EUROPHYSICS LETTERS 1 October 2005

Europhys. Lett., **72** (1), pp. 55–61 (2005)

DOI: 10.1209/epl/i2005-10213-1

Injected power and entropy flow in a heated granular gas

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received 8 July 2005; accepted in final form 2 August 2005
published online 2 September 2005

PACS. 05.40.-a – Fluctuation phenomena, random processes, noise, and Brownian motion.
PACS. 05.20.Dd – Kinetic theory.
PACS. 45.70.-n – Granular systems.

Abstract. – Our interest goes to the power injected in a heated granular gas and to the possibility to interpret it in terms of entropy flow. We numerically determine the distribution of the injected power by means of Monte Carlo simulations. Then, we provide a kinetic-theory approach to the computation of such a distribution function. Finally, after showing why the injected power does not satisfy a fluctuation relation *à la* Gallavotti-Cohen, we put forward a new quantity which does fulfill such a relation, and is not only applicable in a variety of frameworks outside the granular world, but also experimentally accessible.

In the realm of non-equilibrium statistical physics, universal or generic results are scarce. Landmarks in the field are Einstein's seminal contribution [1] exhibiting a relation between particle current fluctuations and a response function, followed by Onsager's reciprocity [2] and the Green-Kubo relations [3,4]. The recent discovery by Evans, Cohen and Morris [5] formalized into a mathematical theorem of general scope by Gallavotti and Cohen [6] of a symmetry property, that we will call Gallavotti-Cohen relation (GC), bearing on the entropy flux distribution therefore stands as a major progress. Similar results have been established for Markov processes by Kurchan [7] and Lebowitz and Spohn [8], with much lighter mathematics than for dynamical systems. However, mathematical as well as physical difficulties, that we shall later describe, have prevented this result to find its way towards experimental confirmation.

From the point of view of probing the validity of the Gallavotti-Cohen theorem outside its mathematical domain of validity, granular gases will prove instrumental. This was indeed already realized by Aumaître *et al.* [9]. Yet, in the absence of a first-principle definition of entropy, a physical one, albeit heuristic, was proposed: the energy injected by the thermostat divided by the granular temperature. This is precisely the quantity simulated in [9], and considered in a recent experimental work [10]. Besides, the idea of using a macroscopic and global observable for characterizing the state of a system, instead of resorting to local probes (velocity field, correlations, structure factor) has proved a valuable tool *per se* for the identification of generic features in non-equilibrium systems [11].

In this letter we consider a paradigmatic model of a granular gas maintained in a steady state by external heating, namely hard-sphere (or hard-disk) particles undergoing inelastic collisions, each of these particles being independently subjected to a random force $\boldsymbol{F}_i$ which we take to be Gaussian distributed with variance Γ. The equation of motion for particle i with velocity $\boldsymbol{v}_i$ then reads $\mathrm{d}\boldsymbol{v}_i/\mathrm{d}t = \boldsymbol{F}_{\text{coll}} + \boldsymbol{F}_i$, where $\boldsymbol{F}_{\text{coll}}$ is the force due to inter-particle collisions, and acts at contact only [12]. This model preserves essential features of standard experimental setups, like the inelastic collisions, and a heating mechanism independent of the particles' velocities. It moreover bypasses experimental difficulties like the lack of translational invariance and has been the subject of intense investigations both on the numerical and analytical sides [12], therefore its putative limitations are controlled.

The results we have obtained are as follows: First, by means of Monte Carlo simulations, we pinpoint the numerical hazards that pave the way to the full determination of the injected power probability distribution function (pdf) and its symmetry properties. Second, we show how kinetic theory can be extended to describe the large deviation function of the injected power thus allowing for an explicit test of GC. This constitutes the first analytical result of a distribution function for a global observable in a many-body, non-Gaussian, far-from-equilibrium system. Finally, we explain the reasons why the injected power cannot satisfy a Gallavotti-Cohen relation. This leads us to proposing a new quantity, with the properties of a Gibbs entropy flow, that not only avoids the aforementioned difficulties, but that should also be accessible in specific granular gases experiments, and could possibly be generalized to other non-equilibrium systems.

We define the time-integrated injected power over the time interval $[0,t]$ as the total work $\mathcal{W}(t)$ provided by the thermostat:

$$\mathcal{W}(t) = \int_0^t \mathrm{d}t \sum_i \boldsymbol{F}_i \cdot \boldsymbol{v}_i. \tag{1}$$

The granular temperature is defined by $T_g = 1/\beta = \langle \boldsymbol{v}_i^2 \rangle / d$, where d is the space dimension and the angular brackets denote a statistical average in the steady state. The central object of our study is the pdf of $\mathcal{W}(t)$, $P(\mathcal{W},t)$, and its related large deviation function

$$\pi_\infty(w) = \lim_{t\to\infty} \pi_t(w) \qquad \text{with} \quad \pi_t(w) = \frac{1}{t} \ln P(wt,t). \tag{2}$$

The generating function $\hat{P}(\lambda,t) = \langle \mathrm{e}^{-\lambda \mathcal{W}} \rangle$ and its related large deviation function $\mu(\lambda) = \lim_{t\to\infty} \frac{1}{t} \ln \hat{P}(\lambda,t)$ will provide equivalent information, as we may usually go from one to the other by Legendre transform, $\pi_\infty(w) = \max_\lambda \{\mu(\lambda) + \lambda w\}$.

We now recall the content of the GC relation. In phenomenological thermodynamics [13], one writes an evolution equation for the entropy S,

$$\frac{\mathrm{d}S}{\mathrm{d}t} = \sigma - \int_{\text{system}} \mathrm{d}V \nabla \cdot \boldsymbol{J}_S \tag{3}$$

which, in a steady state, expresses a balance of an entropy production term (a measure of intrinsic irreversibility) with an entropy flux $\boldsymbol{J}_S$ produced by an external drive (typically, a boundary condition imposing energy or matter flow). The central result of Gallavotti and Cohen is to have shown in a particular setting that the pdf $P(\mathcal{S},t)$ of a quantity $\mathcal{S}(t)$ playing the role of the time-integrated flux term $\int \mathrm{d}t\mathrm{d}V \nabla \cdot \boldsymbol{J}_S$ verifies, in the limit of asymptotically large times,

$$\ln \frac{P(\mathcal{S}, t)}{P(-\mathcal{S}, t)} = \mathcal{S}. \tag{4}$$

Nevertheless, the assumptions underlying GC are microscopic reversibility and the identification of $\dot{\mathcal{S}}$ with the phase space contraction rate. In granular materials, the former is violated and the latter definition is doomed to fail, since the phase space volume can only decrease if the heating mechanism is velocity independent. This has led to the idea that $\beta\mathcal{W}$ could possibly play the role of $\mathcal{S}$ [9]. In the heated granular gas the fluctuating total kinetic energy $E(t) = \sum_i \boldsymbol{v}_i{}^2/2$ varies according to

$$E(t) - E(0) = \mathcal{W}(t) - \mathcal{D}(t), \tag{5}$$

where $\mathcal{D}(t) \geq 0$ is the energy dissipated through collisions up until time t. Of course on average $\langle \mathcal{W}(t) \rangle = \langle \mathcal{D}(t) \rangle = 2\mathrm{d}\Gamma t > 0$, yet there will be individual realizations for which $\mathcal{W}$ will be negative. If the GC relation (4) held for $\mathcal{W}$, it would take the following form [14]:

$$\pi_\infty(w) - \pi_\infty(-w) = \beta w, \ \mu(\lambda) = \mu(\beta - \lambda). \tag{6}$$

Remark, though, that the left-hand side in (5) is bounded in time (while $\mathcal{W}$ and $\mathcal{D}$ grow typically linearly with time), therefore [15] both the injected power and the dissipated power have the same (cumulant) generating function. A straightforward consequence of that fact is the absence of $w < 0$ events at large times: $\pi_\infty(w < 0) = -\infty$, hence (6) cannot be correct [16].

Let us see now how this rigorous fact comes about in numerical studies. We have simulated a model of N inelastic hard disks under the effect of a homogeneous thermostat. The collisions between two disks i and j conserve the total momentum and reduce the normal component of the relative velocity, *i.e.* $(\boldsymbol{v}'_i - \boldsymbol{v}'_j) \cdot \hat{\boldsymbol{n}} = -\alpha(\boldsymbol{v}_i - \boldsymbol{v}_j) \cdot \hat{\boldsymbol{n}}$, where the primes mark the post-collisional velocities and $\hat{\boldsymbol{n}}$ is the direction joining the colliding particles. The driving force $\boldsymbol{F}_i$ mentioned above obeys $\langle F_i^\gamma(t) F_j^\delta(t') \rangle = 2\Gamma \delta_{ij} \delta^{\gamma\delta} \delta(t - t')$. Molecular chaos is enforced through the use of a Direct Simulation Monte Carlo [17] algorithm. The restitution coefficient α takes values between 0 and 1 (elastic gas). The gas rapidly reaches a stationary state with a granular temperature $T_g = 4\Gamma/(1 - \alpha^2)$, where the mean free time is used as a time unit, which will be the case in the subsequent analysis. We have measured the fluctuations of the work exerted by the thermostat $\mathcal{W}(t)$ as defined in eq. (1) using an integration time t. $P(\mathcal{W}, t)$ clearly shows non-Gaussian tails, which can be regarded as a hint that the true large deviations are being probed (since central-limit theorem requires small deviations to be Gaussian). The resulting function $\pi_t(w)$ is shown (see fig. 1) to verify almost perfectly a relation such as (6). When decreasing α a slight departure (about 10%) from the slope β can be recognized. And yet the plot of $\pi_t(w) - \pi_t(-w)$ stays linear in w. The inset of fig. 1 is of particular interest: it is numerically the proof that the slope does not depend upon the time of integration for the considered range of t values. More interestingly, it highlights the dramatic decay of the number of observable negative events as t is increased: even with such a simple and fast to simulate model, obtaining large statistics at large t is difficult. This observation poses a crucial question: has the numerical investigation reached the true asymptotics, *i.e.* can we believe that $\pi_t(w) \sim \pi_\infty(w)$ for the values of t shown in the figure? In the following we exploit further numerical studies and a novel analytical approach to demonstrate that a time much longer should be waited and that this first numerical result is misleading. It is nevertheless important to discover that at values of t small enough to observe some negative injected power the GC relation appears to be satisfied.

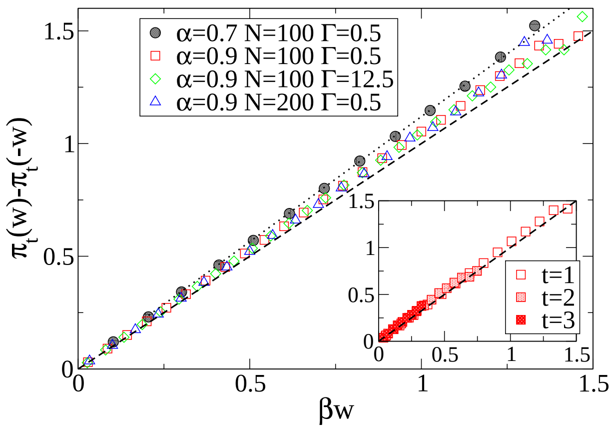

Fig. 1 – (Color online) Plot of $\pi_t(w) - \pi_t(-w)$ as a function of βw. The dashed line has slope 1, the dotted line has slope 1.1. The inset contains the same graph for different values of t, for the case $\alpha = 0.9$, $N = 100$ and $\Gamma = 0.5$.

We now sketch the analytical strategy that allowed us to find the pdf of the injected power. We start from an extended Liouville equation for the probability $\rho(\Gamma_N, \mathcal{W}, t)$ that the system is in state Γ_N with $\mathcal{W}(t) = \mathcal{W}$ at time t. The second step is to convert the Liouville equation in terms of the generating function $\hat{\rho}(\Gamma_N, \lambda, t) = \int \mathrm{d}\mathcal{W} \mathrm{e}^{-\lambda \mathcal{W}} \rho$. Recall that, for $\lambda = 0$, projection of the Liouville equation onto the one-particle subspace yields an equation coupling the one-particle distribution function to the two-particle distribution function, which is factorized through the molecular-chaos hypothesis. In our case, the situation is very similar when it comes to determining the largest eigenvalue $\mu(\lambda)$ of the evolution operator for $\hat{\rho}$ (which, in physical words, is the generating function for the cumulants of $\mathcal{W}(t)/t$): projecting onto the one-particle subspace yields an equation coupled to the two-particle subspace. By means of a molecular-chaos–like closure procedure we arrive at an equation for both the eigenvalue μ and its related eigenfunction. The extensive mathematical analysis of this program is cumbersome and will be reported elsewhere [18]. We concentrate here on the results that are as follows. First we find that the large deviation function of $\mathcal{W} = wt$ has the graph depicted in fig. 2. The tails are given by

$$\pi_\infty(w \to 0^+) \sim -w^{-1/3}, \qquad \pi_\infty(w \to +\infty) \sim -w \tag{7}$$

with, as expected, no $w < 0$ contribution. While the $w \to 0^+$ regime appears to be thermostat dependent, the exponential right tail of $P(\mathcal{W}, t)$ seems to be a robust property related to the presence of a branch cut in the complex λ plane for $\mu(\lambda)$.

We now come back to our previous numerical results. The observation of a clean linear behaviour for $\pi_t(w) - \pi_t(-w)$, with slope β, apparently independently of time (see inset of fig. 1), as though GC were satisfied, is in contrast with our analytical results indicating that the truly asymptotic $\pi_\infty(w)$ has no $w < 0$ contribution. At the level of simulations or experiments it is impossible to distinguish between non-Gaussian tails due to spurious short-time effects and real asymptotic large deviation tails. Nevertheless, the numerical study of cumulants with time, which are integrals and therefore benefit from a larger statistics, is decisive both to prove the validity of our analytical approach and to get rid of all doubts about which is the true asymptotic regime. We see (inset of fig. 2) that the third cumulant reaches a stable value at times of order ~50, much larger than the times used in fig. 1. Moreover, this stable value is in

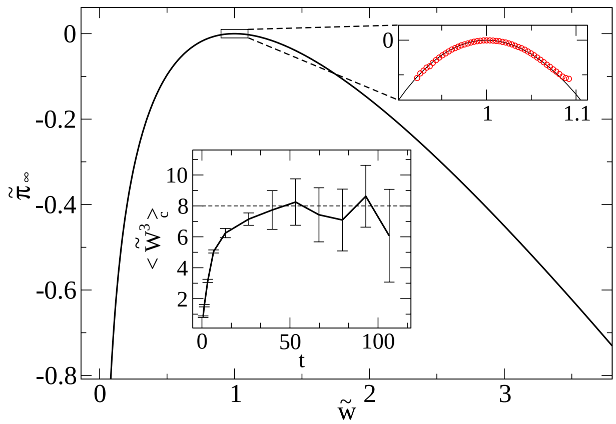

Fig. 2 – The large deviation function π_∞ of the rescaled quantity $\mathcal{W}/\langle\mathcal{W}\rangle$ obtained from the Legendre transform of the largest eigenvalue $\mu(\lambda)$ (see text and [18] for details). The inset shows the dimensionless third cumulant $\langle\tilde{\mathcal{W}}^3\rangle_c = \langle\mathcal{W}^3\rangle_c\beta^2/\langle\mathcal{W}\rangle$ relaxing towards its predicted theoretical value, which is 8. The part of the curve close to $w/\langle w\rangle$ is magnified to show the agreement between simulations and theory on the limited accessible range of values at $t = 40$.

very good agreement with the value expected from our theory $\langle\mathcal{W}^3\rangle_c = -t\,[\partial^3\mu(\lambda)/\partial\lambda^3]_{\lambda=0}$. We recall that this estimate of the third cumulant is highly non-trivial. At such large t values, however, the numerically accessible range of w is very small, limiting the possibility of a detailed comparison between analytics and numerics (see fig. 2).

Having reached the conclusion that the injected power cannot fulfill the GC relation, in this final paragraph we propose an alternative quantity which is, by its very definition, a Gibbs entropy flow, and satisfies the GC fluctuation relation. The sequel applies both to the original experimental system in which particles contained in a closed box are vigorously shaken and to our random thermostat. We now tag one of these particles that we follow along its path, which is similar in spirit to the work reported in [19]. The rest of the particles act as a thermostat for the tagged particle. Note, however, that the states of the particle bath evolve according to dynamical rules that do not fulfill the detailed balance condition. Similarly, the trajectory in the phase space of the tagged particle does not fulfill the detailed balance condition (this is a key difference with [19]). It is now possible to view the time evolution of the tagged particle as a Markov process. In the tagged-particle phase space, to every non-zero transition rate between two velocity states one can associate a non-zero rate for the backward move. This is the core of the difference with following the dynamics in the phase space of the whole system. There, due to irreversible microscopic dynamics (inelastic collisions), for a given forward-in-time trajectory in phase space, there is no corresponding, however extremely unlikely, backward-in-time trajectory. Hence for the tagged particle it is perfectly legitimate to define an integrated entropy flow *à la* Lebowitz and Spohn [8] (see also Maes [20] or Gaspard [21] for alternative presentations):

$$\mathcal{S}(t) = \sum_{i=1}^{n(t)} \ln \frac{K(\boldsymbol{v}_i \to \boldsymbol{v}_{i+1})}{K(\boldsymbol{v}_{i+1} \to \boldsymbol{v}_i)}, \tag{8}$$

where $n(t)$ is the number of collisions undergone by the tagged particle over the time interval $[0,t]$, $\boldsymbol{v}_i$ is its velocity after the i-th collision, and $K(\boldsymbol{v} \to \boldsymbol{v}')$ is the velocity transition rate of a particle undergoing a collision. Expression (8) may be experimentally accessible in the following way: the monitoring of a large number of collisions (and of the velocities before and after collision) first gives an estimation of the velocity transition rates $K(\boldsymbol{v} \to \boldsymbol{v}')$, that can be tabulated with an appropriate discretization of velocities; it is then possible to follow one given tagged particle, to measure its successive pre- and post-collision velocities and thus to compute $\mathcal{S}$. In the elastic limit for the thermostat the transition rates $K(\boldsymbol{v} \to \boldsymbol{v}')$ verify the detailed balance condition with respect to a Maxwellian tagged-particle velocity pdf [19], hence there is no entropy flow anymore, and $\mathcal{S}(t)/t \overset{t\to\infty}{\to} 0$ (the tagged particle is in equilibrium within its own phase space). Fully explicit expressions for the transition rate $K(\boldsymbol{v} \to \boldsymbol{v}')$, and hence for $\mathcal{S}(t)$ [18] can be derived for an inelastic thermostat, *e.g.* using Sonine expansions. By construction, the pdf of the instantaneous entropy flow (8) will verify a GC relation, with the ensuing consequences in terms of Green-Kubo relations.

We have provided the first computation of the large deviation function of the injected power in a system driven far from equilibrium, for which no general theory has hitherto been coined, as opposed to systems weakly driven out of equilibrium [22]. This computation allowed us to pinpoint numerical limitations and yet to extract reliable data. We have shown why the injected power cannot satisfy a GC relation, thus revealing a scenario sharing many features in common with the equilibrium toy model considered by Farago [23]. However, even if π_∞, the large-t limit of $\pi_t(w)$, cannot exhibit a GC symmetry due to the absence of a negative tail, it appears that from a practical point of view, $\pi_t(w)$ seems to obey a GC-like relation (see fig. 1). An important consequence of the analytical work outlined here is that such a "finite-time" property cannot be considered as an extension of GC theorem. Finally, we have put forward a new approach, based upon a Lagrangian point of view, that leads to a definition of an entropy flow possessing all the properties requested by the systematic approach of Lebowitz and Spohn [8], and which may be experimentally accessible. We are confident that not only the new extensions of kinetic theory developed here, but also the proposal for an entropy function, will trigger new theoretical investigations and will lend themselves to experimental confirmations far beyond the granular community, in the spirit of recent experiments on turbulent flows resting on Lagrangian viewpoint investigations [24].

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The authors acknowledge several useful conversations with S. Aumaître, J. Farago and S. Fauve. AP acknowledges the Marie Curie grant No. MEIF-CT-2003-500944. ET thanks the EC Human Potential program under contract HPRN-CT-2002-00307 (DYGLAGEMEN).

REFERENCES

[1] Einstein A., *Ann. Phys. (Leipzig)*, **17** (1905) 549.
[2] Onsager L., *Phys. Rev.*, **37** (1931) 405; **38** (1931) 2265.
[3] Green M. S., *J. Chem. Phys.*, **22** (1954) 398.
[4] Kubo R., *J. Phys. Soc. Jpn.*, **12** (1957) 570.
[5] Evans D. J., Cohen E. G. D. and Morriss G. P., *Phys. Rev. Lett.*, **71** (1993) 2401; 3616(E).
[6] Gallavotti G. and Cohen E. G. D., *Phys. Rev. Lett.*, **74** (1995) 2694.
[7] Kurchan J., *J. Phys. A*, **31** (1998) 3719.
[8] Lebowitz J. L. and Spohn H., *J. Stat. Phys.*, **95** (1999) 333.
[9] Aumaître S., Fauve S., McNamara S. and Poggi P., *Eur. Phys. J. B*, **19** (2001) 449.
[10] Feitosa K. and Menon N., *Phys. Rev. Lett.*, **92** (2004) 164301.
[11] Labbé R., Pinton J.-F. and Fauve S., *J. Phys. II*, **6** (1996) 1; Bramwell S. T., Holdsworth P. C. W. and Pinton J.-F., *Nature*, **396** (1998) 552.

[12] Williams D. R. M. and MacKintosh F. C., *Phys. Rev. E*, **54** (1996) R9; Peng G. and Ohta T., *Phys. Rev. E*, **58** (1998) 4737; van Noije T. P. C., Ernst M. H., Trizac E. and Pagonabarraga I., *Phys. Rev. E*, **59** (1999) 4326; Henrique C., Batrouni G. and Bideau D., *Phys. Rev. E*, **63** (2000) 011304; Moon S. J., Shattuck M. D. and Swift J. B., *Phys. Rev. E*, **64** (2001) 031303.

[13] de Groot S. R. and Mazur P., *Non-Equilibirum Thermodynamics* (North-Holland, Amsterdam) 1969.

[14] A direct although non-trivial consequence would be that $\langle \mathrm{e}^{-\beta\mathcal{W}} \rangle = 1$ which would be hinting to the existence of a free-energy–like state function (see, *e.g.*, Jarzynski C., *J. Stat. Mech.* (2004) P09005).

[15] This argument was brought to our attention by J. Farago.

[16] Relation (6) may nevertheless be observed experimentally (see [10]) or numerically at finite time (transient effect). For more details, see Puglisi A. *et al.*, to be published in *Phys. Rev. Lett.* (2005).

[17] Bird G. A., *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Clarendon, Oxford) 1994.

[18] Visco P., Puglisi A., Trizac E. and van Wijland F., submitted to *J. Stat. Phys.*; Puglisi A., Visco P. and van Wijland F., submitted to *Phys. Rev. E.*

[19] Martin P. A. and Piasecki J., *Europhys. Lett.*, **46** (1999) 613.

[20] Maes C., *J. Stat. Phys.*, **95** (1999) 367.

[21] Gaspard P., *Chaos, Scattering and Statistical Mechanics* (Cambridge University Press, Cambridge) 1998.

[22] Derrida B. and Bodineau T., *Phys. Rev. Lett.*, **92** (2004) 180601.

[23] Farago J., *J. Stat. Phys.*, **107** (2002) 781.

[24] Ott S. and Mann J., *J. Fluid. Mech.*, **422** (2000) 207; Yeung P. K., *Annu. Rev. Fluid Mech.*, **34** (2002) 115; Chevillard L., Roux S. G., Levêque E., Mordant N., Pinton J.-F. and Arneodo A., *Phys. Rev. Lett.*, **91** (2003) 214502.