Fluctuations of entropy production in driven glasses

Mauro Sellitto

Dipartimento di Scienze Fisiche and Unità INFM,
Università “Federico II”, Mostra d’Oltremare, Pad. 19, I-80125 Napoli, Italy

(Received 1 January 1998; revised 15 January 1998)

We study by Montecarlo simulation the non-equilibrium stationary behavior of a three-dimensional stochastic lattice gas with reversible kinetic constraints and in diffusive contact with two particle reservoirs at different chemical potential. When one of the boundaries is placed in the “glassy phase”, the statistics of entropy production fluctuations driven by the chemical potential gradient satisfy the Gallavotti-Cohen fluctuation theorem provided that an “effective” entropy production is introduced.

05.20-y, 05.70.Ln, 5.40+j

Introduction. The Gallavotti-Cohen fluctuation theorem (FT) is a result of remarkable generality concerning the distribution of entropy production fluctuations over long time intervals in stationary open systems. It states that the ratio of the probabilities of observing a given average entropy production \( \sigma \), over a time interval \( \tau \), to that of observing the opposite value \(-\sigma\) is \( e^{-\sigma \tau} \). It has been recently shown [1] that this result implies the fluctuation-dissipation theorem (FDT) and Onsager’s reciprocity relations in the limit of vanishing temperature or high-density phase (i.e., in equilibrium). Therefore, the FT appears as an important stepping stone towards the generalization of thermodynamics to situations out of equilibrium.

The FT was inspired by a pioneering numerical experiment on a thermostated fluid under shear flow [2]. It has been further confirmed by the numerical simulation of an electrical conduction model [3], and heat diffusion in a Fermi-Pasta-Ulam chain [4], while a turbulent Rayleigh-Bénard convection experiment is still under analysis [5]. Although the theorem was originally proved for thermostated Hamiltonian systems driven by external forces, under certain “chaoticity” assumptions for the dynamics [6], it also holds for rather “generic” stochastic systems endowed with Langevin [7], and diffusive dynamics [8].

It is well known, however, that violations of FDT appear in a wide class of conservative systems, since their relaxational dynamics after a quench in the low-temperature or high-density phase is so slow that prevents them from reaching equilibrium on finite time scales [9]. In the attempt to formulate a thermology of aging systems, the FDT violation has been related to scales [9]. In the attempt to formulate a thermology of aging systems, the FDT violation has been related to scales [9].

The driven glass. To corroborate this conjecture we consider a three dimensional lattice-gas model of hard-core particles kept away from equilibrium by a chemical potential gradient (see fig. 1). At the top and bottom layer of the system particles are inserted and removed according the usual Montecarlo rule, mimicking the contact of the system with a particle reservoir \( \mathcal{R}_\pm \): we randomly choose a site on the layer; if it is empty, we add a new particle; otherwise we remove the particle with probability \( e^{-\beta \mu} \) (\( \mu \geq 0 \)). The global effect of the reservoirs is to fix the boundary densities at two different values \( \rho_+ \) and \( \rho_- \), driving a current through the system. A similar setup was previously consider by Spohn [10] with the aim of studying analytically long-range correlations in a simple model of non-equilibrium fluid subject to temperature gradients. The link of the microscopic theory with the fluctuating hydrodynamics was also investigated, see [11] and, for a review, [12]. Here, we consider a bulk dynamics implementing the cage effect in supercooled liquids [13]. Therefore, the sweeps of creation/destruction of particles on the edges are alternated with the following diffusive sweep. A particle and one of its neighbouring sites are chosen at random; the particle moves if the three following conditions are all met: 1) the neighbouring site is empty; 2) the particle has less than 4 nearest neighbours; 3) the particle will have less than 4 nearest neighbours after it has moved. The rule is symmetric in time and, unlike the usual driven diffusive systems where detailed
balance is broken \cite{18,19}, the system is microscopically reversible.

The dynamical behavior of the system when the two reservoirs are at same chemical potential has been investigated in \cite{20,21}. It is worth to recall briefly some results. Although the equilibrium thermodynamics of the model is trivial, a purely dynamical transition takes place when the system is quenched in the glassy phase, namely above the threshold value \( \mu_c \approx 2.0 \): the density approaches by a power-law an asymptotic value \( \rho_c \approx 0.88 \), different from the equilibrium value allowed by the dynamical evolution rule, and the diffusion coefficient of the particles vanishes roughly as the inverse of the time elapsed after the quench \cite{20,22}. Consequently the system ages, and the mean-square displacement and the conjugated response function satisfy a generalized FDT with a FD ratio given by \( X \approx 0.79 \) \cite{22}.

We are interested here to the case where a boundary is in the fluid phase \( (\mu_- < \mu_c) \) and the other one in the glassy phase \( (\mu_+ > \mu_c) \). The numerical experiment is performed in the following way. The system consists of a cubic lattice of size \( L^2 \times 2L \) with \( L = 10 \). The reservoir \( R_+ \) is located at \( z = 0 \) while \( R_- \) at \( z = \pm L \). In this way we can take periodic boundary conditions in all directions and avoid spurious edge effects \cite{23}. We start with a low-density uniform distribution of particles and let the system reach a stationary state characterized by a time-translation invariant correlation function of current fluctuations. We then follow the dynamical trajectory of the motion for a time of \( 10^8 \) Montecarlo sweeps (MCs) along which the observables of interest are evaluated. In particular we consider the particle current \( J(t) \), defined as an extensive quantity (proportional to the transverse surface \( L^2 \)) by:

\[
J(t) = \frac{1}{2L} \sum_{z=-L}^{L-1} [j_+(z,t) - j_-(z,t)],
\]

where \( j_+(z,t) \) and \( j_-(z,t) \) are the number of jumps taking place at time \( t \) through the layer \( z \) in the direction of, and opposite to, respectively, the externally imposed chemical potential gradient.

Fluctuation theorem and effective entropy production. In order to study the statistics of current fluctuations we consider the average particle current over a time interval of duration \( \tau \):

\[
J_\tau(t) = \frac{1}{\tau} \sum_{s=t+1}^{t+\tau} J(s),
\]

which in a steady state does not depend on \( t \). We then compute the probability distribution \( \pi_\tau(p) \) of the adimensional variable

\[
p = \frac{J_\tau}{J}
\]

where \( J = \lim_{\tau \to \infty} J_\tau \). The function \( \pi_\tau(p) \) also gives the distribution of entropy production fluctuations since, according the thermodynamics of linear irreversible processes \cite{13}, the average entropy production \( \sigma_\tau \) over a time interval \( \tau \) is simply related to the corresponding average particle current \( J_\tau \) by:

\[
\sigma_\tau = J_\tau (\mu_+ - \mu_-).
\]

Fig. 2 shows the distribution \( \pi_\tau(p) \) for different values of the time interval, \( \tau = 1, 2, 5, 10 \) MCs. The chemical potential of the reservoir is \( \mu_+ = 2.2 \) and \( \mu_- = 0 \). Being the system in the “large deviation” regime it can appear surprising that the shape of \( \pi_\tau(p) \), is compatible with a gaussian distribution, even though no a priori relation is expected with the Sinai limit theorem \cite{13}. For a discussion see \cite{24}, where a similar result was also obtained; while a skew distribution was found in \cite{25}.

Once determined the probability distribution \( \pi_\tau(p) \) of entropy-production fluctuations it is simple to check the Gallavotti-Cohen FT, that in our case reads:

\[
\log \frac{\pi_\tau(p)}{\pi_\tau(-p)} = \tau \, p \, J (\mu_+ - \mu_-).
\]

Fig. 3 shows that the lhs and rhs of the relation (5) are linearly related but are not equal. However, an equality is obtained by taking into account the “effective chemical potential” \( \mu_{\text{eff}} = X \mu \) (or, equivalently, the FD ratio \( X \)) of the glassy boundary in the calculation of the entropy production:

\[
\sigma_\tau = J_\tau (\mu_{\text{eff}} - \mu_-).
\]

When the reservoirs are both placed in the fluid phase, where \( X = 1 \) (and \( \mu_{\text{eff}} = \mu_+ \)), the FT should be recovered. The inset of fig. 3 shows, consistently, that for \( \mu_+ = 1.8, \mu_- = 0 \), and \( \tau = 1, 2, 5 \) MCs the FT is well satisfied.

To rule out that these results are a mere coincidence we have also performed extensive numerical simulations with different values of the chemical potential \( \mu_- \). In fig. 4, we show the results for \( \mu_- = -0.4, -0.2, 0.0, 0.2, 0.4 \), and \( \mu_+ = 2.2 \), with \( \tau = 1 \) MCs, plotted against the effective entropy production. We see that also this plot supports the conjecture of a generalized form of FT.

We now give an heuristic argument showing how the appearance of the FD ratio here should not be surprising. Let us observe that our experimental setup is nothing else than a device to perform measurements of the effective chemical potential, \( \mu_{\text{eff}} \), of the system \cite{26}. Indeed, suppose that we want to measure the value of \( \mu_{\text{eff}} \) for an aging system in contact with a reservoir \( R_+ \) at \( \mu_+ > \mu_c \). We start with the stationary system in contact with \( R_+ \) and \( R_- \), with \( \mu_- < \mu_c \), the last reservoir acting as a “thermometer”. Then, if we disconnect the system from \( R_- \) and let it relax, the density of the corresponding layer will increase until the average particle current
is zero (the value of \( \mu \) where this condition is first met defines \( \mu_{\text{eq}} \)). However, since the system is unable to fully equilibrate with the reservoir \( \mathbb{R}_+ \) (being \( \mu_+ > \mu_c \)), such a density will be lower than \( \rho_c \) and therefore the corresponding chemical potential will be reduced by a factor \( X \), i.e., \( \mu_{\text{eq}} = X \mu_+ \). In principle, this method represent a possible way to measure the FD ratio of aging systems and gives some insight into the notion of effective temperature as partial equilibration factor \( \mu_{\text{eff}} \).

It is also interesting to observe that the stationary density profile can be predicted by a non-linear diffusion equation [21]. However, this matter as well as the validity of Einstein relation between diffusivity and conductivity will be discussed elsewhere.

Conclusions and perspectives. We have investigated by Monte Carlo simulation non-equilibrium stationary behavior of a constrained lattice-gas model driven by a chemical potential gradient (driven glass). The approach does not involve fictitious thermostating mechanism allowing dissipation to prevent the heating up of the system [22], neither the question of the interpretation of phase space contraction rate as entropy production, which has not yet received an unanimous answer (see however [23]). The extension to other systems such as driven spin-glasses and to different boundary conditions modelling, e.g., a Couette flow, is also feasible [24].

In particular, we have studied the distribution of entropy production fluctuations when one of the reservoirs is placed in the glassy phase, \( \mu_+ > \mu_c \), and shown that in the stationary state a generalized form of FT is satisfied which takes into account the effective entropy production computed through the FD ratio of the corresponding undriven system. Therefore, the generalized form of FT and FDT should be related by the same limiting procedure exploited in [2]. This vindicates the crucial role played by the notion of “effective temperature” in generic, aging or stationary, out of equilibrium systems.

Although the model considered here is much simpler than a real supercooled liquid in a temperature gradient, it displays interesting phenomena that could be observed, hopefully, also in a “true” experiment.

We conclude by observing that it is not clear what happens in a generic driven glass in which the reservoirs are both placed in the glassy phase, at different values of temperature. In such a strongly non-linear regime of small entropy production the correlation of current fluctuations could exhibit aging and the system never reach a stationary state. What would be the form of Gallavotti-Cohen FT in such a situation, is presently unknown.

The author thanks L. Peliti for a critical reading of the manuscript and F. Bonetto, G. Gallavotti and H. Spohn for discussions. Partial support from INFM through the contract 1229/UDR-NAPO-AMM is acknowledged.

References

[1] G. Gallavotti and E.G.D. Cohen, Phys. Rev. Lett. 74, 2694 (1995); J. Stat. Phys. 80, 1931 (1995).
[2] G. Gallavotti, Phys. Rev. Lett. 77, 4334 (1996); J. Stat. Phys. 84, 899 (1996).
[3] D.J. Evans, E.G.D. Cohen and G.P. Morriss, Phys. Rev. Lett. 71, 2401 (1993); ibid. 71, 3616 (1993). See also: D.J Evans and D.J. Searles, Phys. Rev. E 50, 1645 (1994).
[4] F. Bonetto, G. Gallavotti and P. Garrido, Physica D 105, 125 (1997).
[5] S. Lepri, R. Livi and A. Politi, Physica D 119, 140 (1998).
[6] S. Ciliberto and C. Larocca, in Disorder & Chaos, edited by A. Vulpiani (Editions de Physique, Paris, in press).
[7] J. Kurchan, J. Phys. A: Math. Gen. 31, 3719 (1998).
[8] J.L. Lebowitz and H. Spohn, preprint (1998).
[9] J.-F. Bouchaud, L.F. Cugliandolo, J. Kurchan and M. Mézard, in Spin Glasses and Random Fields, edited by P. Young (World Scientific, Singapore: 1998).
[10] L.F. Cugliandolo, J. Kurchan and L. Peliti, Phys. Rev. E 55, 3898 (1997).
[11] Th.M. Nieuwenhuizen, Phys. Rev. Lett. 80, 5580 (1998).
[12] I. Prigogine, Introduction to Thermodynamics of Irreversible Processes (Wiley, New York: 1962).
[13] Ya.G. Sinai, Lectures in Ergodic Theory (Princeton University Press, Princeton: 1977).
[14] J. Lebowitz and H. Spohn, preprint (1996).
[15] G. Eyink, J.L. Lebowitz and H. Spohn, Comm. Math. Phys. 132, 253 (1990); ibid. 140, 119 (1991).
[16] H. Spohn, Large Scale Dynamics of Interacting Particles (Springer-Verlag, Heidelberg: 1991).
[17] W. Kob and H.C. Andersen, Phys. Rev. E 48, 4364 (1993).
[18] B. Schmittmann and R.K.P. Zia, Statistical Mechanics of Driven Diffusive Systems (Springer-Verlag, Heidelberg: 1995).
[19] G. Eyink, J.L. Lebowitz and H. Spohn, J. Stat. Phys. 83, 385 (1996).
[20] J. Kurchan, L. Peliti and M. Sellitto, Europhys. Lett. 39, 86 (1997).
[21] L. Peliti and M. Sellitto, in Disorder & Chaos, edited by A. Vulpiani (Editions de Physique, Paris, in press).
[22] M. Sellitto, Eur. Phys. J. B 4, 135 (1998).
[23] G.E. Murch, Phil. Mag. 41, 159 (1980).
[24] To pursue better the analogy with usual thermal system consider that particle density, particle current and chemical potential play the same role of energy density, heat flux, and inverse temperature, respectively.
[25] S. Nosé, Prog. Theor. Phys. Suppl. 103, 1 (1991); W.G. Hoover Molecular Dynamics (Springer-Verlag, Heidelberg: 1986).
[26] D. Ruelle, J. Stat. Phys. 85, 1 (1996); ibid. 86, 935 (1997).
[27] A. Coniglio, A. Fierro and M. Sellitto, in preparation.

* Present address: Centro de Física da Matéria Condensada, Av. Prof. Gama Pinto 2, P–1699 Lisboa, Portugal. E-mail: mauro@alf1.cii.fc.ul.pt
FIG. 1. Rayleigh-Bénard experiment to study out of equilibrium stationary states in driven glasses. The system is coupled to two particle reservoir at different chemical potential, the lower one in the glassy phase, $\mu_+ > \mu_c$, and the upper one in the fluid phase, $\mu_- < \mu_c$. Particles flow through the bulk from the bottom to the top.

FIG. 2. Histograms of the probability distribution $\pi_\tau(p)$ of entropy production fluctuations along a trajectory of motion of $10^8$ MCs sampled at time intervals $\tau = 1, 2, 5, 10$ MCs (from top to bottom). The chemical potential on the boundaries is $\mu_+ = 2.2$ (glassy phase) and $\mu_- = 0$ (fluid phase). The curves are all consistent with a gaussian distribution of average 1.

FIG. 3. Logarithmic probability ratio $\log(\pi_\tau(p)/\pi_\tau(-p))$ vs. the entropy production over a time interval $\tau$, for $\tau = 1$ (diamonds), 2 (stars), 5 (squares), 10 (circles) MCs; and $\mu_+ = 2.2, \mu_- = 0$. The broken line, with slope 1, represents the prediction of the FT. The straight line, with slope $X$, take into account the effective chemical potential $\mu_{\text{eff}} = X\mu_+$ of the glassy boundary. The value of FD ratio, $X = 0.79$, is taken from ref. [22]. Inset: check of FT when both the reservoirs are placed in the fluid phase, $\mu_+ = 1.8$ and $\mu_- = 0$, for $\tau = 1$ (diamonds), 2 (squares), 5 (circles) MCs.

FIG. 4. Logarithmic probability ratio vs. the effective entropy production for $\tau = 1$ MCs, $\mu_+ = 2.2$, and $\mu_- = -0.4$ (asterisks), $-0.2$ (squares), 0 (circles), 0.2 (diamonds), 0.4 (stars). The straight line with slope 1 represents the prediction of generalized FT, where $\mu_{\text{eff}} = X\mu_+$ and the value of FD ratio, $X = 0.79$, is taken from ref. [22].