

Size-polydisperse dust in molecular gas: Energy equipartition versus nonequipartition

Alexander Osinsky ¹, Anna S. Bodrova ^{2,3,4} and Nikolai V. Brilliantov¹

¹*Skolkovo Institute of Science and Technology, 121205, Moscow, Russia*

²*Moscow Institute of Electronics and Mathematics, National Research University Higher School of Economics, 123458 Moscow, Russia*

³*Department of Physics, Humboldt University, 12489 Berlin, Germany*

⁴*Faculty of Physics, M. V. Lomonosov Moscow State University, 119991 Moscow, Russia*



(Received 15 August 2019; accepted 24 January 2020; published 19 February 2020)

We investigate numerically and analytically size-polydisperse granular mixtures immersed into a molecular gas. We show that the equipartition of granular temperatures of particles of different sizes is established; however, the granular temperatures significantly differ from the temperature of the molecular gas. This result is surprising since, generally, the energy equipartition is strongly violated in driven granular mixtures. Qualitatively, the obtained results do not depend on the collision model, being valid for a constant restitution coefficient ε , as well as for the ε for viscoelastic particles. Our findings may be important for astrophysical applications, such as protoplanetary disks, interstellar dust clouds, and comets.

DOI: [10.1103/PhysRevE.101.022903](https://doi.org/10.1103/PhysRevE.101.022903)

I. INTRODUCTION

What is common between very different objects, such as interstellar dust, protoplanetary discs [1–3], comets [4], and dust devils on Mars [5], Earth [6], and possibly other planets? All these systems are made up of size and mass polydisperse dust particles immersed in molecular gas. Interstellar molecular clouds possess high-density regions, so-called clumps. The density of matter there is large enough to trigger a gravitational collapse, which eventually leads to the formation of stars. In the present study, we assume that the density of matter is below this threshold. Moreover, we assume that the granular gas is rarefied, so that the surrounding molecular gas may be treated as a thermostat which is not affected by the granular gas.

The dust particles addressed here are macroscopic, but small enough grains, so that the gravitational interactions between the grains may be neglected. Hence, we have a granular mixture, driven by the molecular gas. Usually, in granular mixtures, the energy equipartition between particles of different sizes is violated. This has been predicted theoretically [7–11] and confirmed in experiments [12,13] and computer simulations [11,14,15]. The same is true for such natural systems as Saturn’s rings, which are essentially granular gas mixtures of particles with a size ranging from 10^{-3} to 1 m [16,17]. The size polydispersity of the rings’ particles stems from the permanent aggregation and fragmentation of the constituents, which keeps the steady-state size distribution [17,18]. The energy equipartition for the rings’ particles does not hold as shown theoretically [19,20] and in computer experiments [21].

Let a granular mixture contain N different sorts of particles, of mass m_k and diameter σ_k with $k = 1, \dots, N$. We assume that the particles are uniform spheres with the mass density of the material ρ , then $m_k = \pi \sigma_k^3 \rho / 6$. Without the loss of generality we assume that all masses are multiples of some minimal mass m_1 , that is, $m_k = km_1$. Let the number

density of particles of mass m_k be equal to n_k . We consider a space uniform system, so that the particles of mass m_k may be characterized by the velocity distribution function $f(\mathbf{v}_k, t)$. It quantifies the number of such particles with velocity \mathbf{v}_k at time t in a unit volume. The number density may be expressed in terms of the distribution function as $n_k = \int d\mathbf{v}_k f(\mathbf{v}_k, t)$. The average energy of particles of mass m_k is characterized by the corresponding granular temperature, T_k , defined as [7,10]

$$\frac{3}{2} n_k T_k = \int d\mathbf{v}_k f(\mathbf{v}_k) \frac{m_k v_k^2}{2}. \quad (1)$$

If all interparticle collisions were elastic, the energy equipartition between all sorts of the particles would hold. The violation of equipartition stems from the dissipative nature of interparticle collisions, which are quantified by the restitution coefficient ε [7],

$$\varepsilon = \left| \frac{(\mathbf{v}'_{ki} \cdot \mathbf{e})}{(\mathbf{v}_{ki} \cdot \mathbf{e})} \right|, \quad (2)$$

where $\mathbf{v}'_{ki} = \mathbf{v}'_k - \mathbf{v}'_i$ and $\mathbf{v}_{ki} = \mathbf{v}_k - \mathbf{v}_i$ are the relative velocities of two particles after and before a collision, correspondingly, and \mathbf{e} is a unit vector connecting their centers at the collision instant. We do not consider very soft particles where the definition of the restitution coefficient is more subtle [22]. The postcollision velocities are related to the precollision velocities \mathbf{v}_k and \mathbf{v}_i as follows [7]:

$$\mathbf{v}'_{k/i} = \mathbf{v}_{k/i} + \frac{m_{\text{eff}}}{m_{k/i}} (1 + \varepsilon) (\mathbf{v}_{ki} \cdot \mathbf{e}) \mathbf{e}. \quad (3)$$

Here $m_{\text{eff}} = m_k m_i / (m_k + m_i)$ is the effective mass of the colliding particles. To date, most studies of granular gases have been focused on the case of a constant restitution coefficient [23–31]. This assumption contradicts, however, experimental observations [32–34], along with basic mechanical laws [35,36], which indicate that ε does depend on the impact velocity [34,35,37–39]. This dependence may be obtained by

solving the equations of motion for colliding particles with the explicit account for the dissipative forces acting between the grains. The simplest first-principle model of inelastic collisions assumes viscoelastic properties of particles' material, which results in viscoelastic interparticle force [37] and finally in the restitution coefficient [35,39,40]:

$$\varepsilon_{ki} = 1 + \sum_{j=1}^{20} h_j (A \kappa_{ki}^{2/5})^{j/2} |(\mathbf{v}_{ki} \cdot \mathbf{e})|^{j/10}. \quad (4)$$

Here h_k are numerical coefficients [40]. The elastic constant

$$\kappa_{ki} = \frac{\kappa}{\sqrt{2}} \frac{k+i}{k^{5/6} i^{5/6} \sqrt{k^{1/3} + i^{1/3}}}, \quad (5)$$

where

$$\kappa = \left(\frac{3}{2}\right)^{3/2} \frac{Y}{1-\nu^2} \left(\frac{6}{\pi \rho m_1^2}\right)^{1/3} \quad (6)$$

is a function of the Young's modulus Y and Poisson ratio ν ; the constant A quantifies the viscous properties of the particles' material [41,42]:

$$A = \frac{1}{Y} \frac{(1+\nu)}{(1-\nu)} \left[\frac{4}{3} \eta_1 (1-\nu+\nu^2) + \eta_2 (1-2\nu)^2 \right], \quad (7)$$

where η_1 and η_2 are the viscosity coefficients.

Recently we have shown that the distribution of granular temperatures in polydisperse mixtures of granular particles follows the power law $T_k = T_1 k^\alpha$, if the size distribution in a mixture is steep enough [43]. The exponent α is universal for all steep size distributions for force-free granular mixtures. For driven granular mixtures, α strongly depends on the agitation mode, in particular on the dependence of the driving force on the particle size. In the current study, we investigate the distribution of temperatures in a mixture of granular particles immersed into a molecular gas. We assume that the particles are very small, similar to, but smaller than, the dust particles in sand devils, tornados on Earth, interstellar dust, comets, and protoplanetary disks. In this case, the presence of a molecular gas becomes important. Moreover, we assume that the action of the molecular gas on the granular mixture keeps it in a steady state.

The adhesion contact forces play an important role for small particles, and they can aggregate at collisions, forming clusters. When such clusters collide at high impact speeds they can break into smaller pieces. If a steady state may be supported, these two processes are balanced resulting in a steady distribution of aggregates size [17]. In the present study we limit ourselves to the range of parameters where aggregative (and respectively disruptive) collisions may be neglected. The analysis of the conditions when the dust particles undergo only bouncing collisions is given below.

We analyze both models of the restitution coefficient: the simplified model of a constant ε , as well as the realistic, first-principle model of visco-elastic particles. In each case, we obtain qualitatively the same and somewhat unexpected result: the energy equipartition for the different granular species, along with the strong violation of the equipartition between the granular mixture and molecular gas. It looks surprising since, generally, a strong violation of the energy equipartition in a driven granular mixture is expected [43].

Our theoretical predictions have been checked by numerical simulations. Namely, we performed direct simulation Monte Carlo (DSMC) and confirmed the analytical findings. Interestingly, our conclusion supports a conjecture of the energy equipartition in a granular mixture, immersed in molecular gas, proposed in Ref. [44]. The rest of the study is organized as follows. In the next section, Sec. II, we specify the model and derive the granular temperatures for all species, which is done for both models of the restitution coefficient. In Sec. III we discuss the details of the numerical simulations and compare the numerical and analytical results. Finally, in Sec. IV we discuss the application of our theory and summarize our findings.

II. TEMPERATURE DISTRIBUTION IN A GRANULAR MIXTURE

We consider a granular mixture, comprising N species of mass $m_k = k m_1$ immersed in a molecular gas with temperature T_g and molecular mass m_g (see Fig. 1). Although being small, the dust particles are still much heavier than the gas molecules, that is, $m_g \ll m_1$. The collisions between the granular particles and gas molecules are elastic. Since the velocity distribution functions are close to Maxwellian distributions [7], we assume for simplicity that $f_k(\mathbf{v}_k, t)$ are Maxwellian:

$$f_k(\mathbf{v}) = \frac{n_k}{\pi^{3/2}} \exp\left(-\frac{v_k^2}{v_{0,k}^2}\right), \quad (8)$$

where $v_{0,k} = (2T_k/m_k)^{1/2}$ is the thermal velocity of particles of mass m_k . The distribution functions evolve according to the Boltzmann equation [7]

$$\frac{\partial}{\partial t} f_k(\mathbf{v}_k, t) = I_k^{\text{coll}} + I_k^{\text{m.g.}} \quad (9)$$

In Eq. (9) I_k^{coll} is the Boltzmann collision integral [7]

$$I_k^{\text{coll}} = \sum_{i=1}^N \sigma_{ki}^2 \int d\mathbf{v}_i \int d\mathbf{e} \Theta(-\mathbf{v}_{ki} \cdot \mathbf{e}) |\mathbf{v}_{ki} \cdot \mathbf{e}| \times [\chi f_k(\mathbf{v}_k'', t) f_i(\mathbf{v}_i'', t) - f_k(\mathbf{v}_k, t) f_i(\mathbf{v}_i, t)], \quad (10)$$

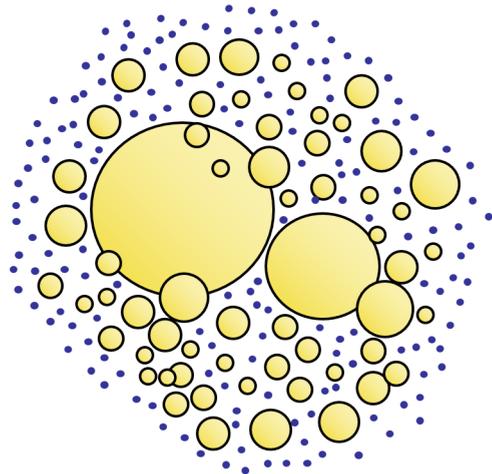


FIG. 1. The granular particles of different masses m_k (depicted with yellow circles) are immersed into a molecular gas composed of molecules of mass $m_g \ll m_k$ (shown as small blue circles).

where $\sigma_{ki} = (\sigma_k + \sigma_i)/2$, with $\sigma_k = [6m_k/(\pi\rho)]^{1/3}$. The summation is performed over all species in the system. \mathbf{v}_k'' and \mathbf{v}_i'' are precollision velocities in the so-called inverse collision, resulting in the postcollision velocities \mathbf{v}_k and \mathbf{v}_i . The Heaviside step function $\Theta(-\mathbf{v}_{ki} \cdot \mathbf{e})$ selects the approaching particles, and the factor χ equals the product of the Jacobian of the transformation $(\mathbf{v}_k'', \mathbf{v}_i'') \rightarrow (\mathbf{v}_k, \mathbf{v}_i)$ and the ratio of the lengths of the collision cylinders of the inverse and the direct collisions [7]. In the case of a constant restitution coefficient $\chi = 1/\varepsilon^2$. For viscoelastic particles it has a more complicated form [7]; in what follows we do not need its explicit expression.

The second term $I_k^{\text{m.g.}}$ describes the driving of the system due to collisions with the surrounding molecular gas. It quantifies the energy injection into the granular mixture to compensate for its losses in dissipative collisions. Since the mass ratio of the gas and grain particles m_g/m_k is very small, the collision integral may be written using the Kramers-Moyal expansion [7]

$$I_k^{\text{m.g.}} = \frac{\partial}{\partial \mathbf{v}_k} \left(\gamma_k \mathbf{v}_k + \bar{\gamma}_k \frac{\partial}{\partial \mathbf{v}_k} \right) f_k(\mathbf{v}_k, t). \quad (11)$$

We investigate the evolution of granular temperatures, defined by Eq. (1). Multiplying the Boltzmann equation (9) by $m_k v_k^2/2$ for $k = 1, \dots, N$ and performing integration over \mathbf{v}_k , we get the following system of equations for evolution of the granular temperatures T_k of species of different masses m_k :

$$\begin{cases} \frac{d}{dt} T_1 = -T_1 \sum_{i=1}^N \xi_{1i} + 2\gamma_1(T_g - T_1) \\ \dots \\ \frac{d}{dt} T_k = -T_k \sum_{i=1}^N \xi_{ki} + 2\gamma_k(T_g - T_k) \\ \dots \\ \frac{d}{dt} T_N = -T_N \sum_{i=1}^N \xi_{Ni} + 2\gamma_N(T_g - T_N) \end{cases}. \quad (12)$$

Here $\gamma_k = \gamma_{0k} \sqrt{T_g}$, $\gamma_{0k} = \frac{4}{3} n_g \sigma_k^2 \sqrt{2\pi m_g/m_k}$, and $\bar{\gamma}_k = \gamma_k T_g/m_k$ [7,44]. The cooling rates ξ_{ki} describe the decrease of temperature of the species of mass m_k due to collisions with the species of mass m_i . For the case of a constant restitution coefficient these quantities read [43]

$$\begin{aligned} \xi_{ki}(t) &= \frac{8}{3} \sqrt{2\pi} n_i \sigma_{ki}^2 \left(\frac{T_k m_i + T_i m_k}{m_i m_k} \right)^{1/2} (1 + \varepsilon) \\ &\times \left(\frac{m_i}{m_i + m_k} \right) \left[1 - \frac{1}{2} (1 + \varepsilon) \frac{T_i m_k + T_k m_i}{T_k (m_i + m_k)} \right]. \end{aligned} \quad (13)$$

We assume that the restitution coefficient ε is the same for the collisions of particles of all sizes. In the case of viscoelastic particles the cooling rates have the form [45]

$$\begin{aligned} \xi_{ki}(t) &= \frac{16}{3} \sqrt{2\pi} n_i \sigma_{ki}^2 \left(\frac{T_k m_i + T_i m_k}{m_i m_k} \right)^{1/2} \left(\frac{m_i}{m_i + m_k} \right) \\ &\times \left\{ 1 - \frac{T_k m_i + T_i m_k}{T_k (m_i + m_k)} \right. \\ &\left. + \sum_{n=2}^{20} B_n \left[h_n - \frac{1}{2} \frac{T_k m_i + T_i m_k}{T_k (m_i + m_k)} A_n \right] \right\}, \end{aligned} \quad (14)$$

where $A_n = 4h_n + \sum_{j+k=n} h_j h_k$ are pure numbers and

$$B_n(t) = (A \kappa_{ki}^{2/5})^{\frac{n}{20}} \left(\frac{2T_k}{m_k} + \frac{2T_i}{m_i} \right)^{\frac{n}{20}} \left[\frac{(20+n)n}{800} \right] \Gamma\left(\frac{n}{20}\right) \quad (15)$$

with $\Gamma(x)$ being the Γ function. Driven granular systems rapidly settle into a nonequilibrium steady state and all granular temperatures attain, after some time constant values, so that $dT_k/dt = 0$. The system of equations (12) turns then into a set of algebraic equations,

$$T_k \sum_{i=1}^N \xi_{ki} = 2\gamma_k(T_g - T_k). \quad (16)$$

Let us assume that the size distribution of the dust particles is steep enough and the number density of the granular mixture scales according to the power law, $n_k = n_1 k^{-\theta}$, with $\theta > 2$. Let the distribution of granular temperatures also scale according to the power law: $T_k = T_1 k^\alpha$. Then the following approximate relation holds [43]:

$$\sum_{i=1}^N \xi_{ki} \sim \begin{cases} k^{\frac{\alpha}{2} - \frac{5}{6}} \int_1^N n_i di & \text{if } \alpha \geq 1 \\ k^{-\frac{1}{3}} \int_1^N i^{\frac{\alpha+1}{2}} n_i di & \text{if } 0 < \alpha < 1 \end{cases}. \quad (17)$$

Substituting Eq. (17) into Eq. (16) and taking into account that $\gamma_k = \gamma_1 k^{-1/3}$, we conclude that the system (17) is compatible only for $\alpha = 0$. This immediately implies the equality of the granular temperatures, $T_k = T_1$, that is, the energy equipartition, and justification of the conjecture of Ref. [44].

We present the sum over the cooling rates in the form

$$\sum_{i=1}^N \xi_{ki} = \sqrt{T_1} \xi_{0k}, \quad (18)$$

where for a constant restitution coefficient:

$$\begin{aligned} \xi_{0k} &= \sum_{i=1}^N \frac{8}{3} \sqrt{2\pi} n_i \sigma_{ki}^2 (1 + \varepsilon) \sqrt{\frac{m_i}{m_k(m_i + m_k)}} \\ &\times \left[1 - \frac{1}{2} (1 + \varepsilon) \right] \end{aligned} \quad (19)$$

and for viscoelastic particles:

$$\begin{aligned} \xi_{0k} &= \sum_{i=1}^N \frac{16}{3} \sqrt{2\pi} n_i \sigma_{ki}^2 \sqrt{\frac{m_i}{m_k(m_i + m_k)}} \\ &\times \sum_{n=2}^{20} B_n \left(\frac{1}{2} \sum_{j+k=n} h_j h_k - h_n \right), \end{aligned} \quad (20)$$

where the coefficients $B_n(t)$ given by Eq. (15) now take the form

$$\begin{aligned} B_n(t) &= (A \kappa_{ki}^{2/5})^{\frac{n}{20}} (2T_1)^{\frac{n}{20}} \left(\frac{m_i + m_k}{m_i m_k} \right)^{\frac{n}{20}} \\ &\times \left[\frac{(20+n)n}{800} \right] \Gamma\left(\frac{n}{20}\right). \end{aligned}$$

The granular temperature of the smallest particles (monomers) T_1 can be found from the equation

$$T_1 \sqrt{T_1} + b \sqrt{T_g} T_1 - b \sqrt{T_g} T_g = 0, \quad (21)$$

where we introduce the notation, $b = 2\gamma_{01}/\xi_{01}$. The quantity b is a function of T_1 for granular particles, colliding with velocity-dependent restitution coefficient, $b = b(T_1)$, so that Eq. (21) is a transcendental equation. However, for the case of a constant restitution coefficient b is constant. Introducing $x = \sqrt{T_1/T_g}$, we recast Eq. (21) in a cubic equation:

$$x^3 + bx^2 - b = 0, \quad (22)$$

with the solution in the form

$$x = \frac{1}{3} \left(-b + zb^2 + \frac{1}{z} \right), \quad (23)$$

where $z = 2^{1/3}(27b - 2b^3 + 3\sqrt{3}\sqrt{27b^2 - 4b^4})^{-1/3}$. This yields the explicit expression for temperatures of granular particles, colliding with constant restitution coefficient, in terms of the molecular gas temperature T_g :

$$T_k = T_1 = B T_g, \quad (24)$$

$$B = \frac{1}{9} \left(-b + zb^2 + \frac{1}{z} \right)^2.$$

It may be shown that $T_k = T_1$ is always smaller than T_g , which also follows from the physical nature of these quantities.

For viscoelastic granular mixture $T_k = T_1$ may be found from the numerical solution of Eq. (21), where the dependence of b on T_1 is to be taken into account. In both cases of constant ε , as well as for ε for viscoelastic particles, the energy equipartition for all granular species is observed. At the same time, the granular temperature significantly differs from the temperature of the molecular gas, $T_k > T_g$. Physically this implies a steady energy flux from the molecular gas to the granular mixture, which permanently loses energy in dissipative collisions.

III. COMPUTER SIMULATION AND SIMULATION RESULTS

To check the prediction of our theory, we perform direct simulation Monte Carlo (DSMC), modified for the application to multispecies systems. The detailed description of the DSMC may be found elsewhere; see, e.g., Ref. [46]. Here we briefly sketch some detail of the simulation method, with the focus on the implementation of the thermostat; see also Refs. [47,48].

We used $N_1 = 3 \times 10^8$ particles of minimal mass m_1 (monomers), so that there were $N_k = \lfloor N_1/k^3 \rfloor = \lfloor 3 \times 10^8/k^3 \rfloor$ particles of mass m_k (k -mers). Initially, the speeds of the particles are generated according to Maxwell distribution for $T = 1$. Therefore, each particle i is associated with its own mass m_i and speed \mathbf{v}_i . Then the speeds change during the collisions and interaction with the molecular gas. The temperatures (determined by particles' kinetic energies) are measured after the system reaches a steady state. Numerically it can be determined by the time when the calculated temperatures stop changing monotonously.

The simulation of collisions between granular particles has been performed according to the following scheme:

(1) Choose the sizes of colliding particles i and k .

(2) Choose the particles with speeds \mathbf{v}_i and \mathbf{v}_k with the probability, proportional to $|\mathbf{v}_i - \mathbf{v}_k| \cdot \mathbf{e}$, where \mathbf{e} is the collision direction (a random unit vector).

(3) Update the speeds of the colliding particles according to the collision rules.

While the particles' collisions are calculated one by one, interaction with molecular gas is performed simultaneously for all particles. We will describe it later in this section. For now, let us briefly go through each step.

1. The sizes of the colliding particles can be determined with the help of the upper bounds on the collision rates C_{ik}

$$C_{ik} = \text{const} N_i N_k \sigma_{ik} (|v_i|_{\max} + |v_k|_{\max}),$$

where $\sigma_{ik} = \left(\frac{\sigma_i + \sigma_k}{2}\right)^2 \sim (i^{1/3} + k^{1/3})^2$ is the collision cross section. Sizes i and k are selected with probability

$$p_{ik} = C_{ik} / \sum_{i,k=1}^M C_{ik},$$

where M is the maximum particle mass in the system.

2. After the sizes are determined, two particles j and l , corresponding to masses i and k , are selected at random. Let us denote their speeds by v_i^j and v_k^l . Then the collision is accepted if

$$|\mathbf{e}(\mathbf{v}_i^j - \mathbf{v}_k^l)| > \text{rand}[0, 1)(|v_i|_{\max} + |v_k|_{\max}),$$

where \mathbf{e} is a random unit vector. Otherwise nothing happens and we choose the sizes again.

3. In case the collision is accepted, postcollision velocities are calculated, like in Eq. (3), with the appropriately defined restitution coefficient.

The action of the molecular gas is described by the term $I_k^{\text{m.g.}}$ of the Boltzmann equation (9). Obviously, this term plays the role of a thermostat. In the lack of collisions between dust particles, the equation for the distribution function reads

$$\frac{\partial f(\mathbf{v}_k, \mathbf{t})}{\partial t} = I_k^{\text{m.g.}}. \quad (25)$$

This equation, with $I_k^{\text{m.g.}}$ given by Eq. (11) is a Fokker-Planck equation, which corresponds to the Langevin equation (see, e.g., Ref. [7]):

$$\frac{d\mathbf{v}_k}{dt} = -\gamma_k \mathbf{v}_k + \mathbf{F}_k^{\text{st}}, \quad (26)$$

$$\langle \mathbf{F}_k^{\text{st}} \rangle = 0, \quad \langle \mathbf{F}_k^{\text{st}}(t) \mathbf{F}_k^{\text{st}}(t') \rangle = \frac{2}{3} \hat{\mathbf{1}} \tilde{\gamma}_k \delta(t - t'), \quad (27)$$

where $\hat{\mathbf{1}}$ is the unit matrix and a direct (dyadic) product is implied in the second part of Eq. (27). The solution of the stochastic Langevin equation may be written as

$$\mathbf{v}_k(t + \Delta t) = \mathbf{v}_k(t) e^{-\gamma_k \Delta t} + \xi \mathbf{e} \cdot \sqrt{3 \frac{T_g}{m_k} (1 - e^{-2\gamma_k \Delta t})},$$

$$\xi \sim \mathcal{N}(0, 1), \quad (28)$$

where $\mathcal{N}(0, 1)$ denotes the normal distribution with zero mean and unit variance.

Numerically the thermostat is implemented by changing the speeds according to Eq. (28). Value of ξ and random direction \mathbf{e} are calculated independently for each particle of size k . The chosen time interval Δt corresponds to the time

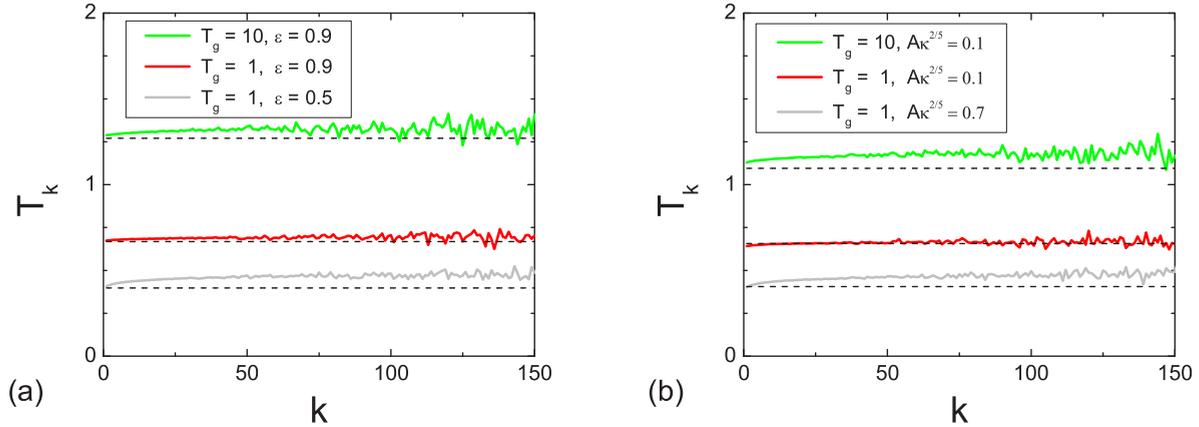


FIG. 2. Granular temperatures T_k of granular particles of mass m_k immersed into a molecular gas of temperature T_g . The granular particles collide with (a) constant restitution coefficient and (b) viscoelastic restitution coefficient. The parameter values are $\sigma_1 = 1$, $m_1 = 1$, $\gamma_{01} = T_g^{-3/2}/2$, $n_k = n_1 k^{-\theta}$ with $n_1 = 1$ and $\theta = 3$. Colored solid lines show simulation results, dashed black lines the analytical results for T_1 [Eq. (24)] for $\varepsilon = \text{const}$ and numerical solution of Eq. (21) for viscoelastic particles. One can clearly see that the temperature distribution in a granular mixture for both cases is close to the equipartition, $T_k \simeq T_1$. There is no energy equipartition between the granular mixture and molecular gas, $T_k < T_g$, since a permanent energy flux from the gas to the mixture supports the steady state.

of Nh collisions, where N is the total number of particles. $h = 0.1$ is a parameter, which should be sufficiently small, to guarantee that each particle experiences several times the action of the thermostat between collisions with other granular particles.

The distribution of granular temperatures T_k , obtained by DSMC for different values of temperature of a molecular gas T_g and restitution coefficient ε is given in Fig. 2. Figure 2(a) corresponds to a constant restitution coefficient, and in Fig. 2(b) the distribution of granular temperatures in a mixture of viscoelastic particles is shown for the steep size distribution $n_k \sim k^{-\theta}$ with $\theta > 2$. The granular temperatures rapidly tend to a steady-state value, where the equipartition in a granular mixture is practically established: $T_k \approx T_1$ for any k . The temperatures of the granular particles T_k differ, however, from the temperature of the molecular gas, $T_k < T_g$, as is predicted by the theory and expected from simple “physical” arguments of the heat flux from the molecular gas to the granular mixture. The smaller the value of the restitution coefficient, the larger the difference between temperatures of the gas and the mixture. For $\varepsilon = 1$ both temperatures become equal and full equipartition is established: $T_k = T_g$. Strictly speaking, the “true” equipartition should follow for $k \gg 1$, as Eq. (17) is valid in this case. In practice, it is observed already for $k > 10$. For other size distributions, e.g., for a flat distribution, $n_k = n_1 \Theta(k_{\max} - k)$, the DSMC also shows constant distribution of temperature, $T_k \approx T_1$ (see Fig. 3).

IV. RESULTS AND DISCUSSION

We investigate numerically and theoretically a size-polydisperse granular gas mixture immersed into a molecular gas. We assume that the molecular gas with temperature T_g is not affected by the granular gas and plays the role of a thermostat. The mixture comprises N different species of masses m_k ($k = 1, \dots, N$). We consider two models of dissipative collisions: a simplified model of a constant restitution coefficient, $\varepsilon = \text{const}$ and a realistic model of viscoelastic

particles, where the restitution coefficient depends on the relative velocities of colliding particles and their masses and sizes. For both models, we observe qualitatively similar behavior: the granular mixture rapidly relaxes to a steady state where granular temperatures of all species become equal, $T_k = T_1$ for all $k = 1, \dots, N$, that is, the energy equipartition is observed. At the same time, the granular temperatures are not equal to the temperature of the molecular gas, $T_k < T_g$. This may be explained by the permanent energy flux from the molecular gas to the granular mixture in the steady state, which compensates the energy losses in dissipative collisions of the grains.

This effect resembles in some respects the experiments of 2D granular gas on a vertically vibrating substrate [49,50]. Here the difference between the “vertical” temperature T_v and horizontal temperature T_h is observed, $T_v > T_g$. The energy is injected into the vertical motion (analogy of the molecular gas) and is converted, though collisions, into the lateral motion (analogy of the dust motion in our system). Since the energy

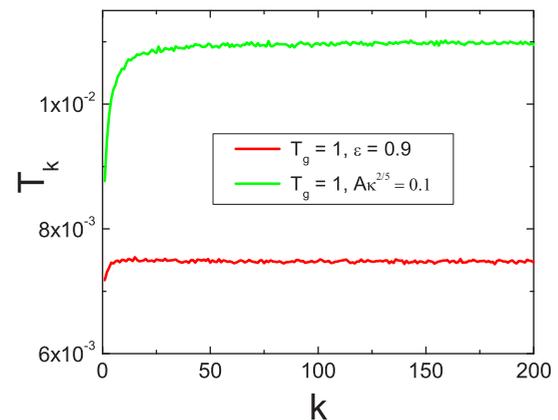


FIG. 3. The temperature distribution for the granular mixture with flat size distribution, $n_k = n_1 \Theta(k_{\max} - k)$, immersed into a molecular gas of temperature T_g .

of the lateral motion is dissipated more intensively than the energy of the vertical motion, which is also pumped by the vibrations, the energy equipartition breaks, that is, $T_v > T_g$.

In our study we neglect the processes of collisional aggregation and fragmentation, assuming that only bouncing collisions take place. Let us estimate the range of parameters, where the conditions of purely bouncing collisions are fulfilled. We assume that sticking collisions occur due to the adhesive interactions of the dust particles at a contact. The critical velocity, demarcating bouncing and sticking collisions, has been reported in a number of studies; see, e.g., Refs. [18,51–53]. It is defined by the work against the adhesive forces W_{ad} , for which we use the explicit expression of Ref. [51]:

$$W_{\text{ad}} = q_0 (\pi^5 \chi^5 R_{\text{eff}}^4 D^2)^{1/3}, \quad (29)$$

where $q_0 = 0.09$ is a pure number, χ is the surface tension, $R_{\text{eff}} = R_1 R_2 / (R_1 + R_2)$, and $D = (3/2)(1 - \nu^2)/Y$ (as previously, ν and Y are the Poisson ratio and the Young modulus, respectively). The condition of bouncing collisions reads

$$T_1 = B k_B T_g > W_{\text{ad}}, \quad (30)$$

where k_B is the Boltzmann constant (the temperature of the gas is in conventional units) and the quantity $B = B(b)$ is defined in Eq. (25). From the definition of $b = 2\gamma_{01}/\xi_{01}$ and Eqs. (22) and (23) follows that $B \sim 1$ for $b \sim 1$ and generally $B \sim b$. Moreover, $b \sim (n_g/n_1)\sqrt{m_g/m_1}$.

Consider some typical quantities for a protoplanetary disk [54] (see also Refs. [55–57]). It contains the molecular gas CO of molecular mass 40 g/mole and dust with size (radius) ranging from 5×10^{-3} to $10 \mu\text{m}$ [54]. We will use the following data for the material parameters of the dust particles [58–60]: $Y = 1\text{--}3 \text{ GP}$, $\rho = 1\text{--}3 \times 10^3 \text{ kg/m}^3$, $\nu = 0.25$, and $\chi = 0.002\text{--}0.025 \text{ J/m}^2$, which corresponds to silica particles, including amorphous aggregates. For these parameters we obtain that $B \sim b \sim 1$, provided the dust fraction belongs

to the interval $n_1/n_g \sim 0.01\%\text{--}1\%$ for the dust particles of submicron to micron size, $\sigma \sim 0.01\text{--}1 \mu\text{m}$. For the gas with temperature of $T_g = 300 \text{ K}$, the dust particles of size $\sigma \sim 0.01\text{--}1 \mu\text{m}$ and smaller undergo pure bouncing collisions. At the same time, for the gas with temperature of $T_g = 1500 \text{ K}$ the bouncing collisions experience particles of size $\sigma \sim 0.1\text{--}5 \mu\text{m}$ and smaller (the lower and upper limits here correspond to the according combination of the constants).

It is also interesting to estimate the relaxation time for the dust temperature, that is, the time needed to attain a steady-state temperature. Taking into account that T_g is commonly much larger than the dust temperature, Eq. (12) for T_1 may be approximated as

$$\dot{T}_1 \approx -2\gamma_1(T_1 - T_g), \quad (31)$$

which yields $(T_1 - T_g) \sim \exp(-t/\tau)$, with the relaxation time $\tau = 2\gamma_1$, where γ_1 has been defined after Eq. (12). Using again the data for a protoplanetary disk [54], $n_g \sim 10^{10}\text{--}10^{16} \text{ m}^{-3}$ and $T_g \sim 50\text{--}400 \text{ K}$, we obtain that the relaxation time for particles of size $\sigma = 1 \mu\text{m}$ ranges from 0.2 hr to 100 yr, and for particles of size $\sigma = 5 \mu\text{m}$ from 1.5 hr to 450 yr.

In conclusion, the observed energy equipartition in granular mixtures is surprising, since generally, the equipartition does not hold in driven granular gases with different particle sizes. The results of our study may be important to understand the properties of molecular gas-dust mixtures: the systems where small dust particles are immersed in the surrounding molecular gas. Our results may be especially useful to understand the properties of protoplanetary disks.

ACKNOWLEDGMENT

We gratefully acknowledge the usage of the Skoltech CDISE HPC cluster (Pardus).

-
- [1] D. Apai and D. S. Lauretta, *Protoplanetary Dust. Astrophysical and Cosmochemical Perspectives* (Cambridge University Press, Cambridge, 2010).
- [2] J. Blum, *Adv. Phys.* **55**, 881 (2006).
- [3] J. Blum and G. Wurm, *Annu. Rev. Astron. Astrophys.* **46**, 21 (2008).
- [4] A.-C. Levasseur-Regourd, J. Agarwal, H. Cottin, C. Engrand, G. Flynn, M. Fulle, T. Gombosi, Y. Langevin, J. Lasue, Th. Mannel, S. Merouane, O. Poch, N. Thomas, and A. Westphal, *Space Sci Rev.* **214**, 64 (2018).
- [5] P. Thomas and P. J. Gierasch, *Science* **230**, 175 (1985).
- [6] N. O. Renno, M. L. Burkett, and M. P. Larkin, *J. Atmosph. Sci.* **55**, 3244 (1998).
- [7] N. V. Brilliantov and T. Pöschel, *Kinetic Theory of Granular Gases* (Oxford University Press, Oxford, 2004).
- [8] J. J. Brey, M. J. Ruiz-Montero, R. García-Rojo, and J. W. Dufty, *Phys. Rev. E* **60**, 7174 (1999).
- [9] J. W. Dufty and J. J. Brey, *New J. Phys.* **7**, 20 (2005).
- [10] V. Garzo and J. W. Dufty, *Phys. Rev. E* **60**, 5706 (1999).
- [11] S. R. Dahl, C. M. Hrenya, V. Garzo, and J. W. Dufty, *Phys. Rev. E* **66**, 041301 (2002).
- [12] R. D. Wildman and D. J. Parker, *Phys. Rev. Lett.* **88**, 064301 (2002).
- [13] K. Feitosa and N. Menon, *Phys. Rev. Lett.* **88**, 198301 (2002).
- [14] A. Bodrova, A. K. Dubey, S. Puri, and N. Brilliantov, *Phys. Rev. Lett.* **109**, 178001 (2012).
- [15] N. Brilliantov, T. Poeschel, and A. Formella, *Nat. Commun.* **9**, 797 (2018).
- [16] J. Schmidt, K. Ohtsuki, N. Rappaport, H. Salo, and F. Spahn, Dynamics of Saturn's dense rings, in *Saturn from Cassini-Huygens*, edited by M. K. Dougherty, L. W. Esposito, and S. M. Krimigis (Springer, Dordrecht, The Netherlands), pp. 413–458.
- [17] N. Brilliantov, P. L. Krapivsky, A. Bodrova, F. Spahn, H. Hayakawa, V. Stadnichuk, and J. Schmidt, *Proc. Natl. Acad. Sci. USA* **112**, 9536 (2015).
- [18] F. Spahn, N. Albers, M. Sremčević and C. Thornton, *Europhys. Lett.* **67**, 545 (2004).
- [19] K. Ohtsuki, *Icarus* **137**, 152 (1999).
- [20] K. Ohtsuki, *Icarus* **183**, 384 (2006).
- [21] H. Salo, *Icarus* **96**, 85 (1992).
- [22] K. Saitoh, A. Bodrova, H. Hayakawa, and N. V. Brilliantov, *Phys. Rev. Lett.* **105**, 238001 (2010).

- [23] P. Haff, *J. Fluid Mech.* **134**, 401 (1983).
- [24] I. Goldhirsch and G. Zanetti, *Phys. Rev. Lett.* **70**, 1619 (1993).
- [25] S. Das and S. Puri, *Europhys. Lett.* **61**, 749 (2003).
- [26] S. K. Das and S. Puri, *Phys. Rev. E* **68**, 011302 (2003).
- [27] H. Nakanishi, *Phys. Rev. E* **67**, 010301(R) (2003).
- [28] T. P. C. van Noije, M. H. Ernst, R. Brito, and J. A. G. Orza, *Phys. Rev. Lett.* **79**, 411 (1997).
- [29] T. P. C. van Noije, M. H. Ernst, and R. Brito, *Phys. Rev. E* **57**, R4891(R) (1998).
- [30] S. R. Ahmad and S. Puri, *Europhys. Lett.* **75**, 56 (2006).
- [31] S. R. Ahmad and S. Puri, *Phys. Rev. E* **75**, 031302 (2007).
- [32] W. Goldsmit, *The Theory and Physical Behavior of Colliding Solids* (Oxford University Press, Oxford, 2004).
- [33] F. Bridges, A. Hatzes, and D. Lin, *Nature (London)* **309**, 333 (1984).
- [34] G. Kuwabara and K. J. Kono, *Jpn. J. Appl. Phys.* **26**, 1230 (1987).
- [35] R. Ramirez, T. Pöschel, N. V. Brilliantov, and T. Schwager, *Phys. Rev. E* **60**, 4465 (1999).
- [36] T. Tanaka, T. Ishida, and Y. Tsuji, *Trans. Jap. Soc. Mech. Eng.* **57**, 456 (1991).
- [37] N. V. Brilliantov, F. Spahn, J. M. Hertzsch, and T. Pöschel, *Phys. Rev. E* **53**, 5382 (1996).
- [38] W. A. M. Morgado and I. Oppenheim, *Phys. Rev. E* **55**, 1940 (1997).
- [39] T. Schwager and T. Pöschel, *Phys. Rev. E* **57**, 650 (1998).
- [40] T. Schwager and T. Pöschel, *Phys. Rev. E* **78**, 051304 (2008).
- [41] N. V. Brilliantov, A. V. Pimenova, and D. S. Goldobin, *Europhys. Lett.* **109**, 14005 (2015).
- [42] D. S. Goldobin, E. A. Susloparov, A. V. Pimenova, and N. V. Brilliantov, *Eur. Phys. J. E* **38**, 55 (2015).
- [43] A. Bodrova, D. Levchenko, and N. V. Brilliantov, *Europhys. Lett.* **106**, 14001 (2014).
- [44] N. Brilliantov and F. Spahn, *Math. Comp. Simul.* **72**, 93 (2006).
- [45] A. S. Bodrova, A. Osinsky, and N. V. Brilliantov, *Sci. Rep.* **10**, 693 (2020).
- [46] T. Poeschel and T. Schwager, *Computational Granular Dynamics: Models and Algorithms* (Springer, Berlin, 2005).
- [47] J. M. Montanero and A. Santos, *Gran. Mat.* **2**, 53 (2000).
- [48] D. R. M. Williams and F. C. MacKintosh, *Phys. Rev. E* **54**, R9 (1996).
- [49] K. Roeller, J. P. D. Clewett, R. M. Bowley, S. Herminghaus, and M. R. Swift, *Phys. Rev. Lett.* **107**, 048002 (2011).
- [50] I. Aranson and L. Tsimring, *Granular Patterns*, (Oxford University Press, Oxford, 2014).
- [51] N. V. Brilliantov, N. Albers, F. Spahn, and T. Pöschel, *Phys. Rev. E* **76**, 051302 (2007).
- [52] N. Albers and F. Spahn, *Icarus* **181**, 292 (2006).
- [53] C. Dominik and A. G. G. Tielens, *Astrophys. J.* **480**, 647 (1997).
- [54] Y. Aikawa and H. Nomura, *Astrophys. J.* **642**, 1152 (2006).
- [55] Y. Aikawa, G. J. van Zadelho, E. F. van Dishoeck, and E. Herbst, *Astron. Astrophys.* **386**, 622 (2002).
- [56] J. P. Williams and C. McPartland, *Astrophys. J.* **830**, 32 (2016).
- [57] S. Kempf, S. Pfalzner, and Thomas K. Henning, *Icarus* **141**, 388 (1999).
- [58] S. Krijt, C. Guttler, D. Heisselmann, C. Dominik, and A. Tielens, *J. Phys. D* **46**, 435303 (2013).
- [59] C. Sorace, M. Louge, M. Crozier, and V. Law, *Mech. Res. Commun.* **36**, 364 (2009).
- [60] H. Kimura, K. Wada, H. Senshu, and H. Kobayashi, *Astrophys. J.* **812**, 67 (2015).