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Stationary state of a heated granular gas: fate of the usual H -functional

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Abstract

We consider the characterization of the nonequilibrium stationary state of a randomly-driven granular gas in terms of an entropy-production based variational formulation. Enforcing spatial homogeneity, we first consider the temporal stability of the stationary state reached after a transient. In connection, two heuristic albeit physically motivated candidates for the non-equilibrium entropy production are put forward. It turns out that none of them displays an extremum for the stationary velocity distribution selected by the dynamics. Finally, the relevance of the relative Kullback entropy is discussed.

Key words: Granular gas; entropy production; H -theorem; nonequilibrium stationary state

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1 Introduction

Apart from being the subject of intense experimental activity, granular gases are also a particularly fertile testing ground for new theoretical ideas and problems, especially within the field of nonequilibrium statistical physics. One such a problem is the role of entropy production as a Lyapunov functional for nonequilibrium steady-states. This problem has its roots in the fifties, in

the works of the Brussels group around Prigogine [1] on the minimum entropy production theorem. The limitations of this theorem, that relies essentially on the linear response formalism (i.e., has a domain of validity that is restricted to close-to-equilibrium situations), were rather clear already at that time, and a first extension to far-from-equilibrium situations was proposed under the form of the phenomenological “general evolution criterion” of Glansdorff and Prigogine (see [2] and references therein).

Since then, there was steady effort, and a huge body of literature, in the search for a variational principle for steady-states that are arbitrarily far from equilibrium. Several candidates for a “nonequilibrium entropy production” with extremal properties at stationarity were proposed in different contexts, and at various levels of coarse-graining of the description – from the microscopic to the phenomenological ones. Some success was encountered for Markovian systems described by a master equation for the probability distribution function of the microstates – starting with the pioneering work of Jiu-li *et al* [3], and intensively studied afterwards (see, e.g., [4,5] to cite only a few). Also, a connection between the phase space contraction rate in dissipative, externally driven systems and an entropy production rate was established in some cases, see e.g. [6] for a critical discussion. An extension of Jaynes’ maximum entropy inference principle (MaxEnt) to nonequilibrium situations was proposed [7], and illustrated recently on several examples [8]. The resulting picture is, however, rather confusing and sometimes even contradictory (e.g., some of the above-mentioned papers speak of a “maximum” entropy production rate at stationarity, while others refer to a “minimum”).

One of the main difficulties of nonequilibrium statistical mechanics is the scarcity of solvable models, on the basis of which one could, eventually, get some clarification on these controversial points. The purpose of the present work is to consider such a solvable model, namely a granular gas modeled as an assembly of inelastic hard-spheres with *constant restitution coefficient*, in which energy is injected by means of random forces acting independently upon the particles. The balance between dissipation and the random kicks allows the system to reach a nonequilibrium steady-state (NESS). In a Boltzmann equation description, one can compute (in some perturbative expansion) the single-particle probability distribution function (pdf). This model is widely-used and very successful in explaining many features of granular systems (see, e.g., [9,10,11]). One of the question is thus whether this model is also appropriate in describing *thermodynamical* properties of granular systems – in particular, the entropy production rate and its eventual relationship with the relaxation to NESS. We propose two heuristic – albeit physically motivated – candidates for the nonequilibrium entropy production rate, as functionals of the pdf, and we discuss their extremal properties in NESS. Such a granular gas has a strong “built-in” irreversible element at the very level of the grain dynamics, which is represented by the inelasticity of the collisions. However,

one may ask whether in the limit of a very weak inelasticity (i.e., for steady-states that are arbitrarily “close to equilibrium”) one could recover a kind of “minimum entropy production theorem” in a stochastic formulation – an equivalent of that described in [3]. We will also address this point here.

In the next section we are introducing the model, and in Sec. 3 we study the nonequilibrium steady-state and its linear stability. Section 4 is devoted to the discussion of the nonequilibrium entropy production issue, and the behavior of the relative Kullback entropy. We conclude in Sec. 5 with a brief discussion of the limitations of this model as far as describing the thermodynamics.

2 The model

We consider a granular gas of inelastic hard spheres in dimension $d \geq 2$, uniformly heated by a stochastic thermostat, as described in detail in [9,10]. The particles undergo binary inelastic collisions, modeled through a *constant restitution coefficient* $\alpha \in [0, 1]$ that is meant to characterize the *degree of inelasticity*; the limit $\alpha = 1$ corresponds to perfectly elastic collisions, while $\alpha = 0$ corresponds to the perfect inelastic ones. Each particle i (of mass m) is subjected to an external Gaussian white noise force $\xi_i(t)$; these forces are uncorrelated for different particles, and homogeneous in space,

$$\langle \xi_{i,\alpha}(t) \xi_{j,\beta}(t') \rangle = m^2 \xi_0^2 \delta_{ij} \delta_{\alpha\beta} \delta(t - t'), \quad \alpha, \beta = 1, \dots, d. \quad (1)$$

We describe the system at the level of the kinetic theory, and for simplicity, without affecting the overall conclusions, we shall concentrate on the *spatially homogeneous* case. For the single particle distribution function $f(\mathbf{r}, \mathbf{v}_1, t) = f(\mathbf{v}_1, t)$, the Boltzmann equation reads then:

$$\partial_t f(\mathbf{v}_1, t) = \chi I[f, f] + \frac{\xi_0^2}{2} \frac{\partial^2}{\partial \mathbf{v}_1^2} f(\mathbf{v}_1, t). \quad (2)$$

The extra term $(\xi_0^2/2)(\partial^2/\partial \mathbf{v}_1^2)f(\mathbf{v}_1, t)$ accounts for the change in the distribution function caused by the random “kicks” the external thermostat is applying on the grains. It corresponds to an injection of energy at constant rate $d\xi_0^2/2$ per unit mass. χ is the pair correlation function at contact and

$$I[f, f] = \sigma^{d-1} \int_{\mathbb{R}^d} d\mathbf{v}_2 \int d\hat{\boldsymbol{\sigma}} \theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12}) (\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12}) \times \left(\frac{1}{\alpha^2} b^{-1} - 1 \right) f(\mathbf{v}_1, t) f(\mathbf{v}_2, t) \quad (3)$$

represents the inelastic two-particle collision operator. Here σ is the diameter of the hard spheres; $\hat{\boldsymbol{\sigma}}$ is a unit vector joining the centers of the particles at

contact; $\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2$; $\theta(\dots)$ is the Heaviside step-function; and b^{-1} is an operator that restitutes the pre-collisional velocities, i.e.,

$$b^{-1}\mathbf{v}_1 = \mathbf{v}_1^{**} = \mathbf{v}_1 - \frac{1+\alpha}{2\alpha}(\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}, \quad (4a)$$

$$b^{-1}\mathbf{v}_2 = \mathbf{v}_2^{**} = \mathbf{v}_2 + \frac{1+\alpha}{2\alpha}(\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}. \quad (4b)$$

Note that the post-collisional velocities are

$$b\mathbf{v}_1 = \mathbf{v}_1^* = \mathbf{v}_1 - \frac{1+\alpha}{2}(\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}, \quad (5a)$$

$$b\mathbf{v}_2 = \mathbf{v}_2^* = \mathbf{v}_2 + \frac{1+\alpha}{2}(\mathbf{v}_{12} \cdot \hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}. \quad (5b)$$

3 Scaling solution and stationary state

3.1 Scaling solution of Boltzmann's equation

It turns convenient to introduce the pdf \tilde{f} of rescaled velocities $\mathbf{c} = \mathbf{v}/v_T$:

$$f(\mathbf{v}, t) = \frac{n}{v_T(t)^d} \tilde{f}(\mathbf{c}, t), \quad (6)$$

where n is the number particle density and

$$v_T(t) = \sqrt{\frac{2k_B T(t)}{m}} \quad (7)$$

is the thermal velocity associated to the kinetic temperature of the particles,

$$\frac{d}{2}k_B T(t) = \frac{1}{n} \int_{\mathbb{R}^d} d\mathbf{v} \frac{m}{2} v^2 f(\mathbf{v}, t) \quad (8)$$

(k_B is Boltzmann's constant).

For inelastic collisions, $\tilde{f}(\mathbf{c}, t)$ is different from a Gaussian

$$\phi(\mathbf{c}) = \frac{1}{\pi^{d/2}} e^{-c^2}, \quad (9)$$

and it is customary to characterize its deviation from a Gaussian through a series development in terms of Sonine polynomials $S_n(c^2)$, which, in practice,

is truncated to the first non-zero term [11],

$$\tilde{f}(c, t) = \phi(c) \left[1 + a_2(t) S_2(c^2) \right], \quad (10)$$

where

$$S_2(c^2) = \frac{1}{2}c^4 - \frac{d+2}{2}c^2 + \frac{d(d+2)}{8}. \quad (11)$$

The possible explicit temporal dependence of $\tilde{f}(c, t)$ appears through the time-dependent coefficient $a_2(t)$ of the Sonine polynomial $S_2(c^2)$.

For consistency of the description, it is found that the kinetic temperature $T(t)$ and the coefficient $a_2(t)$ obey a set of two coupled nonlinear first-order differential equations:

$$\begin{aligned} \frac{dT(t)}{dt} = \frac{m\xi_0^2}{k_B} - \sqrt{\frac{k_B}{\pi m}} \frac{n\chi\sigma^{d-1}(1-\alpha^2)S_d}{d} T^{3/2}(t) \\ \times \left[1 + \frac{3}{16}a_2(t) + \frac{9}{1024}a_2^2(t) \right], \quad (12) \end{aligned}$$

$$\begin{aligned} \frac{da_2(t)}{dt} + \frac{2m\xi_0^2}{k_B T(t)} a_2(t) + \sqrt{\frac{k_B T(t)}{\pi m}} \frac{4n\chi\sigma^{d-1}(1-\alpha^2)S_d}{d(d+2)} \\ \times \left[1 + \frac{3}{16}a_2(t) + \frac{9}{1024}a_2^2(t) \right] \left[1 + \frac{d(d+2)}{8}a_2(t) \right] \\ = \sqrt{\frac{2k_B T(t)}{\pi m}} \frac{4n\chi\sigma^{d-1}S_d}{d(d+2)} \left[\frac{1-\alpha^2}{1+\alpha^2} + D_1 a_2(t) + D_2 a_2^2(t) \right]. \quad (13) \end{aligned}$$

Here $S_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface of the unit-radius sphere in dimension d , Γ being Euler's Gamma function. Equation (12) follows from the definition (8) of the kinetic temperature, while Eq. (13) is obtained from the limit of vanishing velocities of the Boltzmann equation (2), see [12]. The coefficients D_1 and D_2 are given, respectively, by [12]:

$$\begin{aligned} D_1 = \frac{1-2d-d^2}{8} + \frac{1}{8(1+\alpha^2)^3} \left[2(1+\alpha^2)^2(d^2-2d-5) \right. \\ \left. + 4(d-1)(\alpha-1)^2(1+\alpha^2) + 8(\alpha^4+6\alpha^2+1) \right], \quad (14) \end{aligned}$$

$$\begin{aligned} D_2 = \frac{d(d+2)}{64} + \frac{1}{32(1+\alpha^2)^5} \left[12\alpha^3(1+\alpha^2)(d-1)(d-2) \right. \\ \left. - 4\alpha^2(1+\alpha^4)(24+4d-d^2) + 4\alpha(1+\alpha^6)(d+6)(d-1) \right. \\ \left. - (1+\alpha^8)(26+28d+9d^2) \right]. \quad (15) \end{aligned}$$

3.2 Stationary state

In the asymptotic limit, the granular system will reach a stationary state, that results from the balance between the energy injection by the external thermostat, and the energy dissipation through inelastic collisions between the particles. The stationary temperature T_0 is thus related both to the restitution coefficient α and to the amplitude ξ_0^2 of the Gaussian thermostat. Or, to state it differently, in order to ensure a given value of T_0 (for a fixed value of α), as resulting from the stationary form of Eq. (12), one has to tune the amplitude ξ_0^2 of the stochastic thermostat to

$$\xi_0^2 = \frac{n\chi\sigma^{d-1}(1-\alpha^2)S_d}{d\sqrt{\pi}} \left(\frac{k_B T_0}{m}\right)^{3/2} \times \left(1 + \frac{3}{16}a_{20} + \frac{9}{1024}a_{20}^2\right). \quad (16)$$

Here a_{20} is the stationary value of the coefficient of the first correction to the Gaussian. Its expression can be obtained from the stationary form of Eq (13) and it is the solution of the third order nonlinear equation (see e.g. [11] for a discussion concerning the relevance of the corresponding three roots in the case of a force-free system):

$$(1-\alpha^2) \left(1 + \frac{3}{16}a_{20} + \frac{9}{1024}a_{20}^2\right) \left[1 + a_{20} \frac{(d+2)(d+4)}{8}\right] = \sqrt{2} \left(\frac{1-\alpha^2}{1+\alpha^2} + D_1 a_{20} + D_2 a_{20}^2\right). \quad (17)$$

The coefficient a_{20} can be obtained in a closed analytical form through a Taylor expansion of the above equation. It was however shown in previous works [12,10] that there are some ambiguities from this linearization procedure that may affect a_{20} . We therefore chose the linearizing scheme that yields the closest result to the Monte Carlo simulations of Ref. [12]:

$$a_{20} = -16(1-\alpha^2)(1+\alpha^2)(1-\sqrt{2}+\alpha^2) \times \left\{16\sqrt{2}+13+4d(3\sqrt{2}+1)+2d^2(\sqrt{2}-1) + \alpha^2(-75+44d-2d^2) - \alpha^4 [16\sqrt{2}-3+2d(d+6)(\sqrt{2}-1)] + \alpha^6(-5+4d+2d^2)\right\}^{-1}. \quad (18)$$

Considering instead the expression derived by van Noije and Ernst in [9] would not alter the following discussion. Note that a_{20} becomes zero in the elastic limit $\alpha = 1$, when the stationary probability distribution recovers trivially the Gaussian, equilibrium shape.

The corresponding stationary probability distribution function is therefore

$$f_0(\mathbf{v}) = \frac{n}{v_{T_0}^d} \tilde{f}_0(c) = \frac{n}{v_{T_0}^d} \phi(c) \left[1 + a_{20} S_2(c^2) \right], \quad (19)$$

where $v_{T_0} = \sqrt{2k_B T_0/m}$ is the stationary value of the thermal velocity.

3.3 Linear stability analysis of the stationary state

The stability of the aforementioned steady state has not been investigated in the literature, even if the hydrodynamic-like equations have been derived recently for the (dilute) system considered here [13]. A complete linear stability analysis (and its eventual comparison with the existing results for the homogeneous cooling state [14]) is a tedious task, and a separate research subject that we shall not address here further. Instead, we shall consider a simplified version of it, in which the homogeneity of the state is not affected by the perturbations. This will by no mean influence our general conclusions.

Let us then consider small deviations of the temperature and of the coefficient a_2 from their stationary values,

$$T = T_0(1 + \delta\theta), \quad a_2 = a_{20} + \delta a_2, \quad (20)$$

with $|\delta\theta| \ll 1$, $|\delta a_2| \ll |a_{20}|$.

The linearized evolution equations of these perturbations result from Eqs. (12) and (13),

$$\frac{d}{dt}(\delta\theta) = -\frac{m\xi_0^2}{k_B T_0} \left[\frac{3}{2} \delta\theta + \frac{3/16 + (9/512)a_{20}}{1 + (3/16)a_{20} + (9/1024)a_{20}^2} \delta a_2 \right], \quad (21)$$

$$\begin{aligned} \frac{d}{dt}(\delta a_2) = & -\frac{m\xi_0^2}{k_B T_0} \left\{ a_{20} \delta\theta + \left\{ \frac{d+4}{2} + \frac{4}{d+2} \right. \right. \\ & \times \left[\left(1 + a_{20} \frac{d(d+2)}{8} \right) \left(\frac{3}{16} + \frac{9}{512} a_{20} \right) \right. \\ & \left. \left. - \frac{\sqrt{2}}{1-\alpha^2} (D_1 + 2D_2 a_{20}) \right] \left[1 + \frac{3}{16} a_{20} + \frac{9}{1024} a_{20}^2 \right]^{-1} \right\} \delta a_2 \}. \end{aligned} \quad (22)$$

In Fig. 1 we have represented the two eigenvalues of the corresponding stability matrix as a function of the restitution coefficient α , for both $d = 2$ and $d = 3$ cases.

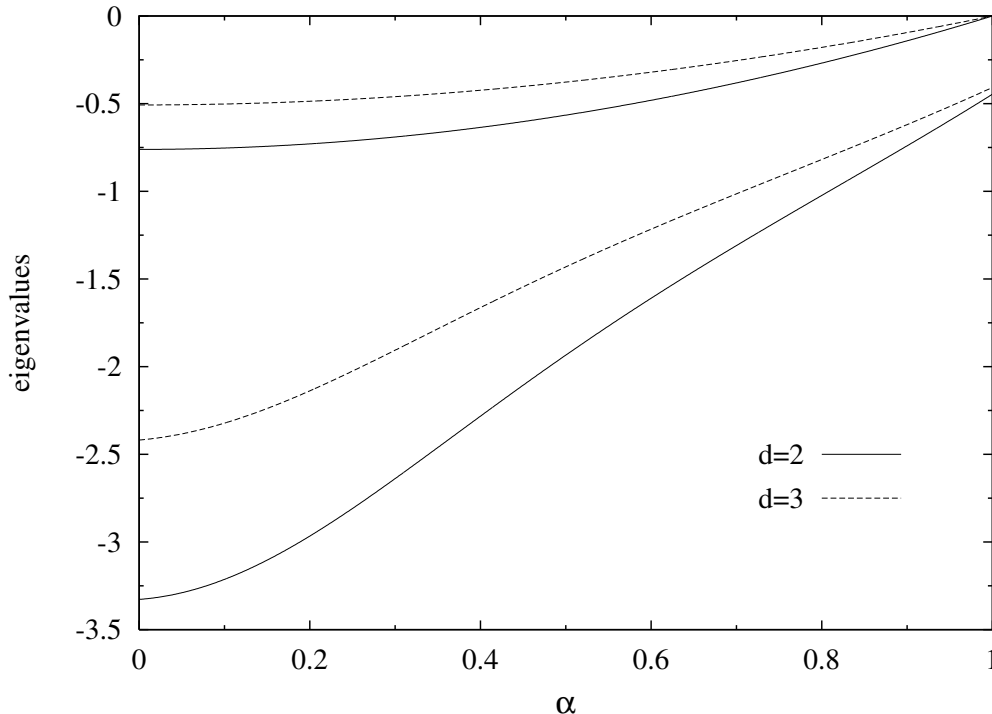


Fig. 1. The eigenvalues of the linear stability matrix for the stationary state as a function of α for $d = 2$ and $d = 3$. The eigenvalues are measured in units $t_0^{-1} = n\sigma^{d-1}\chi S_d v_{T_0}/\sqrt{2\pi}$.

One notices that the two eigenvalues are strictly negative for $\alpha < 1$, which indicates the *stability* of the stationary state with respect to small perturbations in the temperature and in the shape of the probability distribution function (in the scaling form). We emphasize again that spatial homogeneity has been enforced here. As expected, in the elastic limit $\alpha = 1$ one of the eigenvalues becomes zero (while the other one remains negative) – which corresponds to the temperature becoming a marginal mode, and to a relaxation of the distribution function to its equilibrium Gaussian shape.

4 Entropy production

We now turn to the issue of entropy. For our *homogeneous* system, we consider the Shannon information entropy

$$S(t) \equiv -k_B \int_{\mathbb{R}^d} d\mathbf{v}_1 f(\mathbf{v}_1, t) \ln \left(\frac{f(\mathbf{v}_1, t)}{eh^d} \right) \quad (23)$$

(with Euler's number e and Planck's constant h , and eh^d the volume of the semiclassical elementary phase-space cell)." It is known that in the elastic limit $\alpha = 1$ (and in the absence of an external drive) this reduces to the

appropriate expression of the usual thermodynamic entropy and leads to the classical “ H -theorem”. We now consider the time evolution of $S(t)$ as governed by the Boltzmann equation (2), which reads

$$\begin{aligned}
\frac{dS}{dt} &= -k_B \int_{\mathbb{R}^d} d\mathbf{v}_1 \frac{\partial f(\mathbf{v}_1, t)}{\partial t} \ln \left(\frac{f(\mathbf{v}_1, t)}{eh^d} \right) \\
&= -\chi k_B \int_{\mathbb{R}^d} d\mathbf{v}_1 I[f, f] \ln \left(\frac{f(\mathbf{v}_1, t)}{eh^d} \right) \\
&\quad - \frac{k_B \xi_0^2}{2} \int_{\mathbb{R}^d} d\mathbf{v}_1 \frac{\partial^2}{\partial \mathbf{v}_1^2} f(\mathbf{v}_1, t) \ln \left(\frac{f(\mathbf{v}_1, t)}{eh^d} \right). \tag{24}
\end{aligned}$$

As mentioned in the Introduction, we wish to introduce a heuristic – albeit physically motivated – entropy production functional that, hopefully, displays extremal properties in NESS. We shall propose two approaches. But before proceeding further, we would like to remind the reader the status of dS/dt within the framework of phenomenological thermodynamics as discussed in standard textbooks [15,16,17], as well as some of its extensions to stochastic systems [3,4,5]. Entropy variations are usually split into two parts:

$$\frac{dS}{dt} = \sigma_{\text{irr}} + \sigma_{\text{flux}}, \tag{25}$$

where $\sigma_{\text{irr}} \geq 0$ is the entropy production arising due to the dissipative processes that take place inside the system (that is positively-defined according to the second principle of thermodynamics), while the entropy flux $\sigma_{\text{flux}} = -\int_V dV \nabla \cdot \mathbf{J}_S$ accounts for the external forces driving the system into a nonequilibrium state (the related contribution is often reduced to boundary terms). The “art” of phenomenological thermodynamics precisely bears on \mathbf{J}_S and on how to decompose it in terms of the energy, particle, momentum, chemical, *etc.*, currents. This is done, usually, on the basis of the local equilibrium hypothesis. In a similar way, σ_{irr} often appears as a bilinear form in the fluxes running through the system and the conjugate affinities. In the near-to-equilibrium regime, the fluxes are usually proportional to the conjugated affinities, with the Onsager coefficients as proportionality factors, and one recovers Prigogine’s minimum theorem for σ_{irr} under the hypothesis of time-reversibility of the underlying microscopic dynamics.

However, in view of the local character of the energy injection mechanism, as well as of the spatial homogeneity of the system, the situation is completely different in the case we are considering. Indeed, unlike the above-mentioned “conventional” NESS, there are neither macroscopic, however weak, currents running across the system, nor the related phenomenological Onsager response coefficients. Therefore, the separation into “source” and “flow” for the entropy variation is much more tricky.

First approach.— A first proposed choice of the “entropy production” is

$$\sigma_{\text{irr}} = \frac{k_B \chi \sigma^{d-1}}{4} \int d\mathbf{v}_1 d\mathbf{v}_2 d\hat{\boldsymbol{\sigma}} \theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12}) \hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12} \\ \times (f_1^{**} f_2^{**} - f_1 f_2) \ln \left(\frac{f_1^{**} f_2^{**}}{f_1 f_2} \right) + \frac{\xi_0^2}{2} \int d\mathbf{v} \frac{(\nabla_{\mathbf{v}} f)^2}{f}, \quad (26)$$

the form of the first r.h.s. term being simply chosen by analogy with the elastic-limit case. The second term has been chosen by analogy with standard diffusion processes. In those processes this term vanishes at equilibrium because the gradients disappear. Note however that here the diffusion process happens in the velocity space, and thus the vanishing of this term at equilibrium is not due to the system becoming homogeneous in \mathbf{v} -space, but because of the energy source strength ξ_0^2 being tuned to 0. The above σ_{irr} appears to be the sum of two positive definite terms, and it is therefore also positive definite. Furthermore, σ_{irr} can only be zero *at equilibrium*, namely when both the energy source (the random kicks) and the energy sink (the dissipative collisions) are tuned to zero. In that respect, it fulfills the properties expected from standard phenomenological thermodynamics.

On the other hand, the form of the entropy flux σ_{flux} is now constrained to be

$$\sigma_{\text{flux}} = \frac{k_B \chi \sigma^{d-1}}{4} \int d\mathbf{v}_1 d\mathbf{v}_2 d\hat{\boldsymbol{\sigma}} \theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12}) \hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12} \\ \times f_1 f_2 \ln \left[\frac{(f_1^{**} f_2^{**})(f_1 f_2)^{1-\alpha^2}}{(f_1^* f_2^*)^{2-\alpha^2}} \right], \quad (27)$$

where we have used the shorthand notations $f_{1,2} = f(\mathbf{v}_{1,2}, t)$, respectively $f_{1,2}^{**} = f(\mathbf{v}_{1,2}^{**}, t)$ for the distribution functions corresponding to the pre-collisional velocities (4). The above functional of f is negative for a large class of trial functions, and must definitely assume a negative value $\sigma_{\text{flux}} \sim -\frac{1-\alpha^2}{\ell} T_0^{1/2}$ in the steady state ($\ell \sim \frac{1}{\chi \sigma^{d-1}}$ is the mean free path). However, aside from conveying the shrinking of phase space volumes, we must dismiss $\sigma_{\text{irr/flux}}$ as relevant candidates for extremum entropy functionals. Indeed, in the spirit of phenomenological thermodynamics, the splitting of dS/dt into σ_{irr} and σ_{flux} is motivated by the desire to isolate the driving processes (the source and sink referred to above) from the irreversible processes inside the system. However there is no simple and univoque manner to do so, and definitely this first choice is not accomplishing this physically-motivated requirement. It must be noted that the last term of eq.(26) could have also chosen as a part of σ_{flux} , which would then have featured both the source and the sink, at the price of abandoning its negative definiteness.

Second approach.— We now propose an alternative and perhaps more pragmatic route, which consists in isolating as the only driving mechanism the random kicks provided by the thermostat. The inelastic collisions, viewed above as an

energy sink, are now incorporated into a term describing the system's intrinsic dissipative microscopic dynamics. Along those lines we henceforth write that

$$\frac{dS}{dt} = \sigma_{syst} + \sigma_{ext}. \quad (28)$$

The first contribution σ_{syst} corresponds to the entropy production inside the system, i.e., it comes from the changes of the particles velocities during the binary inelastic collisions,

$$\begin{aligned} \sigma_{syst} = \frac{k_B \chi \sigma^{d-1}}{2} \int_{\mathbb{R}^d} d\mathbf{v}_1 \int_{\mathbb{R}^d} d\mathbf{v}_2 \int d\hat{\boldsymbol{\sigma}} \theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12}) \\ \times (\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{12}) f_1 f_2 \ln \left(\frac{f_1 f_2}{f_1^* f_2^*} \right), \end{aligned} \quad (29)$$

where we have used the shorthand notation $f_{1,2}^* = f(\mathbf{v}_{1,2}^*, t)$ for the distribution functions corresponding to the post-collisional velocities (5). Of course, in the limit of elastic collisions $\alpha = 1$ the expression of σ_{syst} reduces to the usual positive-definite expression of the hard-disk gas that enters the H -theorem. However, in general σ_{syst} does not have a definite sign. One can imagine the entropy production inside the system as resulting from two antagonist (although actually undissociated) mechanisms, namely a generic disordering effect of any particle collisions (e.g., that is also present for elastic hard spheres) in $d \geq 2$, and an ordering effect due to the inelastic character of the collisions (i.e., to the reduction of the translational agitation of the particles). Depending on the actual shape of the distribution function, one of these two mechanisms may prevail on the other, thus determining the sign of the instantaneous value of σ_{syst} .

The second contribution σ_{ext} is determined by the effect of the thermostat on the distribution function of the particles of the system. It corresponds to an energy injection into the system, and to a disordering effect of the particles velocities (through "random kicking"), and therefore, as expected, is always a *positively-defined* quantity,

$$\sigma_{ext} = \frac{k_B \xi_0^2}{2} \int_{\mathbb{R}^d} d\mathbf{v} \frac{1}{f(\mathbf{v}, t)} [\nabla_{\mathbf{v}} f(\mathbf{v}, t)]^2. \quad (30)$$

Introducing the dimensionless quantities

$$\tilde{\sigma}_{syst,ext} = \frac{2\sigma_{syst,ext}}{\chi \sigma^{d-1} v_{T_0} n^2}, \quad (31)$$

one obtains the expressions for the dimensionless time-dependent entropy pro-

duction sources:

$$\begin{aligned} \tilde{\sigma}_{syst} = & \left[\frac{T(t)}{T_0} \right]^{1/2} \int_{\mathbb{R}^d} d\mathbf{c}_1 \int_{\mathbb{R}^d} d\mathbf{c}_2 \int d\hat{\boldsymbol{\sigma}} \theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{c}_{12}) \\ & \times (\hat{\boldsymbol{\sigma}} \cdot \mathbf{c}_{12}) \tilde{f}(\mathbf{c}_1, t) \tilde{f}(\mathbf{c}_2, t) \ln \left[\frac{\tilde{f}(\mathbf{c}_1, t) \tilde{f}(\mathbf{c}_2, t)}{\tilde{f}(\mathbf{c}_1^*, t) \tilde{f}(\mathbf{c}_2^*, t)} \right], \quad (32) \end{aligned}$$

respectively

$$\begin{aligned} \tilde{\sigma}_{ext} = & \left[\frac{T_0}{T(t)} \right] \frac{(1-\alpha^2)S_d}{2d\sqrt{2\pi}} \left(1 + \frac{3}{16}a_2(t) + \frac{9}{1024}a_2^2(t) \right) \\ & \times \int_{\mathbb{R}^d} d\mathbf{c} \frac{1}{\tilde{f}(\mathbf{c}, t)} \left[\nabla_{\mathbf{c}} \tilde{f}(\mathbf{c}, t) \right]^2. \quad (33) \end{aligned}$$

In the stationary regime at temperature T_0 one has, obviously, $\tilde{\sigma}_{syst} = -\tilde{\sigma}_{ext} \equiv -\tilde{\sigma}_0$. The quantity $\tilde{\sigma}_0$ is positive and decaying monotonously with α , as illustrated in Fig. 2. Note that $\tilde{\sigma}_0$ is nonzero as long as the collisions are inelastic,

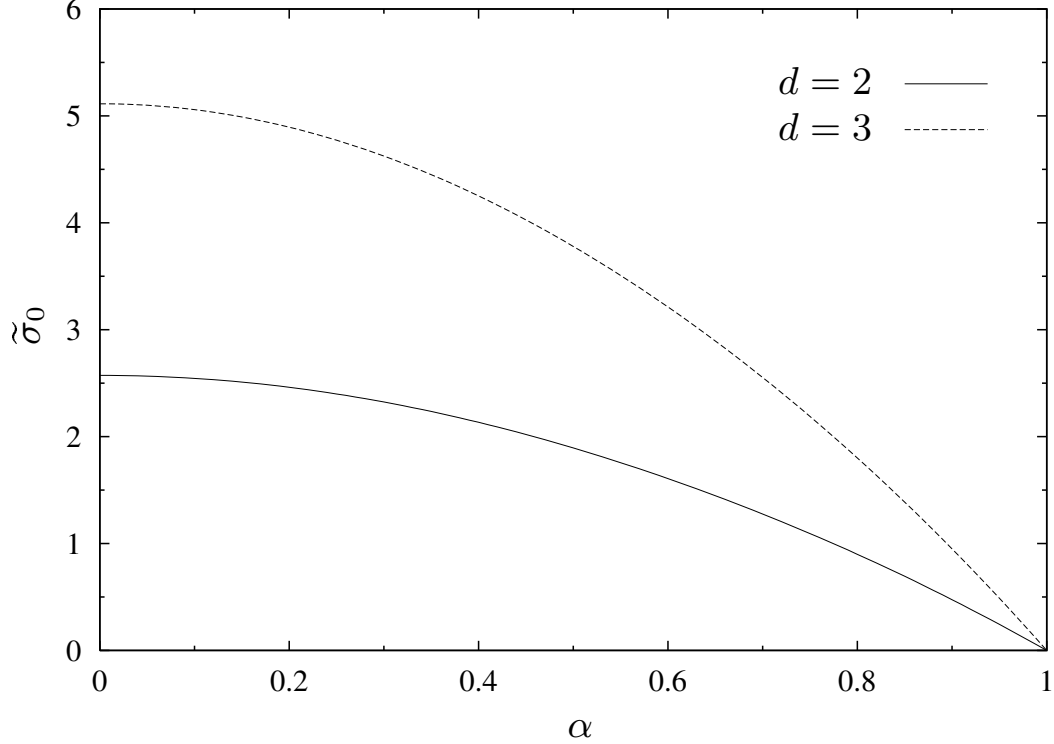


Fig. 2. The dimensionless stationary entropy production $\tilde{\sigma}_0$ as a function of α in $d = 2$ and $d = 3$.

i.e., as long as the stationary probability distribution is non-Gaussian. Note also the negativity of $\tilde{\sigma}_{syst}$ in the stationary state – the ordering effect due to the inelastic character of the collisions prevails on the generic disordering effect of the collisions.

Let us now address the question whether the entropy production (as a whole, or one of its parts $\tilde{\sigma}_{syst}$ or $\tilde{\sigma}_{ext}$) can play the role of some kind of “nonequilibrium potential” for the system, i.e., whether or not it can account for the linear stability of the stationary state of the system. The particular case of the quasi-elastic limit $\varepsilon \equiv 1 - \alpha \ll 1$ is especially interesting, given that the stationary state is close to equilibrium. One might then expect *a priori* that a “minimum entropy production theorem” (in the spirit of the “extended Prigogine theory” [3]) might be valid in this case.

Consider thus small perturbations of the temperature and of the coefficient a_2 around their stationary values, as in Eq. (20). A Taylor development of the entropy production terms $\tilde{\sigma}_{syst}$ and $\tilde{\sigma}_{ext}$ leads to nonzero linear contributions in the perturbations $\delta\theta$ and δa_2 ,

$$\begin{aligned} \tilde{\sigma}_{syst} - (-\tilde{\sigma}_0) &= -\delta\theta \left(\frac{\tilde{\sigma}_0}{2} \right) + \delta a_2 \int_{\mathbb{R}^d} d\mathbf{c}_1 \int_{\mathbb{R}^d} d\mathbf{c}_2 \int d\hat{\boldsymbol{\sigma}} \\ &\quad \times \theta(\hat{\boldsymbol{\sigma}} \cdot \mathbf{c}_{12})(\hat{\boldsymbol{\sigma}} \cdot \mathbf{c}_{12}) \tilde{f}_0(c_1) \tilde{f}_0(c_2) \left\{ \left[\frac{S_2(c_1^2)}{1 + a_{20} S_2(c_1^2)} + \right. \right. \\ &\quad \times \left. \frac{S_2(c_2^2)}{1 + a_{20} S_2(c_2^2)} - \frac{S_2(c_1^{*2})}{1 + a_{20} S_2(c_1^{*2})} - \frac{S_2(c_2^{*2})}{1 + a_{20} S_2(c_2^{*2})} \right] \\ &\quad \left. + \left[\frac{S_2(c_1^2)}{1 + a_{20} S_2(c_1^2)} + \frac{S_2(c_2^2)}{1 + a_{20} S_2(c_2^2)} \right] \ln \left[\frac{\tilde{f}_0(\mathbf{c}_1) \tilde{f}_0(\mathbf{c}_2)}{\tilde{f}_0(\mathbf{c}_1^*) \tilde{f}_0(\mathbf{c}_2^*)} \right] \right\} \\ &\quad + O(\delta\theta^2, \delta a_2^2), \quad (34) \end{aligned}$$

respectively

$$\begin{aligned} \tilde{\sigma}_{ext} - (\tilde{\sigma}_0) &= -\delta\theta(\tilde{\sigma}_0) + \delta a_2 \left\{ \frac{3/16 + (9/512)a_{20}}{1 + (3/16)a_{20} + (9/1024)a_{20}^2} \tilde{\sigma}_0 \right. \\ &\quad \left. + \frac{(1-\alpha^2)S_d}{2d\sqrt{2\pi}} \left(1 + \frac{3}{16}a_{20} + \frac{9}{1024}a_{20}^2 \right) \right. \\ &\quad \times \int_{\mathbb{R}^d} d\mathbf{c} \left[\frac{2(\nabla_{\mathbf{c}} \tilde{f}_0(\mathbf{c})) \cdot [\nabla_{\mathbf{c}} (e^{-c^2} S_2(c^2))]}{\pi^{d/2} \tilde{f}_0(\mathbf{c})} \right. \\ &\quad \left. \left. - \frac{(\nabla_{\mathbf{c}} \tilde{f}_0(\mathbf{c}))^2 (e^{-c^2} S_2(c^2))}{\pi^{d/2} \tilde{f}_0^2(\mathbf{c})} \right] \right\} + O(\delta\theta^2, \delta a_2^2). \quad (35) \end{aligned}$$

The total entropy production $\tilde{\sigma}_{syst} + \tilde{\sigma}_{ext}$ also contains linear terms in the perturbations $\delta\theta$ and δa_2 .

The same holds true even in the quasielastic limit $\varepsilon \equiv 1 - \alpha \ll 1$, when one can evaluate explicitly to $O(\varepsilon^2)$ the expression of the coefficients of the

perturbations. More precisely,

$$\begin{aligned} \tilde{\sigma}_{ext} - (-\tilde{\sigma}_0) &= -\delta\theta \left(\frac{\tilde{\sigma}_0}{2} \right) - \delta a_2 \frac{\sqrt{2} \pi^{\frac{d-1}{2}}}{\Gamma(d/2)} \\ &\quad \times \left[2(d-1) a_{20} + \frac{4d+5}{8} \varepsilon + O(\varepsilon^2) \right], \\ \tilde{\sigma}_{syst} - \tilde{\sigma}_0 &= -\delta\theta (\tilde{\sigma}_0) + \delta a_2 \left[\frac{3}{16} \tilde{\sigma}_0 + O(\varepsilon^2) \right], \end{aligned} \quad (36)$$

where the stationary values are

$$\tilde{\sigma}_0 = \frac{2\sqrt{2}\pi^{\frac{d-1}{2}}}{\Gamma(d/2)} \varepsilon + O(\varepsilon^2), \quad (37)$$

and

$$a_{20} = -\frac{\sqrt{2}(\sqrt{2}-1)}{d-1} \varepsilon + O(\varepsilon^2). \quad (38)$$

The meaning of this result is that the entropy production as defined above cannot be used for a variational description of the relaxation of the system towards the stationary state, not even in the quasi-elastic limit.

One may argue that the choice of the definition of the entropy production inside the system might be inappropriate, since it refers only to the translational degrees of freedom, and it does not take into account properly the internal degrees of freedom of the particles – that are, in fact, responsible for the inelastic character of the collisions. The description of the inelasticity through a constant restitution coefficient α might thus be incompatible with a thermodynamic description of the system in terms of entropy production. We note that it is known that such a model, although being a useful approximation which captures important physical effects, is in fact incompatible with basic mechanical laws (see e.g. chapter 3 of Ref. [11]).

Let us now discuss briefly another issue that draw attention recently, see Refs. [18,19], namely that of the *Kullback relative entropy*, defined as

$$\begin{aligned} S_R(t) &= -k_B \int_{\mathbb{R}^d} d\mathbf{v} f(\mathbf{v}, t) \ln \left(\frac{f(\mathbf{v}, t)}{f_0(\mathbf{v})} \right) \\ &= -\frac{k_B n}{v_T^d} \int_{\mathbb{R}^d} d\mathbf{c} \phi(c) [1 + a_2 S_2(c^2)] \ln \left(\frac{v_{T_0}^d}{v_T^d} \frac{1 + a_2 S_2(c^2)}{1 + a_{20} S_2(c^2)} \right). \end{aligned} \quad (39)$$

$S_R(t)$ is a measure of the “distance” between the actual pdf $f(\mathbf{v}, t)$ and its stationary profile $f_0(\mathbf{v})$, and, of course, is equal to zero at the stationary state. Following Ref. [19], one can parametrize $S_R(t)$ through the two sets of parameters, $\{\gamma_1 = a_2(t), \gamma_2 = T(t)\}$ for the nonstationary state, respectively

$\{\gamma_{10} = a_{20}, \gamma_{20} = T_0\}$ for the stationary pdf. Considering as above (sec. 3.3) small deviations of the temperature and of the coefficient a_2 (that result in a small deviation $\delta f(\mathbf{v}, t)$ of the pdf) from their stationary values, one finds:

$$\delta S_R \approx -\frac{k_B}{2} \int_{\mathbb{R}^d} d\mathbf{v} \frac{1}{f_0(\mathbf{v})} [\delta f(\mathbf{v}, t)]^2 = -\frac{1}{2} \sum_{i,j=1,2} F_{ij} \delta\gamma_1 \delta\gamma_2 \leq 0, \quad (40)$$

where $\delta\gamma_1 = \delta a_2$, $\delta\gamma_2 = T_0 \delta\theta$, and F_{ij} is the positively-defined Fisher information matrix [20],

$$F_{ij} = k_B \int_{\mathbb{R}^d} d\mathbf{v} f_0(\mathbf{v}) \left(\frac{\partial \ln f_0(\mathbf{v})}{\partial \gamma_{i0}} \right) \left(\frac{\partial \ln f_0(\mathbf{v})}{\partial \gamma_{j0}} \right). \quad (41)$$

It looks therefore as if this relative entropy has the required property of extremum at the steady-state (and monotonous exponential asymptotic relaxation towards it). This property has already been demonstrated for other types of nonequilibrium stochastic systems (e.g., in Ref. [18], the one-dimensional Ornstein-Uhlenbeck and Rayleigh processes, noise-perturbed harmonic oscillator, dichotomous noise). The question arises about its relationship with the thermodynamic entropy production; in Ref. [19] it was shown that in the case of the usual Smolukhowski diffusion the Kullback entropy time-variation rate coincides with the Shannon entropy production rate. However, some further case-study (in particular, on systems described by kinetic Boltzmann-like equations) are necessary before generalizing this important conclusion to other nonequilibrium situations. In particular, although very appealing, the Kullback entropy does not reduce to the usual H -functional in the limit of an elastic gas of particles relaxing to equilibrium. Besides that, computing Kullback entropy requires the knowledge of the steady-state pdf, while the expected approach would be to define a proper Lyapunov functional of the system from which to *deduce* the stationary state.

5 Conclusions

We illustrated on the well-known model of a randomly driven granular gas with constant restitution coefficient the difficulties that one encounters when trying to construct a variational principle for NESS based on an “entropy production”. Two approaches were proposed for the interpretation of the entropy balance equation in terms of “sources” and “flows”, but none of them lead to the formulation of such a principle. The main reason for this failure seems to be the intrinsic irreversible microscopic dynamics of the granular gas. Modeling the internal degrees of freedom of the grains (that are responsible for the inelasticity of the collisions) through a constant restitution coefficient is thus

not appropriate for a thermodynamic description. This shows thus a major limitation of this model. A further step in the rather involved question of the refinement of the description would be the use of *random restitution coefficients* (as done, e.g., in [21]). These are meant to describe the possible flow of energy (at the collision) both towards and *from* the internal degrees of freedom to the translational degrees of freedom. Such a model, however, cannot be treated analytically, and no simple analytic conclusions can be therefore drawn on the fate of the corresponding H -functional. Numerical results are left for further studies.

Moreover, the problem of the Kullback relative entropy, its monotonous relaxation to the steady-state, and its relationship with the thermodynamic entropy production of a nonequilibrium system is a very promising direction for further studies.

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