Validity of Gallavotti-Cohen Fluctuation Relation in driven granular gases

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ABSTRACT: In a recent experiment it has been claimed that the Gallavotti and Cohen's Fluctuation Relation (FR) is satisied by the fluctuations of power injection in a vibrated granular gas. Anyway, by simple reasoning, it can be shown that for a granular gas such a relation cannot be true. We have studied numerically and analytically the fluctuations of power injection in different models. FR never holds. In the case of boundary driving it can be calculated the behavior at intermediate, observable times, of internal power injection, obtaining quantitative agreement with the experiment. In the case of homogeneous driving a general theory can be obtained, predicting the behavior of the large deviation function of the fluctuations of power injected by the thermostat. Finally we suggest a possible route to define an entropy production, measurable in granular gases, which must satisfy the FT.

1 INTRODUCTION

1.1 Granular gases

A granular gas is the perfect tool for investigating statistical mechanics in out-of-equilibrium regimes (1). It proves to be a simple and rich model, open to analytical and numerical insights, and at the same time accessible by experiments. From the theoretical point of view, a granular gas is a collection of hard objects (rods, disks or spheres), moving in a container, which lose a fraction of their relative energy in instantaneous binary collisions. In the physical world it can be found under the form of fluidized sand or grains of any kind, where the fluidization is usually provided by a high frequency vibration. When speaking of a granular *gas* we refer to setups dilute enough, in order to keep the excluded volume effects small with respect to the other mechanisms determining the transport properties. Granular gases display an astonishing plethora of different behaviors, depending upon the external conditions. A large class of instabilities leading to spontaneous symmetry breakings is observed, such as clustering and shear, surface waves, convection rolls and shocks (2). An inelastic gas does not satisfy the fundamental hypothesis of equilibrium gases, mainly because of energy dissipation which implies the presence of an external energy injection and therefore a non-trivial flow of energy between a source/thermostat and an energy sink. This leads to the breakdown of many typical equilibrium assumptions: a driven granular gas exhibits non-Gaussian velocity distributions, does not obey to equipartition of energy (among different degrees of freedom or among different components of a mixture), and if the energy driving is modeled as a homogeneous thermostat with temperature T_{bath} and a granular temperature $T_{gran} = \langle v^2 \rangle / D$ (D the dimensionality) is measured, it is usually found $T_{gran} < T_{bath}$.

1.2 The Fluctuation Theorem

Recently, in experiments and numerical simulations, the validity of the so-called Gallavotti-Cohen Fluctuation Relation (FR), stated for the first time in (3), has been probed in vibrated granular gases. The FR is a theorem (4) proved for chaotic dynamical systems with microscopic reversibility, when the entropy production (in the form of the phase space contraction rate) is measured, and for Markov processes (5; 6) when the fluctuations of a well suited function of the phase space trajectories, taken as a measure of violation of the detailed balance, i.e. of entropy production, are measured. FT roughly says that, being σ_τ the measured fluctuating quantity integrated on a time τ, and $f(\sigma_\tau)$ its probability density function, then

$$\ln[f(\sigma_\tau)/f(-\sigma_\tau)] = \sigma_\tau \tag{1}$$

when $\tau \to \infty$.

The FT gives a measure of the relative weight of transient violations of the second principle of thermodynamics, which requires entropy production to be non-negative (11). The FT has been experimentally verified in a few setups (12). More recently it has been verified in an experiment on granular gases (8).

2 The experiment

The experiment performed by Menon and Feitosa (8) consisted of a $2D$ box containing N identical grains of glass, vibrated at frequency f and amplitude A. The authors observed the kinetic energy variations Δ_τ, during windows of time τ, in a central subregion of the system characterized by an almost homogeneous temperature and density. They divided this variation into two contributions:

$$\Delta_\tau = Q_\tau - D_\tau, \tag{2}$$

where D_τ is the energy dissipated in inelastic collisions and Q_τ is the energy flux through the borders, due to the kinetic energy transported by particles going in and going out. The authors of the experiment have conjectured that Q_τ, being a measure of injected power in the sub-system, can be related to the entropy flow or the entropy produced by the thermostat constituted by the rest of the gas (which in the steady state is equal to the internal entropy production). They have measured its probability density function (pdf) $f(Q_\tau)$ and found that

$$\ln \frac{f(Q_\tau)}{f(-Q_\tau)} = \beta Q_\tau \tag{3}$$

with $\beta \neq 1/T_g$. Lacking a reasonable explanation for the value of β, the authors have claimed to have experimentally verified the FR with an "effective temperature" $T_{eff} = 1/\beta$, suggesting it as possible non-equilibrium generalization of usual temperature.

There is a first major objection to this reasoning: in the limit of zero inelasticity (i.e. in the case of ideal elastic grains) the pdf $f(Q_\tau)$ becomes symmetric with respect to the average injected power through the borders of the central region, which is 0, so that $\beta \to 0$, i.e. the effective temperature would diverge instead of coinciding with the equilibrium temperature. There is also a more subtle problem in this experiment: from Equation 2, it can be demonstrated that the large deviation function of $f(Q_\tau)$ is equal to the large deviation function of $f(D_\tau)$. We recall that when $\tau \to \infty$, $f(Q_\tau) \sim exp(\tau\pi(Q_\tau/\tau))$ and $\pi(q)$ is the large deviation function of $f(Q_\tau)$. Since D_τ is *always positive*, it follows that the relation 3 cannot hold when $\tau \to \infty$.

3 THE EXPLANATION OF THE EXPERIMENT

We have reproduced the experiment by means of molecular dynamics simulations of inelastic hard disks (13), recovering all the experimental results with a good quantitative agreement. Moreover we have analytically studied the fluctuations of Q_τ. It appears that the injected power measured in the experiment can be written as

$$Q_\tau = \frac{1}{2}\left(\sum_{i=1}^{n_+} v_{i+}^2 - \sum_{i=1}^{n_-} v_{i-}^2\right), \tag{4}$$

where n_- (n_+) is the number of particles leaving (entering) the window during the time τ, and v_{i-}^2 (v_{i+}^2) are the squared moduli of their velocities. In order to analyze the statistics of Q_τ we take n_- and n_+ as Poisson-distributed random variables with average $\omega\tau$, neglecting correlations among particles entering or leaving successively the central region. Supported by direct observation in the simulation we assume the velocities $\mathbf{v}_{i+}$ and $\mathbf{v}_{i-}$ to come from populations with different temperatures T_+ and T_- respectively. Indeed, compared with the population entering the central region, those particles that leave it have suffered on average more inelastic collisions, so that $T_- < T_+$. Finally we assume Gaussian velocity pdfs (while non-Gaussian tails are quite common in granular gases (14), we have checked that they play a negligible role here). We have analytically calculated the generating function of $f(Q_\tau)$, obtaining $g(z) = \exp(\tau\mu(z))$ for any τ, with

$$\mu(z) = \omega\left(-2 + (1 - T_+ z)^{-D/2} + (1 + T_- z)^{-D/2}\right), \tag{5}$$

which also automatically coincides with the large deviation function of $g(z)$. We recall that the two large deviation functions $\mu(z)$ and $\pi(q)$ are related by a Legendre transform. An FR with a slope β implies that $\mu(z) = \mu(\beta - z)$ and this relation is evidently not satisfied by Eq. 5. Anyway it has been observed (7) that $\pi(q) - \pi(-q) \approx 2\pi'(0)q + o(q^3)$ at small values of q. This means that the linear relation 3 with $\beta_{eff} = 2\pi'(0)$ can be observed if the range of Q_τ is small, which is usually the case since in experiments and simulations the statistics of negative events is very poor. From equation 5 a formula for the slope β follows:

$$\beta_{eff} = 2\frac{\gamma^\delta - 1}{\gamma + \gamma^\delta}\frac{1}{T_-} \tag{6}$$

with $\gamma = T_+/T_-$ and $\delta = 2/(2 + D)$. When $\gamma = 1$ (i.e. when the gas is elastic) $\beta_{eff} = 0$. This formula is in good agreement with the slope observed in the simulations and in the experiment.

We remark that, in order to be consistent with the second objection given at the end of the introduction, the assumption of non-correlated velocities in the expression 4 must be violated at large times $\tau \to \infty$. The fact that expression 5 is in good quantitative agreement with the experiment is consistent with the observation of negative events. We can argue that the experiment and the simulations have considered times large enough to test the validity of formula 6, but not too much large, so that correlations may be disregarded.

4 A SIMPLE MODEL OF HOMOGENEOUSLY DRIVEN GRANULAR GAS

It is natural, in a theoretical research, to focus on simple models, in order to catch the essential ingredients of a phenomenon. We have therefore studied one of the most investigated models of homogeneously driven granular gases (9). In this model N hard disks collide inelastically and each particle, between collisions, is coupled to an external thermostat so that its equation of motion reads

$$\frac{d\mathbf{v}_i(t)}{dt} = \mathbf{F}_i(t) \tag{7}$$

with $\mathbf{F}$ a random force with covariance $\langle F_i^\alpha(t) F_j^\beta(t') \rangle = 2\Gamma \delta_{ij} \delta_{\alpha\beta} \delta(t-t')$. We assume Molecular Chaos and, in the simulations, we enforce it through the use of a Direct Simulation Monte Carlo algorithm (10). The collisions happen with a restitution coefficient α that takes values between 0 (perfectly inelastic gas) and 1 (elastic gas). The gas rapidly reaches a stationary state with a granular temperature $T_g = 4D/(1-\alpha^2)$, if the mean free time is used as a measure unit for time. Our interest (15) went to the fluctuations of the work exerted by the thermostat

$$\mathcal{W}(\tau) = \int_0^\tau dt \, \sum_i \mathbf{F}_i \cdot \mathbf{v}_i \tag{8}$$

Again, the equation 2 holds, with $Q_\tau \equiv \mathcal{W}(\tau)$, so that the possibility of observing FR, i.e. a linear relation such as the one in Eq. 3 at large τ, is ruled out. Anyway we are interested in the way this “violation” of FR comes out from a direct analysis of the pdf of $\mathcal{W}$ in the model . We started from an extended Liouville equation for the probability $\rho(\Gamma_N, \mathcal{W}, t)$ that the system is in a point Γ_N of the N-velocity phase space, with $\mathcal{W}(t) = \mathcal{W}$ at time t. The second step is to convert the Liouville equation in terms of the generating function $\hat{\rho}(\Gamma_N, \lambda, t) = \int d\mathcal{W} \exp(-\lambda \mathcal{W})\rho$. We are interested in the largest eigenvalue $\mu(\lambda)$ of the evolution operator for $\hat{\rho}$, which is the generating function for the cumulants of $\mathcal{W}(t)/t$. The eigenvalue equation is then projected onto the one-particle subspace, which couples to the two-particle subspace, as the Boltzmann equation limit $\lambda \to 0$ already features. By means of a molecular-chaos like closure procedure we arrive at an equation for both the eigenvalue μ and its related eigenfunction. The we are able to show that the large deviation function of $\mathcal{W} = wt$ has tails given by

$$\pi(w \to 0^+) \sim -w^{-1/3}, \;\; \pi(w \to +\infty) \sim -w \tag{9}$$

with, as expected, no $w < 0$ contribution. While the $w \to 0^+$ regime looks 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 $\mu(\lambda)$. Moreover, using that $\frac{d^4\mu}{d\lambda^4} = \langle \mathcal{W}^4 \rangle_c / t$ we could compare $\mathcal{W}$'s first cumulants with their numerical estimates, obtaining good quantitative agreement.

In an experiment, i.e. in this case in a numerical simulation, it is extremely difficult to gather a decent statistics for negative events, so that one is obliged to use not too high values of τ, usually not much larger than the mean free time which is the characteristic time of the dynamics. Again this leads to an apparent agreement with FR: a linear relation such as the one in Eq. 3 is obtained. It appears that in this model $\beta \approx 1/T_g$ when α is near 1. As α is decreased the linear relation is still observed, with a slope slightly larger (and growing as α gets smaller and smaller) than $1/T_g$. Such a slope would be consistent with a Gaussian pdf of $\mathcal{W}$ (centered in $\langle \mathcal{W} \rangle \neq 0$), but the pdf's show clear deviations from the Gaussian also in the interested region. We are investigating the possibility of reproducing this slope through a reasoning similar to the one already sketched in the previous section.

5 DETAILED BALANCE FOR A TAGGED PARTICLE

Up to now we have shown that, even if simulations and experiments, due to limited resolution, suggest the contrary, the Gallavotti-Cohen FR cannot hold for the fluctuations of power injection in a granular gas. A question remains about the possibility of finding a quantity playing the role of entropy production in stationary granular gases and therefore satisfying the FR. In the derivation of FR for stochastic systems given by Lebowitz and Spohn (6) it has been put in evidence that, if one knows the transition probabilities of the Markovian process governing the dynamics, then it can be defined a functional $W(\tau)$ of the trajectories of length τ which can be identified with the Gibbs entropy flow. Anyway, to follow this path, some kind of “reversibility” is needed, i.e. for each possible jump in the space of phases its reversed jump must be possible (of course with different probability). This is not the case for granular gases, as a consequence of inelastic collision rules. If two particles have collided, doing the transition $(\mathbf{v}_1,\mathbf{v}_2) \to (\mathbf{v}'_1,\mathbf{v}'_2)$ there is not any collision such that $(\mathbf{v}'_1,\mathbf{v}'_2) \to (\mathbf{v}_1,\mathbf{v}_2)$. Symmetry is restored only when $\alpha = 1$, i.e. when the gas is elastic. To circumvent this problem, we have conjectured that a tagged particle may be representative of the mixing properties of the whole gas. We imagine that the gas, made of $N \ll 1$ particles, is in contact with the same thermostat modeled in Eq. 7, while the tagged particle is not. It simply collides inelastically with the gas particles without perturbing its stationary state. The velocity pdf of the tagged particle is well described by a linear-Boltzmann equation. Then it is possible to describe the dynamics of the particle as a Markov chain of successive collisions. Each jump $\mathbf{v} \to \mathbf{v}'$ has a transition probability $K(\mathbf{v},\mathbf{v}')$ and the inverse jump $\mathbf{v}' \to \mathbf{v}$ is always possible, thanks to fact that the collision-mate degree of freedom has been integrated out. Following the recipe of Lebowitz and Spohn (6), we are able to obtain an explicit expression for the entropy production $W(\tau)$ associated to the tagged particle. It of course depends upon the particular stationary velocity pdf of the gas, which is usually different from a Gaussian. It is interesting to observe that the inelastic tagged particle model has a simple solution in the case that the gas has a Gaussian velocity pdf: the tagged particle has exactly a Gaussian velocity pdf with a temperature *different* from the one of the gas (16). In this case the Markov process followed by the tagged particle satisfies the detailed balance with respect to this Gaussian measure and the entropy production is zero. As soon as the velocity pdf of the gas deviates from the Gaussian (which is the most physical situation) then the detailed balance is violated, $W(\tau)$ assumes positive as well as negative values, and the Fluctuation Relation holds.

6 CONCLUSIONS

We have studied by numerical simulations and analytical calculations the fluctuations of injected power in driven granular gases in different experimental setup, driven at the boundaries or homogeneously. This has proved to be useful in order to understand the real possibility of probing the large time limit of the integral of these fluctuations in experiments. It seems that such limit is almost impossible to be obtained and that the information at the available times may be misleading. Mainly a "false" verification of the Gallavotti-Cohen Fluctuation Relation can be observed. We have concluded suggesting a route to define an entropy production in driven granular gases.

A. P. acknowledges the Marie Curie grant No. MEIF-CT-2003-500944. E.T. thanks the EC Human Potential program under contract HPRN-CT-2002-00307 (DYGLAGEMEN).

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