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Homogeneous States in Granular Fluids Driven by Thermostats

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Abstract. The dynamics of a homogeneous granular gas fluidized by a stochastic bath with friction is analyzed in the context of the Enskog-Boltzmann equation. After a transient regime, the system evolves towards a (scaled) distribution function φ that does not only depend on the dimensionless velocity $\mathbf{c} \equiv \mathbf{v}/v_0(T)$ ($v_0(T)$ being the thermal speed), but also on the (reduced) driven parameters of the model. An approximate expression for φ is constructed by considering the leading order in a Sonine polynomial expansion. The theoretical predictions of the (steady) granular temperature and the fourth cumulant of $\varphi(\mathbf{c})$ are compared with those obtained by numerically solving the Enskog-Boltzmann equation from the direct simulation Monte Carlo (DSMC) method. An excellent agreement between theory and simulation is found, even for quite large values of dissipation.

Keywords: Granular gases, driven homogeneous states, thermostats

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INTRODUCTION

Granular systems are constituted by macroscopic grains that collide inelastically so that the total energy decreases with time. In this context, granular matter can be considered as a prototype system that inherently is in a non-equilibrium state. This is perhaps one of the main reasons why these systems have received considerable attention in the past few years, apart from its practical interest. Under rapid flow conditions (for instance, when the system is externally vibrated), the motion of grains resembles a granular gas where binary collisions prevail and kinetic theory can be a quite useful tool to study these systems. Thus, in order to maintain the granular medium in a fluidized state an external energy input is needed to compensate for the collisional loss of energy and achieve a *steady* nonequilibrium state. In most of the experiments, energy is supplied through the boundaries causing spatial gradients in the system. To avoid the difficulties associated with inhomogeneous states, it is usual in computer simulations to homogeneously heat the system by the action of an external driving force (thermostat). Nevertheless, in spite of its practical importance, little is known about the influence of the external force (or thermostat) on the properties of the system [1, 2].

The goal of this contribution is to analyze the homogeneous steady state of a driven granular fluid described by the Enskog-Boltzmann kinetic equation. In order to reach a steady state, the particles are assumed to be under the action of an external thermostat composed by two different forces: (i) a stochastic force where the particles are randomly kicked between collisions [3] and (ii) a viscous drag force which mimics the interaction of the particles with an effective viscous “bath” at temperature T_b . One of the main advantages of using this kind of thermostat [4] with respect to others present in the literature [3] is that the temperature of the thermostat T_b (different from the temperature $T < T_b$ of the granular fluid) is always well defined. In particular, for elastic collisions, the fluid equilibrates to the bath temperature ($T = T_b$). This happens because, in addition to the random driving, the thermostat acts on the grains also through a finite drag. Moreover, some recent results [5] suggest that this thermostat is the most appropriate to modelize some experiments.

The present study combines two different but complementary routes. First, a scaling solution φ to the Enskog-Boltzmann equation is proposed at the steady state. The new feature is that the scaling form φ involves two parameters (dimensionless velocity $\mathbf{c} \equiv \mathbf{v}/v_0(T)$ and the reduced noise strength ξ^*) and not only one parameter (dimensionless velocity) as in the free cooling case [6]. Although the exact form of this scaling solution is not known (except for elastic collisions), it is expected that φ is close to a Maxwellian distribution. A reasonable strategy is to expand φ in a complete set of polynomials (Sonine polynomials). Since quite accurate results are obtained in the free cooling case [6] by truncation at first order, a similar approximation is considered here to determine the (steady) granular temperature and the fourth cumulant of φ . The latter quantity measures the deviations of the distribution function on its Maxwellian form. As a second route, we have also performed direct Monte Carlo simulations of the Enskog-Boltzmann equation in the homogeneous state driven by the thermostat suggested in Ref. [4]. Different values of the coefficient of restitution

α and the solid volume fraction ϕ have been considered. In the steady state, the comparison between theoretical and computer simulation results for the steady temperature T_s and the fourth cumulant a_2 shows in general an excellent agreement even for very small values of α and/or moderate densities ϕ .

ENSKOG-BOLTZMANN KINETIC THEORY FOR HOMOGENEOUS DRIVEN STATES

We consider a system of inelastic hard spheres in d dimensions with mass m and diameter σ . Collisions are characterized by a (constant) coefficient of normal restitution $0 < \alpha \leq 1$, with $\alpha = 1$ in the elastic limit. In the special case of a spatially uniform state, the Enskog-Boltzmann equation for the velocity distribution function $f(\mathbf{v}, t)$ reads

$$\partial_t f(\mathbf{v}, t) + \mathcal{F}f(\mathbf{v}, t) = J[\mathbf{v}|f(t), f(t)], \quad (1)$$

where the Boltzmann-Enskog collision operator $J[f, f]$ is

$$J[f, f] = \chi \sigma^{d-1} \int d\mathbf{v}_2 \int d\hat{\sigma} \Theta(\hat{\sigma} \cdot \mathbf{v}_{12}) (\hat{\sigma} \cdot \mathbf{v}_{12}) [\alpha^{-2} f(\mathbf{v}'_1) f(\mathbf{v}'_2) - f(\mathbf{v}_1) f(\mathbf{v}_2)]. \quad (2)$$

In Eq. (1), \mathcal{F} is an operator representing the effect of an external force, χ is the pair correlation function at contact, d is the dimensionality of the system, $\hat{\sigma}$ is a unit vector along the line of centers, Θ is the Heaviside step function, and $\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2$ is the relative velocity of the colliding particles. In addition, $(\mathbf{v}'_1, \mathbf{v}'_2)$ are the precollisional velocities yielding $(\mathbf{v}_1, \mathbf{v}_2)$ as the postcollisional ones, i.e., $\mathbf{v}'_{1,2} = \mathbf{v}_{1,2} \mp \frac{1}{2}(1 + \alpha^{-1})(\hat{\sigma} \cdot \mathbf{v}_{12})\hat{\sigma}$. Note that for uniform states, except for the presence of the factor χ (which accounts for the increase of the collision frequency due to excluded volume effects), the collision operator (2) becomes identical to the Boltzmann collision operator.

As mentioned in the Introduction, in order to reach a steady state, energy injection is needed to compensate for the energy dissipated in collisions. At a theoretical level and for *homogeneous* states, it is quite common to introduce external driving forces acting locally on each particle. Borrowing a terminology often used in nonequilibrium molecular dynamics of ordinary fluids [8], this type of external forces are usually called ‘‘thermostats.’’ Here, we will consider the stochastic bath with friction used in Ref. [4] to determine static and dynamical structure factors in driven granular systems. In general, the equation of motion for a particle i with velocity \mathbf{v}_i can be written as

$$m\dot{\mathbf{v}}_i = \mathbf{F}_i^{\text{th}}(t) + \mathbf{F}_i^{\text{coll}}, \quad (3)$$

where \mathbf{F}_i^{th} is the thermostat force and $\mathbf{F}_i^{\text{coll}}$ is the force due to inelastic collisions. In our case, the total external force \mathbf{F}_i^{th} is given by

$$\mathbf{F}_i^{\text{th}}(t) = -\gamma_b \mathbf{v}_i(t) + \mathbf{F}_i^{\text{st}}(t), \quad (4)$$

where γ_b is a drag coefficient that defines the characteristic interaction time with the external bath, $\tau_b^{-1} = \gamma_b/m$. The viscous drag term $-\gamma_b \mathbf{v}_i$ in the total force (4) models the interaction between each particle and the thermostat. Moreover, the stochastic force \mathbf{F}_i^{st} is assumed to have the form of a Gaussian white noise [3]:

$$\langle \mathbf{F}_i^{\text{st}}(t) \rangle = \mathbf{0}, \quad \langle \mathbf{F}_i^{\text{st}}(t) \mathbf{F}_j^{\text{st}}(t') \rangle = \mathbf{1} m^2 \xi_b^2 \delta_{ij} \delta(t - t'), \quad (5)$$

where $\mathbf{1}$ is the $d \times d$ unit matrix and ξ_b^2 represents the strength of the correlation. The forcing term in the Enskog-Boltzmann equation associated to \mathbf{F}_i^{st} is represented by a Fokker-Planck operator [6] of the form $-\frac{1}{2} \xi_b^2 (\partial/\partial \mathbf{v})^2$. The effect of this latter (random) term is to give frequent kicks to each particle between collisions [3].

Under the above conditions, the corresponding operator \mathcal{F} for this kind of thermostat has the form [4]

$$\mathcal{F}f(\mathbf{v}) = -\frac{\gamma_b}{m} \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{v} f(\mathbf{v}) - \frac{1}{2} \xi_b^2 \left(\frac{\partial}{\partial \mathbf{v}} \right)^2 f(\mathbf{v}), \quad (6)$$

and the kinetic equation (1) becomes

$$\partial_t f - \frac{\gamma_b}{m} \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{v} f - \frac{1}{2} \xi_b^2 \left(\frac{\partial}{\partial \mathbf{v}} \right)^2 f = J[f, f]. \quad (7)$$

The balance equation for the granular temperature $T(t)$ can be easily derived by multiplying both sides of Eq. (7) by $\frac{1}{2}mv^2$ and integrating over velocity. The result is

$$\partial_t T = -\frac{2T}{m}\gamma_b + m\xi_b^2 - \zeta T, \quad (8)$$

where

$$\zeta = -\frac{m}{dnT} \int d\mathbf{v} \mathbf{v}^2 J[f, f] \quad (9)$$

is the cooling rate. We are looking for a *normal* solution [2] to Eq. (7). This means that all the time dependence of $f(\mathbf{v})$ only occurs through its functional dependence on $T(t)$:

$$\partial_t f = \frac{\partial f}{\partial T} \partial_t T = -\left(\frac{2\gamma_b}{m} - \frac{m}{T}\xi_b^2 + \zeta\right) T \frac{\partial f}{\partial T}. \quad (10)$$

Substitution of Eq. (10) into Eq. (7) yields

$$-\left(\frac{2}{m}\gamma_b - \frac{m}{T}\xi_b^2 + \zeta\right) T \frac{\partial f}{\partial T} - \frac{\gamma_b}{m} \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{v} f - \frac{1}{2}\xi_b^2 \left(\frac{\partial}{\partial \mathbf{v}}\right)^2 f = J[f, f]. \quad (11)$$

After a transient regime, the system is expected to reach a steady state characterized by a constant temperature. Thus, according to Eq. (8), the (asymptotic) steady granular temperature T_s is given by the relation

$$\zeta T_s + \frac{2\gamma_b}{m} T_s = m\xi_b^2. \quad (12)$$

This equation establishes a relation between the model parameters γ_b and ξ_b^2 so that only one of the above parameters is independent in the steady state. Here, we will take the noise strength ξ_b^2 as the relevant external parameter. By using (12), Eq. (11) becomes

$$\frac{1}{2}\zeta \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{v} f_s - \frac{m\xi_b^2}{2T_s} \frac{\partial}{\partial \mathbf{v}} \cdot \mathbf{v} f_s - \frac{1}{2}\xi_b^2 \left(\frac{\partial}{\partial \mathbf{v}}\right)^2 f_s = J[f_s, f_s], \quad (13)$$

where f_s denotes the stationary distribution function. According to the left hand side of Eq. (13), it is expected that f_s depends on the model parameter ξ_b^2 .

To get a closed equation for T_s , one needs to evaluate the cooling rate ζ which is defined in terms of f_s through Eq. (9). Although the explicit form of f_s is not known so far, dimensional analysis requires that f_s has the scaled form

$$f_s(\mathbf{v}, \xi_b^2) = n v_0^{-d} \varphi(\mathbf{c}, \xi^*), \quad (14)$$

where $\mathbf{c} \equiv \mathbf{v}/v_0$ and $v_0 = \sqrt{2T_s/m}$ is the thermal speed. In addition, we have introduced the reduced model parameter

$$\xi^* = \frac{m\ell}{T_s v_0} \xi_b^2, \quad (15)$$

where $\ell = 1/(n\sigma^{d-1})$ is the mean free path of a dilute gas of hard spheres. It must be noted that the scaled distribution function φ involves two parameters: the dimensionless velocity \mathbf{c} and the (reduced) noise strength ξ^* . This scaling differs from the one assumed in the case of the homogeneous cooling state [6] where only the dimensionless velocity \mathbf{c} is required to characterize the steady state. Equivalent expressions can be of course chosen, such as $\varphi(\mathbf{c}, \gamma^*)$ if one takes $\gamma^* \equiv \gamma\ell/(mv_0)$ instead of ξ^* as the independent model parameter. A similar scaling solution to the form (14) has been recently proposed [7] for a driven homogeneous granular gas before reaching the stationary regime. In terms of the (reduced) distribution function φ , Eq. (13) can be finally rewritten as

$$\frac{1}{2}\zeta^* \frac{\partial}{\partial \mathbf{c}} \cdot \mathbf{c} \varphi - \frac{1}{2}\xi^* \frac{\partial}{\partial \mathbf{c}} \cdot \mathbf{c} \varphi - \frac{1}{4}\xi^* \left(\frac{\partial}{\partial \mathbf{c}}\right)^2 \varphi = J^*[\varphi, \varphi], \quad (16)$$

where

$$\zeta^* = \frac{\ell\zeta}{v_0}, \quad J^* = \frac{\ell}{n} v_0^{d-1} J. \quad (17)$$

STEADY GRANULAR TEMPERATURE AND FOURTH-CUMULANT. THEORETICAL PREDICTIONS

In the case of elastic collisions ($\alpha = 1$), $\zeta^* = 0$ and the solution to Eq. (16) is a Maxwellian distribution

$$\varphi_M(\mathbf{c}) = \pi^{-d/2} e^{-c^2}. \quad (18)$$

However, if the particles collide inelastically ($\alpha < 1$), the exact form of φ is not known. An *indirect* information on the scaled distribution φ is given through its velocity moments. In particular, the deviation of φ with respect to its Maxwellian form φ_M can be characterized by the kurtosis or the fourth-cumulant

$$a_2 = \frac{4}{d(d+2)} \langle c^4 \rangle - 1, \quad (19)$$

where

$$\langle c^k \rangle = \int d\mathbf{c} c^k \varphi(\mathbf{c}). \quad (20)$$

In order to determine a_2 , we multiply both sides of Eq. (16) by c^4 and integrate over velocity. The result is

$$\frac{d(d+2)}{2} [\zeta^* (1+a_2) - \xi^* a_2] = \mu_4, \quad (21)$$

where

$$\mu_k = - \int d\mathbf{c} c^k J^*[\varphi, \varphi]. \quad (22)$$

Upon writing Eq. (21) use has been made of the relation (12) (in its dimensionless form, i.e., $\zeta^* + 2\gamma^* = \xi^*$) and the result

$$\int d\mathbf{c} c^p \left(\frac{\partial}{\partial \mathbf{c}} \right)^2 \varphi(\mathbf{c}) = p(p+d-2) \langle c^{p-2} \rangle \quad (23)$$

with $p = 4$ and $\langle c^2 \rangle = \frac{d}{2}$. Equation (21) is still exact. To get an approximate expression for a_2 one first assumes that φ can be well described by the leading Sonine approximation:

$$\varphi(\mathbf{c}, \xi^*) \simeq \varphi_M(\mathbf{c}) \left\{ 1 + a_2(\xi^*) \left[\frac{1}{2} c^4 - \frac{d+2}{2} c^2 + \frac{d(d+2)}{8} \right] \right\}. \quad (24)$$

The approximation (24) is justified because the coefficient a_2 is expected to be small [6]. Then, approximate forms for the quantities $\zeta^* = (2/d)\mu_2$ and μ_4 can be obtained when one substitutes Eq. (24) into Eq. (22) and neglects nonlinear terms in a_2 . For μ_2 and μ_4 the results are [6]

$$\mu_2 \rightarrow \mu_2^{(0)} + \mu_2^{(1)} a_2, \quad \mu_4 \rightarrow \mu_4^{(0)} + \mu_4^{(1)} a_2, \quad (25)$$

where

$$\mu_2^{(0)} = \frac{\pi^{(d-1)/2}}{\sqrt{2}\Gamma(\frac{d}{2})} \chi(1-\alpha^2), \quad \mu_2^{(1)} = \frac{3}{16} \mu_2^{(0)}, \quad (26)$$

$$\mu_4^{(0)} = \left(d + \frac{3}{2} + \alpha^2 \right) \mu_2^{(0)}, \quad \mu_4^{(1)} = \left[\frac{3}{32} (10d + 39 + 10\alpha^2) + \frac{d-1}{1-\alpha} \right] \mu_2^{(0)}. \quad (27)$$

With the use of the approximations (25)–(27) and retaining only linear terms in a_2 , the solution to Eq. (21) is

$$a_2 = - \frac{\mu_4^{(0)} - (d+2)\mu_2^{(0)}}{\mu_4^{(1)} - (d+2) \left(\frac{19}{16} \mu_2^{(0)} - \frac{d}{2} \xi^* \right)}. \quad (28)$$

In the case $\gamma_b = 0$ (absence of friction), $\xi^* = (2/d)\mu_2^{(0)}$ and Eq. (28) agrees with the results obtained in the presence of the stochastic thermostat (see Eq. (31) of Ref. [9]).

Once the fourth cumulant is known, the steady temperature can be obtained. First, in terms of a_2 , the cooling rate ζ is given by

$$\zeta = \frac{2}{d} \frac{\pi^{(d-1)/2}}{\Gamma(\frac{d}{2})} (1 - \alpha^2) \chi \left(1 + \frac{3}{16} a_2\right) n \sigma^{d-1} \sqrt{\frac{T_s}{m}}. \quad (29)$$

With this result, Eq. (12) for the reduced temperature $T^* \equiv T_s/T_b$ can be finally written as

$$\frac{2^d}{\sqrt{\pi}} (1 - \alpha^2) \phi \chi \left(1 + \frac{3}{16} a_2\right) T^{*3/2} + 2\bar{\gamma}_b T^* = \bar{\xi}_b, \quad (30)$$

where

$$\bar{\gamma}_b \equiv (mT_b)^{-1/2} \sigma \gamma_b, \quad \bar{\xi}_b \equiv \left(\frac{m}{T_b}\right)^{3/2} \sigma \xi_b^2, \quad (31)$$

and

$$\phi = \frac{\pi^{d/2}}{2^{d-1} d \Gamma(\frac{d}{2})} n \sigma^d \quad (32)$$

is the solid volume fraction. In the case of elastic collisions ($\alpha = 1$), Eq. (30) yields $T^* = 1$ if $2\bar{\gamma}_b = \bar{\xi}_b$.

COMPARISON WITH MONTE CARLO SIMULATIONS

The DSMC method devised by Bird [10] has proven to be a very efficient tool to numerically solve the Boltzmann equation. The method has been extended to the Enskog equation [11] and its application to granular gases in spatially uniform states is very straightforward. In the DSMC method the velocities of the particles are updated from time t to time $t + \delta t$ by following two successive stages: free streaming and collisions. Here, the time step δt is much smaller than the mean free time. In the first step, the velocity \mathbf{v}_i of every particle is changed to $\mathbf{v}_i + \mathbf{w}_i$ according to the external force under consideration. As we pointed out in Section , our thermostat is composed by two different terms: a deterministic external force proportional to the velocity of the particle plus a stochastic force. Thus, $\mathbf{w}_i = \mathbf{w}_i^{\text{drag}} + \mathbf{w}_i^{\text{st}}$, where $\mathbf{w}_i^{\text{drag}}$ and \mathbf{w}_i^{st} denote the velocity increments due to the drag and stochastic forces, respectively. In the case of the (deterministic) drag force,

$$\mathbf{w}_i^{\text{drag}} = \left(1 - e^{\gamma_b \delta t}\right) \mathbf{v}_i, \quad (33)$$

while \mathbf{w}_i^{st} is randomly drawn from the Gaussian probability distribution [9]

$$P(\mathbf{w}) = (2\pi\xi_b^2\delta t)^{-d/2} e^{-\mathbf{w}^2/2\xi_b^2\delta t}. \quad (34)$$

The second step accounts for the collisions among particles. In this stage, a sample of pairs is chosen at random with equiprobability. For each pair ij , the probability of collisions between particles i and j is proportional to the relative velocity between both colliding particles. More details on this stage can be found in Ref. [9]. In our simulations we have typically taken $N = 2 \times 10^6$ simulated particles and a time step $\delta t = 0.005v^{-1}$, where $v = (\sqrt{2}\pi\chi n\sigma^2)^{-1}/v_0$ for hard spheres.

In the following we present a comparison between the DSMC and theoretical results. Here, for the sake of convenience, we introduce the dimensionless quantities (γ_{sim}^* and β_{sim}^*) which are related with the theoretical ones ($\bar{\gamma}_b$ and $\bar{\xi}_b$) as

$$\gamma_{sim}^* = \frac{\gamma_b}{m} v^{-1}(T_b) = \frac{1}{\sqrt{2}\pi\chi(\phi)} \frac{\ell}{v_0(T_b)} \frac{\gamma_b}{m} = \frac{\bar{\gamma}_b}{2\pi\chi(\phi)}, \quad (35)$$

$$\beta_{sim}^* = \xi_b^2 \left[\frac{2T_b}{m} v(T_s)\right]^{-1} = \frac{\bar{\xi}_b}{4\pi\chi(\phi)T^{*1/2}}. \quad (36)$$

Following Ref. [4], the fixed parameters of the simulations are $m = 1$, $\sigma = 0.01$, $T_b = 1$, $\gamma_b = 1$, and $\bar{\xi}_b = 2\bar{\gamma}_b$, and so, $\gamma_{sim}^* = \sigma/(12\phi\chi)$ and $\beta_{sim}^* = \gamma_{sim}^* T^{*-1/2}$. A good approximation for the pair correlation function for spheres is [12]

$$\chi(\phi) = \frac{1 - \frac{1}{2}\phi}{1 - \phi^3}, \quad (37)$$

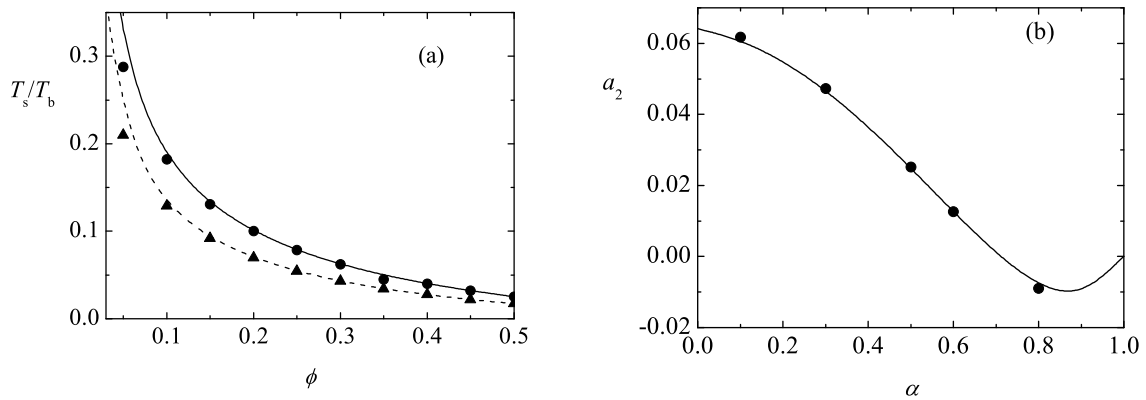


FIGURE 1. Panel (a): Plot of the reduced granular temperature T_s/T_b versus the solid volume fraction ϕ for two values of the coefficient of restitution α : $\alpha = 0.8$ (solid line) and $\alpha = 0.6$ (dashed line). The symbols are Monte Carlo simulations for $\alpha = 0.8$ (circles) and $\alpha = 0.6$ (triangles). Panel (b): Plot of the fourth cumulant a_2 versus the coefficient of restitution α for $\phi = 0.25$. The line is the theoretical result and the symbols are the computer simulation results .

where $\phi = n\pi\sigma^3/6$ for $d = 3$. The panel (a) of Fig. 1 shows the (reduced) granular temperature T_s/T_b versus the volume fraction ϕ , respectively, for two different values of the coefficient of restitution ($\alpha = 0.8$ and $\alpha = 0.6$). We observe an excellent agreement between theory and simulation. As expected, at a given value of density, the steady granular temperature decreases as the gas becomes more inelastic. The dependence of the fourth cumulant a_2 on α is shown in the panel (b) of Fig. 1 for $\phi = 0.25$. The theoretical prediction (28) compares very well with simulation data, even for quite extreme values of dissipation (say for instance, $\alpha = 0.1$). This agreement justifies the approximations (25)–(27) and indicates that the scaled distribution φ is well represented by Eq. (24) in the region of thermal velocities. Moreover, the values of a_2 in the driven case are generally smaller than in the free cooling case [6, 9].

In summary, we have studied the dynamics of a granular fluid driven homogeneously by a stochastic bath with friction. The results have been obtained from the Enskog-Boltzmann equation in the stationary regime. In this regime, the system evolves into a scaling solution φ characterized by two dimensionless parameters: the dimensionless velocity and the reduced noise strength. The distribution function φ has been calculated in the first Sonine approximation and the results derived from it show an excellent agreement with the Monte Carlo simulations. The results derived in this contribution can be used as the starting point to derive the Navier-Stokes transport coefficients of a granular fluid driven by a stochastic bath with friction. They will be further studied in future works.

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