Injected power and entropy flow in a heated granular gas

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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.
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 $F_i$ which
we take to be Gaussian distributed with variance $\Gamma$. The equation of motion for particle $i$
with velocity $v_i$ then reads $dv_i/dt = F_{\text{coll}} + F_i$ where $F_{\text{coll}}$ 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 transla-
tional 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
$W(t)$ provided by the thermostat:

$$W(t) = \int_0^t dt \sum_i F_i \cdot v_i.$$  

(1)

The granular temperature is defined by $T_g = 1/\beta = \langle v_i^2 \rangle/d$ 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 $W(t)$, $P(W, t)$, and its related large deviation function

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

(2)

The generating function $\hat{P}(\lambda, t) = \langle e^{-\lambda W} \rangle$ and its related large deviation function $\mu(\lambda) = \lim_{t \to \infty} \frac{1}{t} \ln P(\lambda, t)$ 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 $S$,

$$\frac{dS}{dt} = \sigma - \int_{\text{system}} dV \nabla \cdot J_S$$  

(3)

which, in a steady-state, expresses a balance of an entropy production term (a measure of
intrinsic irreversibility) with an entropy flux $J_S$ 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 $P(S, t)$ of a quantity $S(t)$ playing
the role of the time-integrated flux term $\int dt dV \nabla \cdot \mathbf{J}_S$ verifies, in the limit of asymptotically
large times,
\[
\ln \frac{P(S, t)}{P(-S, t)} = S. \tag{4}
\]
Nevertheless, the assumptions underlying GC are microscopic reversibility and the identification of $S$ 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 $\beta W$ could possibly play the role of $S$ \[9\]. In the heated granular gas the fluctuating total kinetic energy $E(t) = \sum_i \mathbf{v}_i^2 / 2$ varies according to
\[
E(t) - E(0) = W(t) - D(t) \tag{5}
\]
where $D(t) \geq 0$ is the energy dissipated through collisions up until time $t$. Of course on average $\langle W(t) = \langle D(t) = 2d\Gamma t \rangle > 0$, yet there will be individual realizations for which $W$ will be negative. If the GC relation \[14\] held for $W$, it would take the following form
\[
\pi_{\infty}(w) - \pi_{\infty}(-w) = \beta w, \quad \mu(\lambda) = \mu(\beta - \lambda) \tag{6}
\]
Remark, though, that the left-hand side in \[5\] is bounded in time (while $W$ and $D$ 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. $(\mathbf{v}_i' - \mathbf{v}_j') \cdot \mathbf{n} = -\alpha (\mathbf{v}_i - \mathbf{v}_j) \cdot \mathbf{n}$ where the primes mark the post-collisional velocities and $\mathbf{n}$ is the direction joining the colliding particles. The driving force $\mathbf{F}_i$ mentioned above obeys $\langle F_i^j(t) F_j^j(t') \rangle = 2\Gamma \delta_{ij} \delta^{\gamma \delta} \delta(t - t')$. Molecular Chaos is enforced through the use of a Direct Simulation Monte Carlo \[17\] algorithm. The restitution coefficient $\alpha$ 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 $W(t)$ as defined in Eq. \[1\] using an integration time $t$. $P(W, t)$ 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 $\alpha$ a slight departure (about 10%) from the slope $\beta$ can be recognized. And yet the plot of $\pi_t(w) - \pi_{\infty}(-w)$ 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.
![Graph](image)

Fig. 1 – **Color online**: Plot of $\pi_t(w) - \pi_t(-w)$ as a function of $\beta w$. 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 $\Gamma = 0.5$.

Fig. 2 – The large deviation function $\pi_\infty$ of the rescaled quantity $W/\langle W \rangle$ obtained from the Legendre transform of the largest eigenvalue $\mu(\lambda)$ (see text and [18] for details). The inset shows the dimensionless third cumulant $\langle W^3 \rangle_c = \langle W^3 \rangle / \langle W \rangle$ 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 $t = 40$.

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 $\rho(\Gamma_N, W, t)$ that the system is in state $\Gamma_N$ with $W(t) = W$ at time $t$. The second step is to convert the Liouville equation in terms of the generating function $\hat{\rho}(\Gamma_N, \lambda, t) = \int dW e^{-\lambda W} \rho$. 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 $W(t)/t$): 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 $\mu$ 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 $W = wt$ has the graph depicted in Fig. 2. The tails are given by

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

with, as expected, no $w < 0$ contribution. While the $w \to 0^+$ regime appears to be thermostat-dependent, the exponential right tail of $P(W, t)$ seems to be a robust property related to the presence of a branch cut in the complex $\lambda$ 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 $\beta$, 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 $\sim 50$, much larger than the times used in Fig. 1. Moreover this stable value is in very good agreement with the value expected from our theory $\langle W^3 \rangle_c = -t \partial^3 \mu(\lambda)/\partial \lambda^3 |_{\lambda=0}$. We recall that this estimate of the third cumulant is highly non-trivial. At such large $t$ values, however, the numerically accessible range of $\omega$ 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):

$$S(t) = \sum_{i=1}^{n(t)} \ln \frac{K(v_i \rightarrow v_{i+1})}{K(v_{i+1} \rightarrow v_i)}$$

where $n(t)$ is the number of collisions undergone by the tagged particle over the time interval $[0, t]$, $v_i$ is its velocity after the $i$-th collision, and $K(v \rightarrow v')$ 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 $K(v \rightarrow v')$, 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 $S$. In the elastic limit for the thermostat the transition rates $K(v \rightarrow v')$ verify the detailed balance condition with respect to a Maxwellian tagged particle velocity pdf [19], hence there is no entropy flow anymore, and $S(t)/t \rightarrow 0$ (the tagged particle is in equilibrium within its own phase space). Fully explicit expressions for the transition rate $K(v \rightarrow v')$, and hence for $S(t)$ [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 \( \pi_\infty \), 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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