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Fluctuations relation and external thermostats: an application to granular materials

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Abstract. In this paper we discuss a paradigmatic example of interacting particles subject to non-conservative external forces and to the action of thermostats consisting of external (finite) reservoirs of particles. We then consider a model of granular materials of interest for experimental tests that have recently attracted a lot of attention. This model can be reduced to the previously discussed example under a number of assumptions, in particular that inelasticity due to internal collisions can be neglected for the purpose of measuring the large deviation functional for entropy production rate. We show that if the restitution coefficient in the granular material model is close to one, then the required assuptions are verified on a specific timescale and we predict a fluctuation relation for the entropy production rate measured on the same timescale.

Keywords: transport processes/heat transfer (theory), granular matter, fluctuations (theory), stationary states (theory)

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Contents

1. Non-equilibrium

In studying stationary states in non-equilibrium statistical mechanics [1, 2], it is common to consider d-dimensional systems of particles in a (finite) container Σ_0 forced by non-conservative forces whose work is controlled by thermostats consisting of particles moving outside Σ_0 and interacting with the particles of Σ_0 through interactions across the walls of Σ_0 [3]. If $\mathbf{X}^0 = (\mathbf{x}_1^0, \ldots, \mathbf{x}_{N_0}^0)$ are the particles' positions in an inertial system of coordinates, the equations of motion are determined by their mass m, by the *potential energy* of interaction $V(\mathbf{X}^0)$, by external non-conservative forces $\mathbf{F}_i(\mathbf{X}^0, \boldsymbol{\Phi})$, and by *thermostat* forces $-\boldsymbol{\vartheta}_i$ as

$$m\ddot{\mathbf{x}}_i^0 = -\partial_{\mathbf{x}_i^0} V(\mathbf{X}^0) + \mathbf{F}_i(\mathbf{X}^0; \boldsymbol{\Phi}) - \boldsymbol{\vartheta}_i, \tag{1}$$

where $i = 1, \ldots, N_0$, and $\boldsymbol{\Phi} = (\varphi_1, \ldots, \varphi_q)$ are strength parameters on which the external forces depend (e.g. the components of an external electric field). Forces and potentials will be supposed to be smooth, i.e. analytic, in their variables, aside from *possible* impulsive elastic forces describing shocks; the forces $\mathbf{F}_i$ will be supposed to vanish for $\boldsymbol{\Phi} = \mathbf{0}$. The impulsive forces are allowed here to model possible shocks with the walls of the container Σ_0 or between hard core particles.

Examples of deterministic reservoirs [4] are forces obtained by imposing a non-holonomic constraint via some ad hoc principle, like the Gauss' principle [5] (appendix 9.A4), [6]. A different example will be discussed below extensively.

In general, the forces $\boldsymbol{\vartheta}_i$ can be considered as a set of deterministic 'thermostat forces' if a further property holds: namely that the system evolves according to equation (1) towards a *stationary state*. This means that, for all $(\dot{\mathbf{X}}^0, \mathbf{X}^0)$, *except possibly for a set of zero phase-space volume*, *any* smooth function $f(\dot{\mathbf{X}}^0, \mathbf{X}^0)$ evolves in time so that, denoting $S_t(\dot{\mathbf{X}}^0, \mathbf{X}^0)$ the configuration into which $(\dot{\mathbf{X}}^0, \mathbf{X}^0)$ evolves in time t according

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to equation (1), then the limit

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T f(S_t(\dot{\mathbf{X}}^0,\mathbf{X}^0))\,\mathrm{d}t=\int f(z)\mu(\mathrm{d}z) \tag{2}$$

exists and is independent of $(\dot{\mathbf{X}}^0,\mathbf{X}^0)$. The phase-space probability distribution $\mu(\mathrm{d}z)$ (here $z=(\dot{\mathbf{Y}},\mathbf{Y})$ denotes the coordinates of position and velocity of a generic point in phase space) is then called the *SRB distribution* for the system. It has to be stressed that the condition that thermostat forces be 'effective' enough to impede an indefinite build up of the energy of the system is a strong condition, which we will assume in the models discussed in this note. This imposes on the interaction potentials and on the thermostat conditions, which are not well understood, although they seem empirically verified with the simplest choices of molecular potentials [5].

The maps S_t will have the group property $S_t\cdot S_{t'}=S_{t+t'}$, and the SRB distribution μ will be invariant under time evolution. The SRB distribution is said to describe a stationary state of the system; it depends on the parameters on which the forces acting on the system depend, e.g. $|\Sigma|$ (volume), $\boldsymbol{\Phi}$ (strength of the forcings) and on the model of thermostat forces. The collection of SRB distributions obtained by letting the parameters vary defines a *non-equilibrium ensemble*.

2. A model of external thermostats

Let us now discuss in more detail an important class of thermostats in the context of model equation (1). Imagine that the N_0 particles in the container Σ_0 interacting via the potential $V(\mathbf{X}^0)=\sum_{i<j}\varphi(\mathbf{x}_i^0-\mathbf{x}_j^0)+\sum_j V_0(\mathbf{x}_j^0)$ (where V_0 models external conservative forces such as obstacles, walls, gravity, ...) and subject to the external forces $\mathbf{F}_i$ are also interacting with M other systems Σ_a, of N_a particles of mass m_a, in containers Σ_a contiguous to Σ_0. It will be assumed that $\Sigma_a\cap\Sigma_{a'}=\emptyset$ for $a\neq a'$, $a,a'=0,\ldots,M$.

The coordinates of the particles in the ath system Σ_a will be denoted $\mathbf{x}_j^a$, $j=1,\ldots,N_a$, and they will interact with each other via a potential $V_a(\mathbf{X}^a)=\sum_{i,j}^{N_a}\varphi_a(\mathbf{x}_i^a-\mathbf{x}_j^a)$. Furthermore, there will be an interaction between the particles of each thermostat and those of the system via potentials $W_a(\mathbf{X}^0,\mathbf{X}^a)=\sum_{i=1}^{N_0}\sum_{j=1}^{N_a}w_a(\mathbf{x}_i^0-\mathbf{x}_j^a)$, $a=1,\ldots,M$.

Again, potentials will be assumed to be either hard core or non-singular and V_0 to be at least such that it forbids the existence of obvious constants of motion.

The temperature of each Σ_a will be defined by the total kinetic energy of its particles, *i.e.* by setting $K_a=\sum_{j=1}^{N_a}\frac{1}{2}m_a(\dot{\mathbf{x}}_j^a)^2\stackrel{\mathrm{def}}{=}\frac{1}{2}(dN_a-1)k_{\mathrm{B}}T_a$, where k_{B} is Boltzmann's constant and d is the spatial dimension; the particles of the ath thermostat will be kept at constant temperature by further forces $\boldsymbol{\vartheta}_j^a$. The latter are defined by imposing constancy of K_a via Gauss' least effort principle. This means that equations of motion like

$$\begin{aligned} m\,\ddot{\mathbf{x}}_j^0 &= -\partial_{\mathbf{x}_j^0}\Big(V(\mathbf{X}^0)+\sum_{a=1}^{M}W_a(\mathbf{X}^0,\mathbf{X}^a)\Big)+\mathbf{F}_i(\mathbf{X}^0,\boldsymbol{\Phi})\\ m_a\,\ddot{\mathbf{x}}_j^a &= -\partial_{\mathbf{x}_j^a}(V_a(\mathbf{X}^a)+W_a(\mathbf{X}^0,\mathbf{X}^a))-\boldsymbol{\vartheta}_j^a \end{aligned} \tag{3}$$

and an application of Gauss' principle yields $\boldsymbol{\vartheta}_j^a=m_a(L_a-\dot{V}_a)/(dN_a-1)k_{\mathrm{B}}T_a\,\dot{\mathbf{x}}_j^a\stackrel{\mathrm{def}}{=}\alpha^a\,\dot{\mathbf{x}}_j^a$, where L_a is the work per unit time done by the particles in Σ_0 on the particles of

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Σ_a and V_a is their potential energy [6]. Note that in the first part of equation (3), the forces $-\partial_{\mathbf{x}_i^0} W_a$ play the role of the thermostat forces $\boldsymbol{\vartheta}_i$ in equation (1).

The work L_a appearing in the definition of $\boldsymbol{\vartheta}_j^a$ can be naturally interpreted as *heat* $\dot{Q}_a$ ceded, per unit time, by the particles in Σ_0 to the thermostat Σ_a (because the 'temperature' of Σ_a is constant). If $\mathbf{X} = (\mathbf{X}^0, \mathbf{X}^1, \ldots, \mathbf{X}^M)$, the *entropy creation rate* can be naturally defined as

$$\sigma_0(\dot{\mathbf{X}}, \mathbf{X}) \stackrel{\text{def}}{=} \sum_{a=1}^{M} \frac{\dot{Q}_a}{k_{\text{B}} T_a} \tag{4}$$

hence σ_0 can be called (in model equation (3)) the *average entropy creation rate.* Its time average will be assumed to be $\sigma_{0,+} \stackrel{\text{def}}{=} \langle \sigma_0 \rangle_{\text{SRB}} \neq 0$. Note that now $\langle \cdot \rangle_{\text{SRB}}$ is the average with respect to the stationary measure for the whole system Σ_0 +thermostats.

We shall see that, in ample generality, $\sigma_{0+} \geq 0$: the definition of entropy creation is 'reduced', here, to an 'equilibrium notion', because what is being defined is the entropy increase of the thermostats, which have to be considered to be in equilibrium. No attempt is made to define the entropy of the stationary state. Nor is any attempt made to define the temperature of the non-equilibrium system in Σ_0 (T_a is the temperature of Σ_a, not of Σ_0).

In fact, the above model is a realization of a *Carnot machine*: the machine being the system in Σ_0 on which external forces work, leaving the system in the same state (a special 'cycle') but achieving a transfer of heat between the various thermostats (in agreement with the second law, see equation (4), only if $\sigma_{0,+} \geq 0$).

Another observable that is convenient to introduce is the *phase-space contraction rate* $\sigma(\dot{\mathbf{X}}, \mathbf{X})$, defined as *minus the divergence* of the equations of motion: in the model described by equation (3), this is the sum of the derivatives of the rhs with respect to $\mathbf{X}^0, \mathbf{X}^a, m\dot{\mathbf{X}}^0, m_a\dot{\mathbf{X}}^a$, and it turns out to be

$$\sigma(\dot{\mathbf{X}}, \mathbf{X}) = \sum_a \frac{\dot{Q}_a - \dot{V}_a}{k_{\text{B}} T_a} \equiv \sum_a \frac{\dot{Q}_a}{k_{\text{B}} T_a} - \dot{u}. \tag{5}$$

Therefore, there is a simple and direct relation between the phase-space contraction and the entropy creation rate [6]: they just differ for the total derivative $\dot{u} \stackrel{\text{def}}{=} \sum_a \dot{V}_a / k_{\text{B}} T_a$, whose time average $\langle \dot{u} \rangle_{\text{SRB}}$ vanishes. This implies, in particular, that the time average $\sigma_+ \stackrel{\text{def}}{=} \langle \sigma \rangle_{\text{SRB}}$ is the same as $\sigma_{0,+}$ and, in particular, that it is non-negative, consistent with the interpretation of phase-space volume contraction rate. The $\sigma_+ > 0$ implies that phase space contracts on average, and therefore the SRB distribution will give probability 1 to a zero volume set. Therefore, if $\sigma_+ > 0$, the system is said to be *dissipative.*

The usefulness of introducing the definition of σ is that a *fluctuation theorem* has been established for its large deviations functional in the context of Anosov systems theory. The *chaotic hypothesis* allows us to establish a connection between the fluctuation theorem (valid for the phase-space contraction rate in dissipative Anosov systems) and a *fluctuation relation* for σ and σ_0 in model equation (3), as explained in the next sections.

3. Chaotic hypothesis

In equilibrium statistical mechanics the *ergodic hypothesis* plays an important conceptual role, as it implies that the motions have SRB statistics and that the latter coincides with the Liouville distribution on the energy surface. A role analogous to the *ergodic hypothesis* has been proposed for the *chaotic hypothesis* [7], which states that
A chaotic system can be regarded as an Anosov system for the purpose of computing the time averages of (smooth) observables.

This means that the attracting set of a chaotic system, physically defined as a system with at least one positive Lyapunov exponent, can be regarded as a smooth compact surface Ω on which motion is highly unstable (uniformly hyperbolic) and transitive (there is a dense trajectory). For a mathematically precise definition of an Anosov system, we refer to [8].

We stress that the chaotic hypothesis concerns physical systems: mathematically, *it is easy to find dynamical systems for which it does not hold*, as it is easy (even easier) to find systems in which the ergodic hypothesis fails (e.g. harmonic lattices or black body radiation).

Since physical systems are almost always not Anosov systems, it is very likely that probing motions in extreme regimes will make visible the features that distinguish Anosov systems from non-Anosov systems: much as happens with the ergodic hypothesis.

The ergodic hypothesis provides us with an expression for the averages (as integrals over the normalized Liouville distribution on the energy surface): likewise, the chaotic hypothesis provides us with the existence and a formal expression for the averages (i.e. for the SRB distribution) [8].

The interest in the hypothesis is to provide a framework in which properties such as the existence and formal expression of an SRB distribution is *a priori* guaranteed. One can also say that the role of Anosov systems in chaotic dynamics is similar to the role of harmonic oscillators in the theory of regular motions. They are the paradigm of chaotic systems, as harmonic oscillators are the paradigm of order. Of course, the hypothesis is only a beginning, and one has to learn how to extract information from it, as was the case with the use of the Liouville distribution once the ergodic hypothesis guaranteed that it was the appropriate distribution for the study of the statistics of motions in equilibrium situations [9].

4. Fluctuation theorem

As mentioned above, an important observable in the theory of Anosov systems is the phase-space contraction rate $\sigma(x)$, defined as minus the divergence of the equations of motion, computed in $x \in \Omega$, where Ω is the phase space of the system. A rather general result holds *if* the system is Anosov, dissipative ($\sigma_+ = \langle\sigma\rangle_{\mathrm{SRB}} > 0$), and *furthermore* reversible in the sense that there is an isometry I of phase space such that $IS_t = S_{-t}I$ for all $t \in \mathbb{R}$. Define the *dimensionless phase-space contraction*

$$p(x) = \frac{1}{\tau}\int_0^\tau \frac{\sigma(S_t x)}{\sigma_+}\,\mathrm{d}t \tag{6}$$

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then the SRB average of p is 1 (by definition) and there exists $p^* \geq 1$ such that the probability P_τ of the event $p \in [a, b]$ with $[a, b] \subset (-p^*, p^*)$ has the form

$$P_\tau(p \in [a, b]) = \text{const}\, \mathrm{e}^{\tau \max_{p\in[a,b]} \zeta(p) + \mathrm{O}(1)} \tag{7}$$

with $\zeta(p)$ analytic in $(-p^*, p^*)$ [10, 11]. The function $\zeta(p)$ can be conveniently normalized to have value 0 at $p = 1$ (i.e. at the average value of p).

In Anosov systems which are reversible and dissipative, a general symmetry property, called the *fluctuation theorem* and reflecting the reversibility symmetry, yields the *parameterless* relation [7, 12],

$$\zeta(-p) = \zeta(p) - p\sigma_+ \qquad p \in (-p^*, p^*), \tag{8}$$

where $(-p^*, p^*)$, $p^* \geq 1$, is the largest domain of definition of ζ; it can be shown that ζ is analytic on the whole $(-p^*, p^*)$. This relation is interesting, because it has no free parameters. The relation was discovered in a simulation of shear flow, and it was suggested that it should be related to time reversal symmetry and to Ruelle's ideas on turbulence [13]. A more informal (but imprecise) way of writing equations (7) and (8) is

$$\frac{P_\tau(p)}{P_\tau(-p)} = \mathrm{e}^{\tau p\sigma_+ + \mathrm{O}(1)}, \qquad \text{for all } p \in (-p^*, p^*) \tag{9}$$

where $P_\tau(p)$ is the probability density of p. An interesting consequence of equation (9) is that $\langle \mathrm{e}^{-\tau\, p\, \sigma_+}\rangle_{\text{SRB}} = 1$ in the sense that $(1/\tau) \log \langle \mathrm{e}^{-\tau\, p\, \sigma_+}\rangle_{\text{SRB}} \xrightarrow[\tau\to\infty]{} 0$.

Occasionally, systems with singularities have to be considered: in such cases, the relation equation (8) may change, in the sense that the $\zeta(p)$ may not be analytic; one then expects that the relation holds in the largest analyticity interval symmetric around the origin. In various cases considered in the literature, such an interval appears to contain the interval $(-1, 1)$, and sometimes this can be proved rigorously, for instance in simple, although admittedly special, examples of systems close to equilibrium [9].

The equations (8) and (9) are the first representatives of consequences of the reversibility and chaoticity hypotheses. For instance, given $F_1, \ldots, F_n$ *arbitrary* observables which are (say) odd under time reversal I (i.e. $F(Ix) = -F(x)$) and given n functions $t \in [-\tau/2, \tau/2] \to \varphi_j(t)$, $j = 1, \ldots, n$, one can ask what is the probability that $F_j(S_t x)$ 'closely follows' the *pattern* $\varphi_j(t)$ and, at the same time, $(1/\tau)\int_0^\tau (\sigma(S_\theta x)/\sigma_+)\, \mathrm{d}\theta$ has value p. Then, calling $P_\tau(F_1 \sim \varphi_1, \ldots, F_n \sim \varphi_n, p)$ the probability of this event, which we write in the imprecise form corresponding to equation (9) for simplicity, and defining $I\varphi_j(t) \stackrel{\text{def}}{=} -\varphi_j(-t)$, it is

$$\frac{P_\tau(F_1 \sim \varphi_1, \ldots, F_n \sim \varphi_n, p)}{P_\tau(F_1 \sim I\varphi_1, \ldots, F_n \sim I\varphi_n, -p)} = \mathrm{e}^{\tau\sigma_+ p}, \tag{10}$$

for $p \in (-p^*, p^*)$, which is remarkable because it is parameterless and, at the same time, surprisingly independent of the choice of the observables F_j. The relation equation (10) has far-reaching consequences [5].

Equation (10) can be read as follows: the probability that the observables F_j follow given evolution patterns φ_j, conditioned to entropy creation rate $p\sigma_+$, is *the same* probability that they follow the time-reversed patterns if conditioned to entropy creation rate $-p\sigma_+$. In other words, to change the sign of time, it is *just* sufficient to reverse the sign of the average phase-space contraction p (and we shall see that, in our model, this would amount to changing the sign of the entropy creation rate): no 'extra effort' is needed.

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5. Fluctuation relation

Given a chaotic system for which the chaotic hypothesis can be regarded as valid, it is expected that the fluctuation relation (FR) holds: i.e. that one can define $\zeta(p)$ and that the symmetry equation (8) holds. This is an important check that can be performed on the statistical properties of a stationary non-equilibrium state.

However, it is also important to know whether the quantity p and its fluctuations describe some interesting feature of the dynamical system. The model equation (3), with σ defined as in equation (5), provides an indication of the path to follow in the quest for an interpretation of the fluctuation relation [6, 14].

The remarkable property is that if we accept the chaotic hypothesis for the model equation (3) (i.e. for the whole system Σ_0 + thermostats) and we choose the parameters $\boldsymbol{\Phi}$ and T_a in such a way that $\sigma_+ > 0$, it is expected that the FR holds for p, and this has an immediate physical interpretation because, if we write $p_0(x) \stackrel{\text{def}}{=} (1/\tau)\int_0^\tau (\sigma_0(S_t x)/\sigma_{0+})\,\mathrm{d}t$, then, making use of the property that $p - p_0$ is the variation of u in time τ divided by the elapsed time τ,

$$\begin{aligned} p(x) &= p_0(x) + \frac{u(S_t x) - u(x)}{t} \\ \sigma_{0+} &\equiv \langle \sigma_0 \rangle_{\mathrm{SRB}} \equiv \langle \sigma \rangle_{\mathrm{SRB}} \equiv \sigma_+. \end{aligned} \tag{11}$$

We find that, in the limit $t \to \infty$, p and p_0 have *the same large deviation rate* $\zeta(p)$.

Of course, the thermostats are 'large' (we are even neglecting $O(N_a^{-1})$) and therefore the energies V_a as well as u can be very large, physically of order $O(\sum_a N_a)$. This means that time t that has to pass (in order to see the fluctuation relation equation (8) free of the $O(t^{-1}\sum_a N_a)$ corrections) can be enormous (possibly on an astronomical scale in 'realistic' cases).

This is a situation similar to the one met when considering systems with unbounded stochastic forces [15], or with singular or nearly singular forces and thermostats of isokinetic type [9]. In the present case, we see that the really interesting quantity is the quantity p_0, which is the entropy creation rate, and it is a boundary term *unaffected by the size of the thermostats*. Therefore if one considers and measures only p_0 rather than p, one not only performs a physically meaningful operation (i.e. measuring the average entropy creation rate) but also one can access the large deviation rate $\zeta(p)$ and check the fluctuation relation symmetry on a time that is totally unrelated to the thermostat's size. Furthermore, the more general relations like equation (10) can be naturally extended.

6. A model for granular materials

The current interest in granular materials properties and the consequent availability of experiments, e.g. [16], suggests trying to apply the above ideas to derive possible experimental tests.

The main problem is that, in granular materials, collisions are intrinsically *inelastic*. In each collision, particles heat up, and the heat is subsequently released through thermal exhange with the walls of the container, sound emission (if the experiment is performed in air), radiation, and so on. If one still wants to deal with a *reversible* system, such as the one that we discussed in the previous sections, one should include all these sources of

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dissipation in the theoretical description. Clearly, this is a *very* hard task, and we will not pursue it here.

A simplified description of the system consists of neglecting the internal degrees of freedom of the particles. In this case, the inelastic collisions between point particles will represent the only source of dissipation in the system. Still, the chaotic hypothesis is expected to hold, but in this case the entropy production is strictly positive and there is no hope of observing a fluctuation relation, see e.g. [17], if one looks at the whole system.

Nevertheless, in the presence of inelasticity, temperature gradients are present in the system [16, 18, 19], so that heat is transported through different regions of the container. Then one can try to represent the processes of heat exchange between different regions of the system using the model that we described above; and, assuming that, under suitable conditions, the inelasticity of the collisions can be neglected, one can hope to observe a fluctuation relation for a (suitably defined) entropy production rate. This would be an interesting example of 'ensemble equivalence' in non-equilibrium [5]: we will discuss this possibility in detail in the following.

As a model for a granular material, let Σ be a container consisting of two flat parallel vertical walls covered at the top and with a piston at the bottom that is kept oscillating by a motor, so that its height is

$$z(t) = A \cos \omega t. \tag{12}$$

The model can be simplified by introducing a sawtooth moving piston, as in [19]; however, the results should not depend too much on the details of the time dependence of $z(t)$. The container Σ is partially filled with millimetre-sized balls (a typical size for the faces of Σ is 10 cm and the particle number is about 256): the vertical walls are so close that the balls almost touch both faces, so the problem is effectively two dimensional. The equations of motion of the balls with coordinates (x_i, z_i), $i = 1, \ldots, N$, $z_i \geq z(t)$, are

$$\begin{aligned} m\ddot{x}_i &= f_{x,i} \\ m\ddot{z}_i &= f_{z,i} - mg + m\delta(z_i - z(t))\, 2\,(\dot{z}(t) - \dot{z}_i) \end{aligned} \tag{13}$$

where m = mass, g = gravity acceleration, and the collisions between the balls and the oscillating base of the container are assumed to be elastic [19] (eventually, inelasticity of the walls can be included into the model with negligible changes [17]); $\mathbf{f}_i$ is the force describing the particle collisions and the particle–walls collisions.

The force $\mathbf{f}_i$ has a part describing the particle collisions: this is not necessarily elastic, and in fact we will assume that the particle collisions are inelastic, with restitution coefficient $\alpha < 1$. A simple model for inelastic collisions with inelasticity α (convenient for numerical implementation) is a model in which collisions take place with the usual elastic collision rule, but immediately after the velocities of the particles that have collided is scaled by a factor so that the kinetic energy of the pair is reduced by a factor of $1-\alpha^2$ [17]–[19].

We look at the stationary distribution of the balls: the simplest experimental situation that seems accessible to experiments and simulations is to draw ideal horizontal lines at heights $h_1 > h_2$ delimiting a strip Σ_0 in the container and to look at the particles in Σ_0 as a thermostatted system, the thermostats being the regions Σ_1 and Σ_2 at heights larger than h_1 and smaller than h_2, respectively.

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After a stationary state has been reached, the average kinetic energy of the particles will depend on the height z, and in particular will decrease on increasing z. Given the motion of the particles and a time interval t, it will be possible to measure the quantity Q_2 of (kinetic) energy that particles entering or exiting the region Σ_0 from below (the 'hotter side') carry out of Σ_0 as well as the analogous quantity Q_1 carried out by the particles that enter or exit from above (the 'colder side').

If T_i, $i = 1, 2$, are the average kinetic energies of the particles in small horizontal corridors above and below Σ_0, we see that there is a connection between the model of granular material, equation (13), and the model equation (3) discussed above. Still, model equation (13) cannot be reduced exactly to model equation (3) because of the internal dissipation induced by the inelasticity α and of the fact that the number of particles in Σ_0 depends on time, as particles come and go in the region.

The reason for considering a model for granular material that is not in the class of models of equation (3) is that equation (13) has a closer connection with the actual experiments [16] and with the related numerical simulations. Moreover, under suitable assumptions, which can be expected to hold on a specific timescale, the stationary state of equation (13) is effectively described in terms of the stationary state of equation (3), as discussed below.

Note that real experiments cannot have an arbitrary duration [16]: the particles' movements are recorded by a digital camera and the number of photograms per second is of the order of a thousand, so that the memory for the data is easily exhausted as each photogram has a size of about 1 Mb in current experiments. The same holds for numerical simulations where the accessible timescale is limited by the available computational resources.

Hence each experiment lasts up to a few seconds, starting after the system has been moving for a while, so that a stationary state is reached. The result of the experiment is the reconstruction of the trajectory in phase space of each individual particle inside the observation frame [16].

In order for the number of particles N_0 in Σ_0 to be approximately constant for the duration of the experiment, the vertical size $(h_1 - h_2)$ of Σ_0 should be chosen to be large compared to $(Dt)^{1/2}$, where t is the duration of the experiment and D is the diffusion coefficient. Note that we are assuming that the motion of the particles is diffusive on the scale of Σ_0. In the low-density case, the motion could not be diffusive on the scale of Σ_0: then we would not be able to divide the degrees of freedom between the subsystem and the rest of the system and, moreover, the correlation length would be comparable with (or larger than) the size of the subsystem Σ_0. This would completely change the nature of the problem, and violations to FR could possibly be observed [20, 21].

Given the remarks above, and if

(1) we accept the chaotic hypothesis,

(2) we assume that the result of the observations would be the same if the particles above Σ_0 and below Σ_0 were kept at constant total kinetic energy by reversible thermostats (e.g. Gaussian thermostats) [5, 22, 23],

(3) we neglect the dissipation due to inelastic collisions between particles in Σ_0,

(4) we neglect the fluctuations of the number of particles in Σ_0,

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(5) we suppose that there is dissipation in the sense that

$$\sigma_+ \stackrel{\text{def}}{=} \lim_{t\to+\infty} \frac{1}{t}\left(\frac{Q_1}{T_1}+\frac{Q_2}{T_2}\right) > 0, \tag{14}$$

then we expect the analysis of section 5 to apply to model equation (13).

Note that chaoticity is expected at least if dissipation is small, and evidence for it is provided by the experiment in [16], which indicates that the system evolves to a chaotic stationary state in which dissipation occurs. Dissipation due to internal inelastic collisions will be negligible (for the purpose of checking an FR for σ_0) only on a specific timescale, as discussed below.

Accepting the assumptions above, we then predict that a fluctuation relation is satisfied, see equations (8) and (9), for fluctuations of

$$p = \frac{1}{t\,\sigma_+}\left(\frac{Q_1}{T_1}+\frac{Q_2}{T_2}\right) \tag{15}$$

in the interval $(-p^*, p^*)$, with p^* equal (at least) to 1.

The latter is therefore a property that seems to be accessible to simulations as well as to experimental test. Note, however, that it is very likely that the hypotheses (2)–(4) above will not be *strictly* verified in real experiments—see the discussion in the next section—so we expect that the analysis and interpretation of the experimental results will be non-trivial. Nevertheless, the test would be rather stringent.

7. Relevant timescales

The above analysis assumes the existence of (at least) two timescales. One is the 'equilibrium timescale', θ_e, which is the timescale over which the system evolving at constant energy, equal to the average energy observed, would reach equilibrium in the absence of friction and forcing. An experimental measure of θ_e would be the decorrelation time of self-correlations in the stationary state, and we can assume that θ_e is of the order of the mean collision time. Note that θ_e also coincides with the timescale over which finite time corrections to FR become irrelevant [24]: this means that, in order to be able to measure the large deviations functional for the normalized entropy production rate p in equation (15), one has to choose $t \gg \theta_e$; see also [25] for a detailed discussion of the first-order finite time corrections to the large deviation functional. A second timescale is the 'inelasticity timescale' θ_d, which is the scale over which the system reaches a stationary state if the particles are prepared in a random configuration and the piston is switched on at time $t = 0$. Possibly a third timescale is present: the 'diffusion timescale' θ_D, which is the scale over which a particle diffuses over the size of Σ_0. The analysis above applies only if the time t in equation (15) verifies $\theta_e \ll t \ll \theta_d, \theta_D$ (note, however, that the measurement should be started after a time $\gg \theta_d$, since the piston has been switched on in order to have a stationary state); in practice, this means that the time for reaching the stationary state has to be quite long compared to θ_e. In this case, friction is negligible for the duration of the measurement if the latter is between θ_e and $\min(\theta_D, \theta_d)$. In the setting that we consider, the role of friction is 'just' that of producing the non-equilibrium stationary state itself and the corresponding gradient of temperature: this is reminiscent

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of the role played by friction in classical mechanics problems, where periodic orbits (the 'stationary state') can be selected dynamically by adding a small friction term to the Hamilton equations. Note that, as discussed below, the temperature gradient produced by friction will be rather small: however, smallness of the gradient does not affect the 'FR timescale' over which FR is observable [24].

If internal friction is not negligible (that is, if $t \gtrsim \theta_{\rm d}$), the problem would change nature: an explicit model (and theory) should be developed to describe the transport mechanisms (such as radiation, heat exchange between the particles and the container, sound emission, ...) associated with the dissipation of kinetic energy, and new thermostats should correspondingly be introduced. The definition of entropy production should be changed, by taking into account the presence of such new thermostats. In this case, even changing the definition of entropy production, it is not clear whether FR should be satisfied: in fact, internal dissipation would break the time-reversibility assumption and, even accepting the chaotic hypothesis, nothing guarantees *a priori* the validity of FR.

The validity of $\theta_{\rm e} \ll t \ll \theta_{\rm d}, \theta_{\rm D}$ is not obvious in experiments. A rough estimate of $\theta_{\rm d}$ can be given as follows: the phase-space contraction in a single collision is given by $1-\alpha$. Thus the average phase-space contraction per particle and per unit time is $\sigma_{+,d} = (1-\alpha)/\theta_{\rm e}$, where $1/\theta_{\rm e}$ is the frequency of the collisions for a given particle. It seems natural to assume that $\theta_{\rm d}$ is the timescale at which $\sigma_{+,d}\theta_{\rm d}$ becomes of order 1: on this timescale, inelasticity will become manifest. Thus, we obtain the following estimate:

$$\theta_{\rm d} \sim \frac{1}{1-\alpha}\theta_{\rm e}. \qquad (16)$$

In real materials $\alpha \le 0.95$, so that $\theta_{\rm d}$ can be at most of the order of $20\theta_{\rm e}$. Nevertheless, it is possible that this is already enough to observe a fluctuation relation on intermediate times.

The situation is completely different in numerical simulations where we can play with our freedom in choosing the restitution coefficient α (it can be chosen to be very close to one [17]–[19], in order to have $\theta_{\rm d} \gg \theta_{\rm e}$) and the size of the container Σ_0 (it can be chosen to be large, in order to have $\theta_{\rm D} \gg \theta_{\rm e}$).

To check the consistency of our hypotheses, it has to be shown that it is possible to make a choice of parameters such that $\theta_{\rm e}$ and $\theta_{\rm D}$ are separated by a large time window. Such choices are possible, as discussed below.

If $\delta = h_1 - h_2$ is the width of Σ_0, $\varepsilon = 1-\alpha$, γ is the temperature gradient in Σ_0, and D is the diffusion coefficient, then the following estimates hold:

(a) $\theta_{\rm e} = {\rm O}(1)$, as it can be taken of the order of the inverse collision frequency, which is O(1) if the density is constant and the forcing on the system is tuned to keep the energy constant as $\varepsilon \to 0$.

(b) $\theta_{\rm d} = \theta_{\rm e}{\rm O}(\varepsilon^{-1})$, as implied by equation (16).

(c) $\theta_{\rm D} = {\rm O}(\delta^2/D) = {\rm O}(\delta^2)$, because D is a constant (if the temperature and the density are kept constant).

(d) $\gamma = {\rm O}(\sqrt{\varepsilon})$, as long as $\delta \ll \varepsilon^{-1/2}$. In fact, if the density is high enough to allow us to consider the granular material as a fluid, as in equation (5) of [19], the temperature profile should be given by the heat equation $\nabla^2 T + c\varepsilon T = 0$ with a suitable constant

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c and suitable boundary conditions on the piston ($T = T_0$) and on the top of the container ($\nabla T = 0$). This equation is solved by a linear combination of const $\mathrm{e}^{\pm\sqrt{c\varepsilon}z}$, which has gradients of order $\mathrm{O}(\sqrt{\varepsilon})$, as long as $\delta \ll 1/\sqrt{\varepsilon}$ and the boundaries of Σ_0 are further than $\mathrm{O}(1/\sqrt{\varepsilon})$ from the top.

Now, if we choose $\delta = \varepsilon^{-\beta}$, with $\beta < \frac{1}{2}$, and we take ε small enough, then we have $\theta_{\mathrm{e}} \ll \min\{\theta_{\mathrm{d}}, \theta_{\mathrm{D}}\}$ and $\delta \ll \mathrm{O}(\varepsilon^{-1/2})$, as required by item (d).

Remark. The entropy creation rate due to heat transport into Σ_0, in the presence of a temperature gradient γ, is given by $\sigma_+ = \mathrm{O}(\gamma^2\delta) = \mathrm{O}(\varepsilon\delta)$, because the temperature difference is $\mathrm{O}(\gamma\delta)$ and the energy flow through the surface is of order $\mathrm{O}(\gamma)$ (with $\gamma = \mathrm{O}(\sqrt{\varepsilon})$; see item (d)). The order of magnitude of σ_+ is not larger than the average amount σ_{d} of energy dissipated per unit time in Σ_0 divided by the average kinetic energy T (the latter quantity is of order $\mathrm{O}(\theta_{\mathrm{e}}^{-1}\varepsilon\delta)$ because, at constant density, the number of particles in Σ_0 is $\mathrm{O}(\delta)$); however, the entropy creation due to the dissipative collisions in Σ_0 has fluctuations of order $\mathrm{O}(\varepsilon\delta^{1/2})$, because the number of particles in Σ_0 fluctuates by $\mathrm{O}(\delta^{1/2})$. This is consistent with neglecting the entropy creation inside the region Σ_0 due to the inelasticity, in spite of it being of the same order of the entropy creation due to the heat entering Σ_0 from its upper and lower regions.

This argument supports the proposal that, in numerical simulations, it will be possible to test our ideas by a suitable choice of the parameters. We expect that other choices will be possible: for instance, in the high-density limit it is clear that $\theta_{\mathrm{D}} \gg \theta_{\mathrm{e}}$, because the diffusion coefficient will become very small. To what extent this can be applied to experiment remains an open question.

8. Remarks and conclusions

(1) The model can be given further structure by adding a non-conservative forcing acting on the particles in the region Σ_0: the same relations would follow (in particular the fluctuation relation) if the forced equations of motion are still reversible; see [26] for a (stochastic) example. The above will not hold in general if the forcing is not reversible, e.g. if the inelasticity of the collisions inside Σ_0 cannot be neglected; see below.

(2) An explicit computation of the large deviation function of the dissipated power, in the regime $t \gg \theta_{\mathrm{d}}$ (i.e. when the dissipation is mainly due to inelastic collisions), appeared recently in [27]. However, in the model, only the dissipation due to the collisions was taken into account, so that it is not clear how the heat produced in the collisions is removed from the system; see the discussion above. It turned out that, in this regime, no negative values of p are observed, so that the FR cannot hold. This is interesting and expected on the basis of the considerations above. It is not clear if, including the additional thermostats required to remove heat from the particles and prevent them to warm up indefinitely, the fluctuation relation is recovered. However, this problem is different from the one discussed here, and we leave it for future investigation.

(3) There has also been some debate on the interpretation of the experimental results of [16]. In [17], a simplified model, very similar to the one discussed above, was proposed and shown to reproduce the experimental data of [16]. The prediction of

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the model is that the FR is not satisfied. Note, however, that the geometry considered in [16, 17] is different from the geometry considered here: the whole box is vibrated, so that the temperature profile is symmetric, and a region Σ_0 in the centre of the box is considered. Heat exchange is due to 'hot' particles entering Σ_0 (Q_+) and 'cold' particles exiting Σ_0 (Q_-). One has $Q = Q_+ + Q_- \neq 0$, because of the dissipation in Σ_0, and

$$\sigma_+ = \frac{\dot{Q}_+}{T_+} + \frac{\dot{Q}_-}{T_-} = 0 \tag{17}$$

where T_+ is the temperature outside Σ_0 and T_- is the temperature inside Σ_0; see [17]. Thus the dissipation due to heat exchange between the region Σ_0 and the regions outside Σ_0 vanishes, and the only dissipation is due to the inelasticity of the collisions. In this regime, again, the FR is not expected to hold if the thermostat dissipating the heat produced in the collisions is not included in the model; see above: it is an interesting remark of [17] that partially motivated the present work. We believe that different experiments can be designed in which the dissipation is mainly due to heat exchanges and the inelasticity is negligible, as in the experiment that we proposed above. The main difference between the experiment that we proposed and the experiment in [16] is that the geometry of the box is such that $Q_1/T_1 + Q_2/T_2 > 0$: in this situation, the dissipation due to inelastic collisions should be negligible, as long as $t \ll \theta_{\mathrm{d}}$.

(4) Even in situations in which the dissipation is entirely due to irreversible inelastic collisions between particles, such as those considered in [17, 27], the chaotic hypothesis is expected to hold, and the stationary state is to be described by a SRB distribution. In these cases, the failure of the fluctuation relation is not in contradiction with the chaotic hypothesis, due to the irreversibility of the equations of motion.

Conclusions

We showed that, in a paradigmatic class of mechanical models of thermostatted systems, the phase-space contraction is an interesting quantity. In large systems in contact with thermostats, it may consist of a sum of two quantities: the first with the interpretation of entropy creation rate, and the second is extremely large but equal to a total derivative.

Its fluctuation properties, while asymptotically for large times determining (actually being identical to) the fluctuation properties of the entropy creation rate (*hence implying the fluctuation relation*), may require a very long time to be freed of finite time corrections. But, at the same time, the study of the fluctuation properties of the physical quantity defined by the entropy creation rate can be used to determine the large deviations of the phase-space contraction. The latter, having the *same* large deviation rate, must obey the fluctuation relation, which therefore becomes observable even if the system is in contact with large (or even infinite) thermostats.

The analysis leads us to propose concrete experimental tests as well as tests based on simulations in the context of granular materials. The models that are naturally introduced for the description of granular material experiments are not in the same class of models, for which a relation between the phase-space contraction and entropy production rate was previously discussed. The previous analysis can be applied to granular materials only

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under suitable assumptions, verified on a specific timescale. A fluctuation relation for the entropy production rate, measured on the same timescale, is predicted.

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