# Fluctuation-dissipation relations in driven granular gases

A. Puglisi, A. Baldassarri, and V. Loreto
*Physics Department, "La Sapienza" University in Rome, Piazzale A. Moro 5, 00185 Rome, Italy*
*and INFM, Center for Statistical Mechanics and Complexity, Rome, Italy*
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We study the dynamics of a two-dimensional driven inelastic gas, by means of direct simulation Monte Carlo techniques, i.e., under the assumption of molecular chaos. Under the effect of a uniform stochastic driving in the form of a white noise plus a friction term, the gas is kept in a nonequilibrium steady state characterized by fractal density correlations and non-Gaussian distributions of velocities; the mean-squared velocity, that is the so-called *granular temperature*, is lower than the bath temperature. We observe that a modified form of the Kubo relation, which relates the autocorrelation and the linear response for the dynamics of a system *at equilibrium*, still holds for the off equilibrium, though stationary, dynamics of the systems under investigation. Interestingly, the only needed modification to the equilibrium Kubo relation is the replacement of the equilibrium temperature with an effective temperature, which results equal to the global granular temperature. We present two independent numerical experiments, where two different observables are studied: (a) the staggered density current, whose response to an impulsive shear is proportional to its autocorrelation in the unperturbed system and (b) the response of a tracer to a small constant force, switched on at time $t_w$, which is proportional to the mean-square displacement in the unperturbed system. Both measures confirm the validity of Kubo's formula, provided that the granular temperature is used as the proportionality factor between response and autocorrelation, at least for not too large inelasticities.

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## I. INTRODUCTION

In the past few years, granular materials [1] have become a fast growing field of research. In this framework, a strong interest has arisen in the subject of the so-called granular gases, systems of grains at a very low density so that the collisions can be considered always binary and instantaneous [2]. The collisions among the grains are dissipative, and the amount of energy lost in each collision is parametrized by the so-called restitution coefficient $r$ (see below for a precise definition). Since the energy of the system is not conserved, therefore, an external forcing is usually applied to obtain a dynamic stationary state. For these kind of systems, the analogy with perfect gases allows to introduce a *granular* temperature [3] defined as the mean-square fluctuation of the velocity, that is $T_G=\langle|\mathbf{v}-\langle\mathbf{v}\rangle|^2\rangle$ even though the velocity distribution could not be Gaussian.

In the case of zero external forcing [4] (i.e., the so-called free cooling), granular temperature decreases in time and goes asymptotically to zero when all the particles finally stop. When an energy input feeds the system, instead, the granular temperature may reach a stationary value and several models for the stochastic driving have been proposed employing a constant [5–9] or a random [10] restitution coefficient.

In numerical simulations or in experiments, $T_G$ is often measured taking the average $\langle\cdot\rangle$ on the whole system. However, strong fluctuations in the local granular temperature can be observed [7]. Even considering only the global granular temperature, i.e., for small spatial inhomogeneities, it is not clear to which extent $T_G$ can be considered the "temperature" of the system.

There are of course several possible paths to face this problem. One interesting point of view is that of investigating the response properties of an external thermometer coupled to a granular gas [11]. This corresponds to study the fluctuation-dissipation properties of the system [12]. For a system slightly perturbed from its stationary equilibrium state, linear response theory allows to relate the response to the correlation functions through the fluctuation-dissipation relations [13].

In the simplest case, given a perturbing field $\alpha$, a fluctuation-dissipation relation relates the response of an observable $B$ at the time $t$, after an impulsive perturbation at time 0, to the correlation of the observable $B$ and the field $A$, *conjugated* to $\alpha$, measured in the unperturbed system,

$$\frac{\partial\langle B(t)\rangle}{\partial\alpha}=-\frac{1}{T}\frac{\partial}{\partial t}\langle B(t)A(0)\rangle, \tag{1}$$

where $T$ is the equilibrium temperature of the system.

Recently, Green-Kubo expressions for a homogeneous cooling granular gas have been obtained [14–16] and numerical simulations have confirmed their validity [17]: cooling granulars lack an equilibrium state, therefore the homogeneous cooling state (which is characterized by scaling properties) is used as a reference state to be perturbed, but in this case the Green-Kubo relations must be changed in order to keep into account new terms arising from the time dependence of the reference state and the nonconservative character of collisions (see Ref. [15]). However, in the case of steady state granular gases, a rigorous derivation of Green-Kubo relations has not yet been performed to our knowledge.

In this paper, we perform numerical investigations in order to check the validity of standard Kubo formulas [13,18] to steady state inelastic gases. We perform, in particular, two different sets of numerical experiments on heated granular gases. We choose two different conjugated pairs of variables constituted by the autocorrelation of a given variable and the corresponding response to a perturbation applied to the gas. Kubo's formula, i.e., the proportionality between response and the autocorrelation in the unperturbed system, is verified to hold using the granular temperature as the correct proportionality factor, at least for not too strong inelasticities ($r>0.5$). For stronger inelasticities (smaller values of $r$), Kubo's formula can be verified with a different effective temperature. It should be noted how the adopted simulation scheme [i.e., direct simulation Monte Carlo (DSMC)] represents the numerical implementation of the Boltzmann equation (given, for example, in Ref. [7]), which assumes molecular chaos hypothesis and therefore, neglects short-range correlations. For this reason, for very strong inelasticities, the Boltzmann equation (and the DSMC scheme) cannot be considered realistic and one should use molecular dynamics simulations.

These results differ from the analogous results obtained for dense granular assemblies, where "slow" degrees of freedom thermalize at an effective temperature, which is far higher than the external imposed temperature [19,20]. However the gaslike state of granular matter has nothing to do with these systems, as their stationary state is governed by a rapid decay of the fluctuations and the granular temperature turns out to be the right choice in the description of linear response to slight perturbations.

The outline of the paper is as follows. In Sec. II, we define the model as well as its simulation scheme and give a brief review of known results about the peculiar features of its nonequilibrium stationary state. Section III reviews Kubo's formula and its extension to non-Hamiltonian perturbations. In Sec. IV, we describe numerical experiments using a sinusoidal shear and measuring as a response to the density current. In Sec. V, we perform a diffusion vs mobility experiment upon a tracer (i.e., perturbing a single particle). Finally, Sec. VI is devoted to the conclusions.

## II. THE MODEL

We simulate a gas of $N$ identical particles of unitary mass in a two-dimensional box of side $L=\sqrt{N}$ (in order to have a fixed number density $N/L^2$ when changing $N$) with periodic boundary conditions. The particle collisions are inelastic: the total momentum is conserved, while the component of the relative velocity parallel to the direction joining the center of the particles is reduced to a fraction $r$ (with $0\leqslant r\leqslant 1$) of its initial value, lowering in this way the kinetic energy of the pair:

$$\mathbf{v}_1'=\mathbf{v}_1-\frac{1+r}{2}[(\mathbf{v}_1-\mathbf{v}_2)\cdot\hat{\mathbf{n}}]\hat{\mathbf{n}}, \tag{2a}$$

$$\mathbf{v}_2'=\mathbf{v}_2+\frac{1+r}{2}((\mathbf{v}_1-\mathbf{v}_2)\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}, \tag{2b}$$

where $\mathbf{v}_1'$ and $\mathbf{v}_2'$ are the velocities of the colliding particles *after* the collision.

In the interval between two subsequent collisions, the motion of each particle $i$ is governed by the following Langevin equation [7]:

$$\frac{d}{dt}\mathbf{v}_i(t)=-\frac{\mathbf{v}_i(t)}{\tau_B}+\sqrt{\frac{2T_b}{\tau_B}}\boldsymbol{\eta}_i(t), \tag{3a}$$

$$\frac{d}{dt}\mathbf{x}_i(t)=\mathbf{v}_i(t), \tag{3b}$$

where the function $\boldsymbol{\eta}_i(t)$ is a stochastic process with average $\langle\boldsymbol{\eta}_i(t)\rangle=\mathbf{0}$ and correlations $\langle\eta_i^\alpha(t)\eta_j^\beta(t')\rangle=\delta(t-t')\delta_{ij}\delta_{\alpha\beta}$ ($\alpha$ and $\beta$ being component indices), i.e., a standard white noise. This means that each particle feels a hot fluid with a temperature $T_b$ and a viscosity characterized by a time $\tau_B$.

The question about the most proper way of modeling a stochastic driving is still open. Many authors for instance use Eq. (3) without viscosity [5]. This is equivalent to the limit $\tau_B\to\infty$ and $T_b\to\infty$ with keeping $D=T_b/\tau_B$ constant. In this limit, long- and short-range correlations in the velocity and density fields have been observed [8]. We have measured correlations in the velocity field in the model with viscosity, concluding that they are highly reduced by the viscous term that breaks Galilean invariance (the frame $\mathbf{v}=0$ is preferred) [21]. Our choice of the stochastic driving with viscosity has the following advantages: (a) it guarantees that in the elastic limit ($r=1$), the system after a transient time of the order of $\tau_B$, still reaches a stationary state, characterized by a uniform density and a Gaussian distribution of velocities with temperature $T_b$; (b) it is a heat bath with a well defined finite temperature $T_b$ that can be compared with the granular temperature $T_G$ and the effective temperature $T_{eff}$ measured by means of fluctuation-dissipation relations (see ahead).

In spite of the drastic reduction of velocity correlations, this model exhibits several interesting features, which are parametrized by the restitution coefficient $r$ and the ratio, $\tau_C/\tau_B$, between the mean free time (the average interval of time between two subsequent collisions of the same particle) and the viscosity time. When $\tau_B>\tau_C$ and $r<1$, the system is in a nonequilibrium stationary state with a granular temperature $T_G<T_b$. This state is characterized [7] by fractal density clustering and non-Gaussian distributions of velocities (see Fig. 1) with a dependence upon $r$ and $\tau_C/\tau_B$. This situation persists when direct simulation Monte Carlo (DSMC) [22] is used to perform more rapid and larger simulations of the system. The DSMC simulation scheme consists of a discrete time integration of the motion of the particles. At each time step of length $\Delta t$, the following operations are performed:

(1)*Free streaming*: Equation (3) is integrated for a time step $\Delta t$ disregarding possible interactions among the particles.

(2)*Collisions*: Every particle has a probability $p=\Delta t/\tau_c$ of undergoing a collision. Its collision mate is chosen among the particles in a circle of fixed radius $r_B$ with a probability proportional to its relative velocity. The unitary vector $\mathbf{n}$,

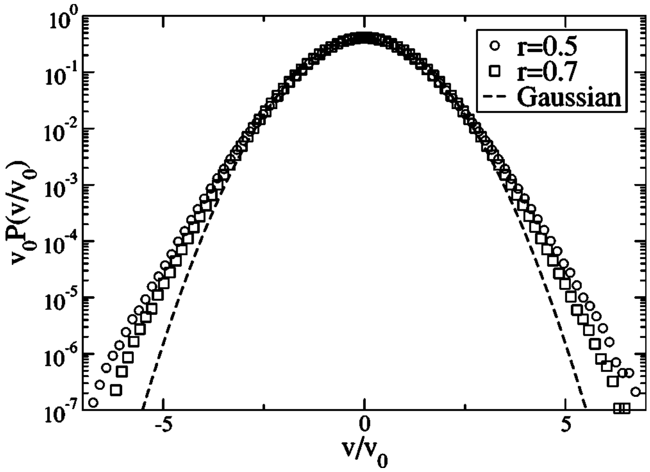


FIG. 1. Rescaled (in order to have unitary variance) distribution of the horizontal component of the velocity of the gas $P(v_x)$ versus $v_x$, with $N=500$, $L^2=N$, heat bath with $T_b=1$, $\tau_b=10$, $\tau_c=1$, and different restitution coefficients. The Gaussian is plotted as a reference for the eye.

which should be parallel to the line joining the centers of particles, is chosen randomly instead and the collision is performed using rule (2).

## III. SHORT REVIEW ABOUT KUBO'S FORMULA

In this section, we review the Kubo's formula, which must hold in the case of equilibrium dynamics. First, we show the case of an Hamiltonian dynamics, and then for non-Hamiltonian equilibrium dynamics of a system subjected to a (impulsive) shear force. The first case is presented just for completeness and to set the notations, the formulas presented in the second case will be numerically checked for an elastic system and extended to the inelastic case in the following sections.

### A. Kubo's formula for Hamiltonian systems

For an Hamiltonian system, the temporal evolution of the phase space distribution $f(p,q,t)$ is ruled by the Liouville equation,

$$\frac{\partial}{\partial t}f(p,q,t)=i[\mathcal{L}+\mathcal{L}_{ext}(t)]f(p,q,t), \tag{4}$$

where $\mathcal{L}$ and $\mathcal{L}_{ext}$ are the Liouville operators relative to the unperturbed Hamiltonian and to its perturbation, respectively. They are defined by means of classical Poisson bracket,

$$i\mathcal{L}f=(\mathcal{H},f)=\sum\left(\frac{\partial\mathcal{H}}{\partial q}\frac{\partial}{\partial p}-\frac{\partial\mathcal{H}}{\partial p}\frac{\partial}{\partial q}\right)f. \tag{5}$$

The perturbation is assumed to be given by coupling a force $\alpha(t)$ with an observable of the system $\hat{A}$, i.e.,

$$\mathcal{H}_{ext}=-\hat{A}(p,q)\alpha(t). \tag{6}$$

The phase space distribution is assumed to be canonical (i.e., at equilibrium) in the infinite past: $f(p,q,-\infty)=f_{eq}(p,q)$. An approximate solution of Eq. (4) to the first order in the perturbation $i\mathcal{L}_{ext}$ is given by

$$f(p,q,t)=f_{eq}(p,q)+\int_{-\infty}^{t}dt'\times\exp[i(t-t')\mathcal{L}](\mathcal{H}_{ext}(t'),f_{eq}(p,q))+\cdots. \tag{7}$$

With this approximation, the deviation, due to the perturbation (6), of the expectation of a physical quantity $\hat{B}$ can be written as the following convolution:

$$\delta\hat{B}(t)=\langle\hat{B}\rangle_t-\langle\hat{B}\rangle_{-\infty}=\int_{-\infty}^{t}dt'\,\Phi_{BA}(t-t')\alpha(t'), \tag{8}$$

where $\langle\ \dots\rangle_t$ denotes averages taken over the ensemble given by $f(p,q,t)$; $\Phi_{BA}(t-t')$, called *response function*, represents the response $\delta\hat{B}(t)$ to the pulsed force $\alpha(t)=\delta(t)$, and reads

$$\Phi_{BA}(t)=\int\int dp\,dq\,f_{eq}(p,q)(\Delta\hat{A}(p,q),\Delta\hat{B}(p_t,q_t))=\langle(\Delta\hat{A},\Delta\hat{B}(t))\rangle, \tag{9}$$

where $\Delta A=\hat{A}-\langle A\rangle$ (and identically for $\Delta\hat{B}$), while $(p_t,q_t)$ is the image of the initial phase point $(p,q)$ determined by the total Hamiltonian (including the perturbation).

Kubo has shown that the response function can be written in a simpler form [13,18],

$$\Phi_{BA}(t)=\beta\left\langle\frac{\partial\Delta\hat{A}}{\partial t}(0)\Delta\hat{B}(t)\right\rangle=-\beta\left\langle\Delta A(0)\frac{\partial\Delta\hat{B}}{\partial t}(t)\right\rangle, \tag{10}$$

where $\beta$ is the inverse of the temperature.

### B. Fluctuation-dissipation for non-Hamiltonian equilibrium systems (the case of shear force)

Let us consider a gas of particles and define a nonconservative perturbation (force) acting on particle $i$ placed at $\mathbf{r}_i(t)$ at time $t$ as

$$\mathbf{F}(\mathbf{r}_i,t)=\gamma_i\boldsymbol{\xi}(\mathbf{r}_i,t),$$

$$\text{with the properties}\quad \nabla\times\boldsymbol{\xi}\neq\mathbf{0},\quad \nabla\cdot\boldsymbol{\xi}=0, \tag{11}$$

where $\gamma_i$ is the particle-dependent part of the force amplitude. For *small enough perturbation* and for any variable ("observable") $O(\mathbf{r})$ such that $\langle O\rangle_{-\infty}=0$, Eq. (8) with the Kubo formula (10) reads [23,24]

$$\langle O(\mathbf{r})\rangle_t=\beta\int d\mathbf{r}'\int_{-\infty}^{t}dt'\left\langle O(\mathbf{r},t)\sum_i \gamma_i\dot{\mathbf{r}}_i(t')\times\delta(\mathbf{r}'-\mathbf{r}_i(t'))\right\rangle_{-\infty}\cdot\boldsymbol{\xi}(\mathbf{r}',t'), \tag{12a}$$

$$\langle\hat{O}(\mathbf{k})\rangle_t=\beta\int_{-\infty}^{t}dt'\left\langle\hat{O}(\mathbf{k},t)\sum_i \gamma_i\dot{\mathbf{r}}_i(t')\times\exp\{i\mathbf{k}\cdot\mathbf{r}_i(t')\}\right\rangle_{-\infty}\cdot\hat{\boldsymbol{\xi}}(\mathbf{k},t'), \tag{12b}$$

where the Fourier transform $G\to\hat{G}$ is defined as

$$\hat{G}(\mathbf{k})=\frac{1}{V}\int d\mathbf{r}e^{-i\mathbf{k}\cdot\mathbf{r}}G(\mathbf{r}). \tag{13}$$

A force satisfying the properties (11) is for instance given by

$$\boldsymbol{\xi}_{\overline{k}}(\mathbf{r},t)=\begin{pmatrix}0\\ \Xi\exp(i\overline{k}_x x)\,\delta(t)\end{pmatrix}, \tag{14}$$

whose spatial Fourier transform reads

$$\boldsymbol{\xi}_{\overline{k}}(\mathbf{k},t)=\begin{pmatrix}0\\ \dfrac{\Xi}{V}\delta(\mathbf{k}-\overline{\mathbf{k}})\,\delta(t)\end{pmatrix}, \tag{15}$$

where $\overline{\mathbf{k}}=(\overline{k}_x,0)$ (having chosen $k_x$ compatible with the periodic boundary conditions, i.e., $k_x=2n_k\pi/L_x$, with $n_k$ integer and $L_x$ the linear horizontal dimension of the box where the particles move). Note that $\Xi$ must have the dimensions of a momentum, i.e., of a velocity (taking unitary masses). With this choice, Eq. (12b) becomes

$$\langle\hat{O}(\mathbf{k})\rangle_t=\frac{\beta\Xi}{V}\left\langle\hat{O}(\mathbf{k},t)\sum_i \gamma_i\dot{y}_i(0)\exp\{i\mathbf{k}\cdot\mathbf{r}_i(0)\}\right\rangle_{-\infty}\times\delta(\mathbf{k}-\overline{\mathbf{k}}). \tag{16}$$

If we now define the staggered $y$ current as

$$J_y^{st}(\mathbf{r},t)=\sum_i \gamma_i\dot{y}_i(t)\,\delta(\mathbf{r}-\mathbf{r}_i(t)), \tag{17a}$$

$$\hat{J}_y^{st}(\mathbf{k},t)=\frac{1}{V}\sum_i \gamma_i\dot{y}_i(t)\exp[-i\mathbf{k}\cdot\mathbf{r}_i(t)], \tag{17b}$$

then, using this current as observable $O$, the relation (16) is written as

$$\langle\hat{J}_y^{st}(\mathbf{k},t)\rangle_t=\frac{\beta\Xi}{V^2}\left\langle\sum_{ij}\gamma_i\dot{y}_i(t)\exp(-i\mathbf{k}\cdot\mathbf{r}_i(t))\,\gamma_j\dot{y}_j(0)\times\exp\{i\overline{k}_x x_j(0)\}\right\rangle_{-\infty}\delta(\mathbf{k}-\overline{\mathbf{k}})$$
$$=\beta\Xi\langle\hat{J}_y^{st}(\mathbf{k},t)\hat{J}_y^{st}(-\mathbf{k},0)\rangle_{-\infty}\delta(\mathbf{k}-\overline{\mathbf{k}}). \tag{18}$$

A real linear combination of forces of the kind in Eq. (14) is

$$\boldsymbol{\xi}(\mathbf{r},t)=\frac{1}{2}(\boldsymbol{\xi}_{\overline{k}}(\mathbf{r},t)+\boldsymbol{\xi}_{-\overline{k}}(\mathbf{r},t))=\begin{pmatrix}0\\ \Xi\cos(\overline{k}_x x)\,\delta(t)\end{pmatrix}. \tag{19}$$

With this choice of the perturbation, the relation (18) becomes

$$\langle\hat{J}_y^{st}(\mathbf{k},t)\rangle_t=\frac{\beta\Xi}{2}\langle\hat{J}_y^{st}(\mathbf{k},t)\hat{J}_y^{st}(-\mathbf{k},0)\rangle_{-\infty}\times(\delta(\mathbf{k}-\overline{\mathbf{k}})+\delta(\mathbf{k}+\overline{\mathbf{k}})). \tag{20}$$

This is a *fluctuation-dissipation* (FD) relation, which expresses the fact that the response of the $\overline{\mathbf{k}}$ component of the transverse current to the perturbing field in Eq. (19) is proportional to the autocorrelation of the same transverse current measured in the system *without perturbation*.

It is useful to remark that for this particular choice of the observables, the right-hand side of the corresponding Fluctuation-dissipation relation, which must be the derivative of the correlation function [see Eq. (1)], takes the simple form of an autocorrelation function [23,24].

The real part of the response calculated at $\overline{\mathbf{k}}$ (per unit of perturbing field) is directly computable and reads

$$\mathrm{Re}\left[\frac{V}{\Xi}\langle\hat{J}_y^{st}(\overline{\mathbf{k}},t)\rangle_t\right]=\frac{1}{\Xi}\left\langle\sum_i \gamma_i\dot{y}_i(t)\cos[\overline{k}_x x_i(t)]\right\rangle_t. \tag{21}$$

From Eq. (20) one obtains the relation,

$$\frac{1}{\Xi}\left\langle\sum_i \gamma_i\dot{y}_i(t)\cos[\overline{k}_x x_i(t)]\right\rangle_t=\frac{\beta}{2}\left\langle\sum_{ij}\gamma_i\gamma_j\dot{y}_i(t)\dot{y}_j(0)\cos\{\overline{k}_x[x_i(t)-x_j(0)]\}\right\rangle_{-\infty}. \tag{22}$$

## IV. FLUCTUATION-DISSIPATION MEASURE I: SHEAR VS CURRENT

The first set of measures we have performed has been aimed to verify relation (22) for a system as described in the previous paragraph. In order to do this, we have used the following recipe proposed in Ref. [23].

(1) Initialize the system $U$ with random positions $\{\mathbf{r}_i^U(0)\}$ and random velocities $\{\dot{\mathbf{r}}_i^U(0)\}$.

(2) Let it evolve with the unperturbed dynamics until time $t_w$, which must be chosen larger than the largest characteristic time of the system (e.g., $\tau_c$ or $\tau_b$). The unperturbed dynamics consists of the time-discretized ($\Delta t$) integration of the Langevin equation (3),

$$\mathbf{v}_i(t+\Delta t)=\mathbf{v}_i(t)-\frac{\Delta t}{\tau_b}\mathbf{v}_i(t)+\sqrt{\frac{2T_b\Delta t}{\tau_b}}\mathbf{R}(t) \qquad (23)$$

plus inelastic collisions with parameter $r$ (restitution coefficient). The collisional step is separated from the Langevin step and is implemented by means of a local Monte Carlo procedure, i.e., random choice of pairs to collide inside a region of diameter $r_B$; the collision probability is proportional to a fixed collision frequency $1/\tau_c$ and to the relative velocity of the particles; $\tau_c$ is chosen to be compatible with an homogeneous gaslike dynamics, i.e., $\tau_c \approx r_B/\sqrt{\langle v^2\rangle_{-\infty}}$.

(3) At time $t_w$, a copy of the system $U$ is created (and named $P$) and the vectors $\{\dot{y}_i(t_w)\}$ and $\{x_i(t_w)\}$ are memorized in order to be used in the computation of the autocorrelation.

(4) The system $U$ is let to evolve with the unperturbed dynamics. The system $P$ is made to evolve with the additional forcing described in Eqs. (11) and (19) for only the time step $[t_w,t_w+\Delta t]$, i.e., the equation for the update of velocities in this particular step being

$$\mathbf{v}_i^P(t_w+\Delta t)=\mathbf{v}_i^P(t_w)-\frac{\Delta t}{\tau_b}\mathbf{v}_i^P(t_w)+\sqrt{\frac{2T_b\Delta t}{\tau_b}}\mathbf{R}(t_w) + \gamma_i\begin{pmatrix}0\\ \Xi\cos[\overline{k}_x x_i^P(t_w)]\end{pmatrix}, \qquad (24)$$

with $\overline{k}_x=2\pi n_k/L_x$. The quantities $\gamma_i$ are chosen to take the random value $\pm 1$ with equal probability (we have checked as different choices produce the same results). Note again that the perturbation intensity $\Xi$ has exactly the dimensions of velocity.

(5) The dynamics of the systems $U$ and $P$ are, thereafter, followed in the unperturbed style, i.e., by using Eq. (23). The functions to be measured are

$$R(\tau)=\frac{1}{N\Xi}\sum_i \gamma_i\dot{y}_i^P(t_w+\tau)\cos[\overline{k}_x x_i^P(t_w+\tau)], \qquad (25a)$$

$$C(\tau)=\frac{1}{N}\sum_{ij}\gamma_i\gamma_j\dot{y}_i^U(t_w+\tau)\dot{y}_j^U(t_w)\cos\{\overline{k}_x[x_i^U(t_w+\tau) - x_j^U(t_w)]\}, \qquad (25b)$$

where $\tau=t-t_w$. It is expected that $R(0)=1/2$ and $C(0)=\langle v^2\rangle$, while $R(\infty)=C(\infty)\to 0$.

(6) The above steps are repeated for many different realizations (or even in the same realization, provided its length is much longer than the typical correlation time) and the averages over those realizations of $R(t-t_w)$ and $C(t-t_w)$ are computed (see Fig. 2).

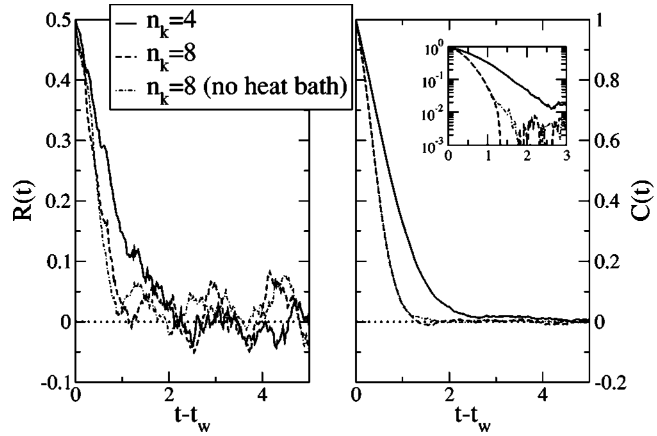


FIG. 2. Left: time dependent response to the impulsive shear perturbation defined in Eqs. (11) and (19): $R(t-t_w)$ vs $t-t_w$ for three simulations with elastic systems, one without thermal bath and two with thermal bath, and with different choices of the wave number $n_k$ of the perturbation. Right: time correlation function $C(t-t_w)$ vs $t-t_w$ for the same systems. In the simulations $r=1$, $N=500$, $\tau_c=1$, and for the two cases with the heat bath $T_b=1$ and $\tau_b=10$. The applied force has $\Xi=0.01$, $\tau_w=100$. The averages have been obtained over 10 000 realizations.

For the aim of checking the whole numerical machinery, we first consider the $r=1$ elastic case. In all the cases investigated, we have checked the linearity of the response by changing the perturbation amplitude in the range $\Xi \in [0.005,0.05]$. Within the specific framework chosen for the observables, the Kubo formula to be verified is given by

$$\langle R(t-t_w)\rangle=\frac{\beta}{2}\langle C(t-t_w)\rangle. \qquad (26)$$

We have performed the following experiments (see Fig. 3): (1) Gas with elastic interactions and absence of thermal bath; (2) Gas with elastic interactions *with* the thermal bath.

From Fig. 2 it can already be appreciated that response and autocorrelations in the elastic gas decay on a time of the order of $\tau_c$ (however this decay is not exponential, as can be observed in the inset of the figure). The parametric plot of the two curves in Fig. 3 shows the perfect agreement with Eq. (26) using $\beta=1/T_b$. In this case, of course, $T_b\equiv T_G$.

We have repeated the same measures on the gas with restitution coefficient $r<1$, i.e., gas with inelastic interactions with the bath (in this case, the bath is essential, to avoid cooling), see Fig. 4.

We obtain again a very good agreement with Eq. (26) using $\beta=1/T_G$. This is the main finding in this set of numerical experiments: even if the gas is out of equilibrium, being driven by a thermal bath at temperature $T_b$, its unperturbed autocorrelation is still proportional to the linear response, and its effective temperature measured by means of fluctuation-dissipation theory is exactly the granular temperature $T_G$.

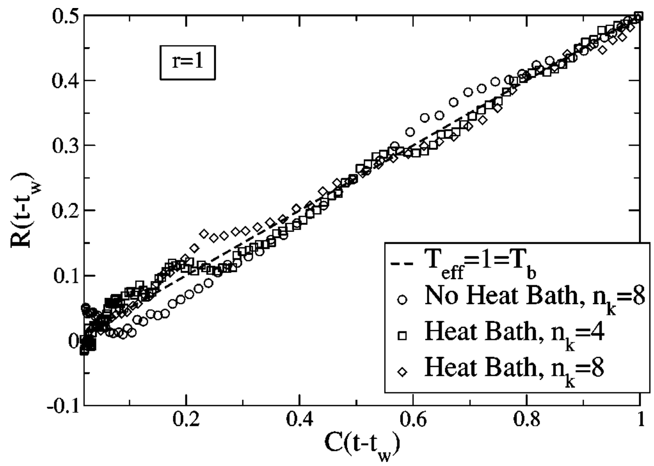


FIG. 3. Parametric plot of $R(t-t_w)$ vs $C(t-t_w)$ for the numerical experiment of type I (impulsive shear perturbation) with $r=1$, with or without heating bath, and for different choices of the wave number $n_k$ of the perturbation. The initial temperature for the case without heat bath is chosen to be 1 while $T_b=1$ and $\tau_b=10$ for the two cases with the heat bath. $N=500$, $\tau_c=1$, $\Xi=0.01$, $n_k=8$, with average over 10 000 realizations using $t_w=100$.

It must also be noted that relation (26) is verified for many values of the wave number $n_k$, i.e., the system does not show a scale dependent effective temperature.

At very large inelasticities, we expect a lack of validity of Eq. (26). This point deserves a deeper investigation.

## V. FLUCTUATION-DISSIPATION MEASURE II: DIFFUSION

Another independent confirmation of the validity of the modified linear response theory for a granular gas comes from the study of the diffusion properties, i.e., of the large

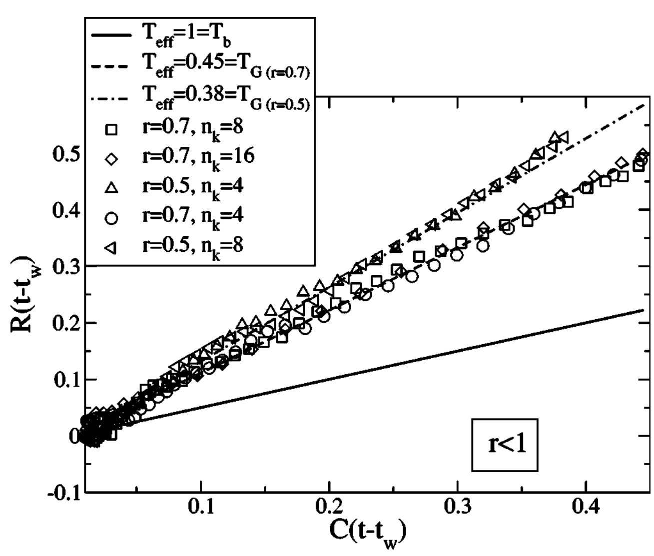


FIG. 4. Parametric plot of $R(t-t_w)$ vs $C(t-t_w)$ for the numerical experiment of type I (impulsive shear perturbation) with $r<1$, with heating bath, and for different choices of the wave number $n_k$ of the perturbation. $T_b=1$, $\tau_b=10$, $N=500$, $\tau_c=1$, $\Xi=0.01$, $n_k=8$, with averages over 10 000 realizations, using $t_w=100$.

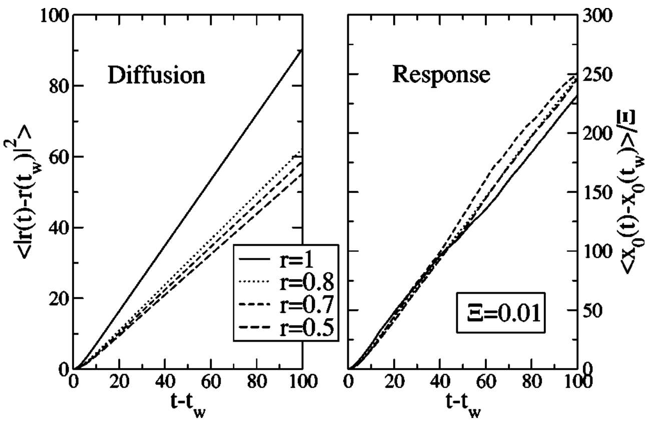


FIG. 5. Simulations of systems coupled to a thermal bath with elastic or inelastic collisions. $N=500$, $\tau_c=1$, $T_b=0.1$, $\tau_b=10$, $\Xi=0.01$, $\tau_w=100$. The results are obtained by averaging over 10 000 realizations. Left: mean squared displacement $B(t,t_w)$ vs $t-t_w$. Right: integrated response $\chi(t,t_w)$ to a constant force applied to the particle numbered as 0 vs $t-t_w$.

time behavior of the mean-squared displacement $B(t,t_w) = \langle|\mathbf{r}(t)-\mathbf{r}(t_w)|^2\rangle \sim 2D(t-t_w)$. In this case, the Einstein relation is expected to hold $D=\langle|\mathbf{v}|^2\rangle\tau_{corr}$, where $\tau_{corr} = \beta\int d\tau\langle v(t_w+\tau)v(t_w)\rangle$: this relation however, often addressed as a sort of FD relation, is always verified and just represents a check of the correctness of the simulation. Instead, some surprise could arise from mobility measurements: a small static drag force (switched on at time $t_w$) of intensity $\Xi$ (in the direction of the unitary vector $\hat{\mathbf{x}}$ of the $x$ axis) is applied to a given particle (tracer, e.g., particle with index 0 and position $\mathbf{r}_0$). The tracer reaches, as a result of the viscous force generated by the gas surrounding it, a limit constant velocity such that $\chi(t,t_w)\equiv\langle|(\mathbf{r}_0(t)-\mathbf{r}_0(t_w))\cdot\hat{\mathbf{x}}|\rangle \sim \Xi\mu t$, where $\mu$ is the mobility, which is expected to be related to the diffusion coefficient through the Einstein relation $\mu=D/\langle\mathbf{v}_x^2\rangle=2D/T$ (if the force is applied on the direction $x$ in the two-dimensional system).

Figure 5 shows the mean-squared displacement (in the unperturbed system) and the $x$ displacement of the tracer (when it is accelerated) divided by the intensity of the perturbing force versus time: it can be appreciated how both these quantities grow linearly with time, defining the diffusion coefficient and the mobility.

In our experiments, we have checked the linearity of the relation between $\langle|x_0(t)-x_0(t_w)|\rangle\equiv\langle|[\mathbf{r}_0(t)-\mathbf{r}_0(t_w)]\cdot\hat{\mathbf{x}}|\rangle$ and $\langle|\mathbf{r}(t)-\mathbf{r}(t_w)|^2\rangle$. In particular, if Kubo's formula was valid, one should have

$$\frac{\langle|x_0(t)-x_0(t_w)|\rangle}{\Xi}=\beta\frac{\langle|\mathbf{r}_i(t)-\mathbf{r}_i(t_w)|^2\rangle}{4}, \qquad (27)$$

with $\beta=1/T$ if the system is in thermodynamic equilibrium at temperature $T$.

In all the simulations, we have checked the linearity of the response by changing the perturbation amplitude in the range $\Xi\in[0.005,0.05]$.

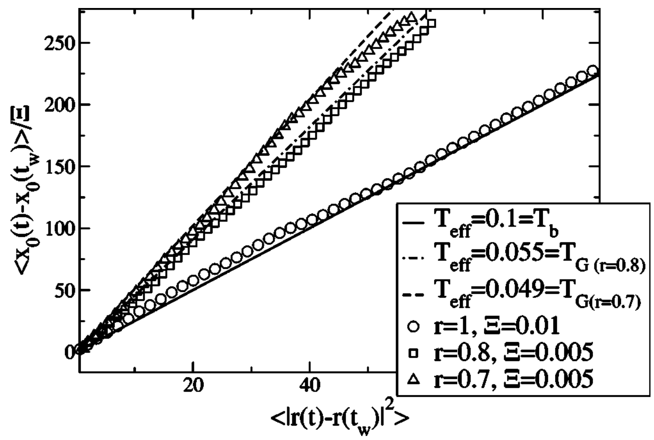


FIG. 6. Parametric plot of $\chi(t,t_w)$ vs $B(t,t_w)$ for the numerical experiment of type II (constant force applied on one particle) with $r=1$, $r=0.8$, and $r=0.7$, with heating bath, and for different choices of the intensity $\Xi$ of the perturbation, using $T_b=0.1$, $\tau_b=10$, $N=500$, $\tau_c=1$, $t_w=100$. The results are obtained by averaging over 10 000 realizations.

Figure 6 reports the parametric plot of the response to the force versus the mean-squared displacement in the unperturbed system, showing how relation (27) is very well satisfied at different inelasticities. Also in this case one could expect a breakdown of FD relation at large inelasticities due to cluster formation (i.e., spatial lack of homogeneity), which is present even in the case of DSMC solutions of Boltzmann equation (see for example Ref. [7]). This hypothesis should deserve a deeper investigation.

It should be noted that the coincidence of the results obtained with the two methods of Secs. IV and V is not obvious in a nonequilibrium context and it should not always be expected.

## VI. CONCLUSIONS

In conclusion, in this paper, we have investigated the validity of Kubo's relations in driven granular gases in two dimensions. We have compared, in particular, two sets of measures. On one hand, we have measured the proportionality factor between the response of the staggered density current to an impulsive shear forcing and its autocorrelation function in the unperturbed system. On the other hand, we have monitored the velocity of a tracer by checking the proportionality between its response to a small constant force, switched on at time $t_w$, and its mean-squared displacement in the unperturbed stationary state.

In both cases, a proportionality is observed, in analogy with the linear response theory for equilibrium dynamics. Furthermore, the proportionality factor in the Kubo formulas is equal to the inverse of th granular temperature (at least for not so small restitution coefficients), which hence plays the role of the equilibrium temperature in the elastic case. It is important to remark how these results are recovered by two completely independent measurement schemes.

Several remarks are in order. First of all, though a granular gas is a nontrivial out-of-equilibrium system, from the point of view of its thermodynamics it exhibits properties, which seem much simpler than the corresponding properties observed in a compacting granular medium. In this case, in fact, apparently no slow modes are present or at least their presence does not give rise to the existence of several effective temperatures depending on the time scales investigated [12]. On the other hand, the proportionality factor, we have found, between response and autocorrelation cannot be considered as a temperature from the point of view of equilibrium thermodynamics since it does not rely on any known statistical ensemble.

Another point to stress concerns the validity of the zeroth principle of thermodynamics. The question that immediately arises could be summarized as follows: if the granular temperature represents the correct temperature from the point of view of the fluctuation-dissipation theorem, should we expect that it rules the thermalization properties of two different granular gases put in contact? As already mentioned, the answer to this question is far from being trivial as witnessed by all recent results obtained on mixtures [25–35], where a lack of equipartition is observed. However, these results (validity of fluctuation-dissipation relations and lack ofequipartition) can coexist simply because heated granular gases have not only a thermal source but also a thermal sink (dissipative collisions) and therefore, any zero principle should be stated in terms of a balance equation among energy fluxes instead of a strict equivalence between temperature of systems in contact.

We again remark that there are also other common ways of driving a granular gas in a stationary state, e.g., stochastic driving without viscosity [8], stochastic restitution coefficient models [10], multiplicative noise models [9], and so on. In some of these models, a more pronounced departure from homogeneity (for example, correlations in the velocity field [8]) and therefore, a breakdown of fluctuation-dissipation relations should be investigated.

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