}$$

where

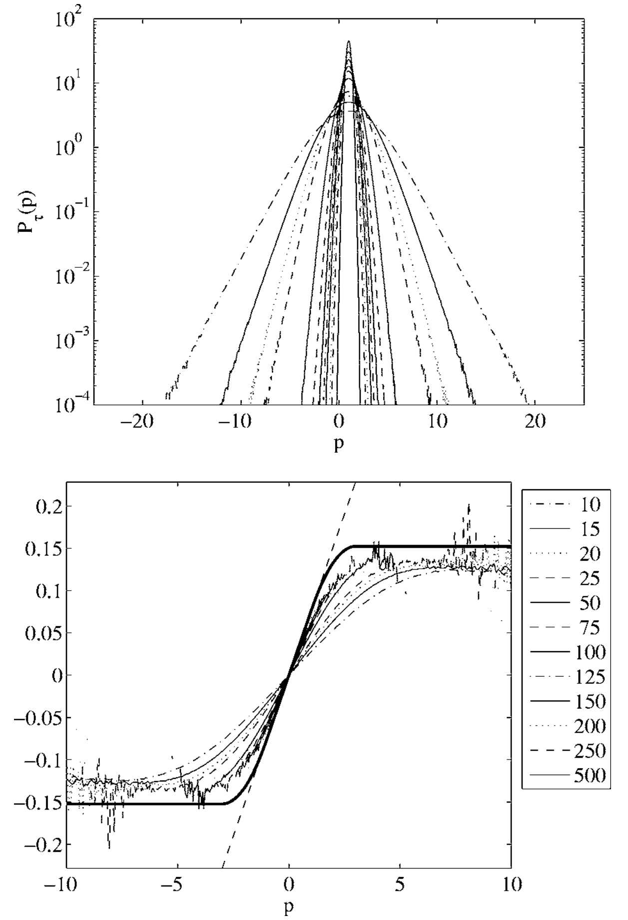

FIG. 2. The same as Fig. 1 for $\mathbf{E}=(0.5,0)$. The average phase-space contraction rate $\langle 2\zeta\rangle = 7.62\times 10^{-2}$ was measured over a total of $\approx 3\times 10^{8}$ collisions.

$$f(p) = \begin{cases} p, & 0 \leqslant p < 1, \\ p-(p-1)^2/4, & 1 \leqslant p < 3, \\ 2, & p \geqslant 3. \end{cases} \tag{5}$$

For negative p, $f(p)$ is odd, $f(-p)=-f(p)$.

According to [5], the fluctuations of the time averages of σ_0 for the Nosé–Hoover Lorentz gas are Gaussian [12], which, given that the kinetic-energy probability distribution is canonical in the presence of the Nosé–Hoover thermostat, entitles us to use the result of [11], Eqs. (4) and (5). We present in Figs. 1 and 2 the results of numerical simulations on a hexagonal lattice with intercell distance unity and disk radius 0.44 (consistent with the finite horizon condition). That is, we take the fundamental lattice translation vectors to be (1, 0) and $(1/2,\sqrt{3}/2)$. Two different values of the external field are considered, both along the x axis, $\mathbf{E}=(0.1,0)$ and $\mathbf{E}=(0.5,0)$. The numerical integration was performed using an algorithm similar to that used in [13]. As seen from the figures, the numerical data is entirely consistent with Eq. (2). Indeed, as times become large, the small fluctuation amplitudes have a linear slope which approaches asymptotically the value given by the RHS of Eq. (2). The data are compared to the prediction in Eqs. (4) and (5) and show a rather

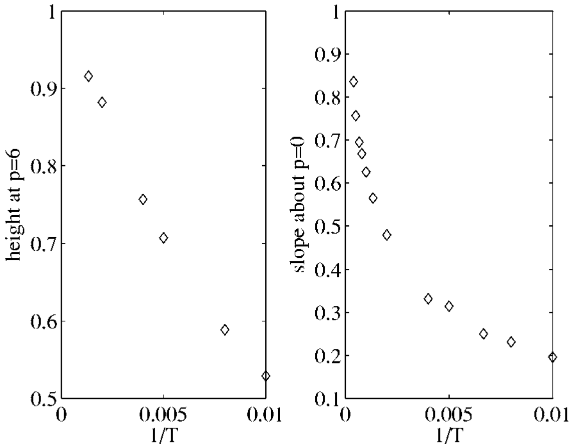

FIG. 3. Height of saturation measured at $p=6$ (for times $T=100,\ldots,750$) (left), and slope measured about $p=0$ vs $1/T$ of the curves shown in the bottom panel of Fig. 1 for the external forcing $\mathbf{E}=(0.1,0)$. The vertical coordinates are renormalized to the asymptotic values predicted by Eq. (5). Both curves can be linearly extrapolated to 1 as $T\rightarrow\infty$. These data confirm that $\mathcal{O}(1/T)$ corrections affect the finite-time measurements.

good agreement, albeit $f(p)=2$ seems to slightly overestimate the saturation level. As illustrated on the left panel of Fig. 3, this apparent discrepancy is only a finite-time correction, expected to be $\mathcal{O}(1/T)$ [14]. Likewise, the right panel of Fig. 3 shows that the slope in the linear regime of fluctuations approaches the predicted asymptotic value as average lengths increase. Figures 1 and 2 moreover show the linear regime of fluctuations persists irrespective of the strength of the driving field. That is to say, the field strength is relevant to the asymptotic regime only through σ_+, which is quadratic in the field strength, consistent with Eqs. (4) and (5). Similar results were obtained for field values as low as $\mathbf{E}=(0.05,0)$, the main difficulty being that the length of the time averages in Eq. (2) needs to be increased significantly in order for the slope to converge to the asymptotic value predicted by Eq. (2).

In summary, the driven periodic Lorentz gas with Nosé–Hoover thermostating provides a simple example of a fully deterministic model whose work and phase-space contraction rate fluctuations obey relations similar to those found in [11] for the work and heat fluctuations of a Brownian particle in a potential well. Similar results were obtained in [15] for the nonequilibrium fluctuations of a *RC* circuit. This suggests an identification between phase-space contraction rate and heat dissipation in this framework. The numerical evidence we presented is entirely consistent with the phase-space contraction rate fluctuation theorem as stated in [10]. The sharp constrast between this observation and the conclusion drawn by [5] (similar claims can be found in [7]), that the fluctuation theorem does not hold if the driving is small, can be attributed to two reasons: (i) these authors did not consider properly the saturation of the fluctuation at larger $p>p^*$, and (ii) they did not run the simulation long enough to observe the small but clear linear region at $p<p^*$. The small deviations between our data and the form predicted by Eqs. (4) and (5) should be attributed to finite-time corrections. We hope to further report on this issue in a future publication.

The author wishes to thank M. Dolowschiák, Z. Kovács, G. Nicolis, G. Gallavotti, and R. van Zon for helpful comments, as well as F. Zamponi who pointed out the relevance of Eqs. (4) and (5). The author would also like to thank P. Gaspard and J. R. Dorfman for their continuing support. The author is chargé de recherches with the F. N. R. S. (Belgium).

[1] D. J. Evans, E. G. D. Cohen, and G. P. Morriss, Phys. Rev. Lett. **71**, 2401 (1993).
[2] D. J. Evans and D. J. Searles, Phys. Rev. E **50**, 1645 (1994).
[3] G. Gallavotti and E. G. D. Cohen, Phys. Rev. Lett. **74**, 2694 (1995); J. Stat. Phys. **80**, 931 (1995).
[4] B. Moran and W. G. Hoover, J. Stat. Phys. **48**, 709 (1987).
[5] M. Dolowschiák and Z. Kovács, Phys. Rev. E **71**, 025202(R) (2005).
[6] D. J. Evans and D. J. Searles, J. Chem. Phys. **113**, 3503 (2000).
[7] D. J. Evans, D. J. Searles, and L. Rondoni, Phys. Rev. E **71**, 056120 (2005).
[8] The role of T as temperature is consistent as long as the external field is nonzero. For zero field, the system has a limit cycle. It is therefore not ergodic and the notion of temperature is ill defined.
[9] The Lorentz gas or Gaussian thermostated driven Lorentz gas is strictly speaking not Anosov because of the instantaneous collisions with the scatterers.
[10] F. Bonetto, G. Gallavotti, A. Giuliani, and F. Zamponi, e-print cond-mat/0507672.
[11] R. van Zon and E. G. D. Cohen, Phys. Rev. Lett. **91**, 110601 (2003).
[12] We could check this observation to very good accuracy. For instance, the distributions of σ_0 corresponding to the data presented in Figs. 1 and 2 have kurtosis (fourth moment divided by second moment squared) equal to 3, the Gaussian value, within one percent (and similarly for higher moments 6 and 8). Likewise the skewness (third moment squared by second moment to the cube) is zero within one thousandth.
[13] K. Rateitschak, R. Klages, and W. G. Hoover, J. Stat. Phys. **101**, 61 (2000).
[14] A. Giuliani, F. Zamponi, and G. Gallavotti, J. Stat. Phys. **119**, 909 (2005).
[15] N. Garnier and S. Ciliberto, Phys. Rev. E **71**, 060101(R) (2005).