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The Effects of Heating Mechanism on Granular Gases with a Gaussian Size Distribution *

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Two-dimensional event-driven simulations are employed to gain insight into the granular energy and segregation in granular gases with a Gaussian particle size distribution when exposed to a differential heating mechanism. It is found that the bulk value of the temperature ratio depends on the choice of differential boundary heating, while the segregation behavior is insensitive to the differential heating mechanism. Moreover, by studying the numerical model without spatial degrees of freedom, differential boundary heating is found to affect nonequipartition in the bulk of the system even where heating events are rare compared to collisions.

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Granular gases,[1] i.e., gases of particles interacting through dissipative collisions, represent an important paradigm in the study of nonequilibrium physics. Due to the intrinsic dissipative character of interparticle collisions, an energy supply is requested to fluidize a granular gas to maintain a steady state. This can be carried out, for instance, by vibrating or shaking the grains. When exposed to a boundary heating, gradients in density and temperature develop in a granular system. In granular mixtures, segregation generally results from spatial variations in the granular temperature and the application of external forces. Larger denser particles tend to accumulate in regions of low granular temperature.[2,3] Experiments, theory, and simulations have recently shown that in a granular mixture with two species of particles, as soon as the interparticle collisions dissipate energy, the equipartition of energy among the mixture components is lost[4–16] even in the tracer limit.[17] The granular temperature T defined as the mean kinetic energy per degree of freedom does not have the properties required by standard thermodynamics. In recent experiments,[4–6] it is observed that two species of a mixture arrive at a ratio of granular temperature $\gamma \neq 1$, which is affected strongly by the particle mass ratio and weakly by the inelasticity. These observations have been more comprehensively investigated by event-driven simulations of vibration-fluidized systems.[9–13] Likewise, the theoretical results obtained by homogeneously heated models[14–16] have been compared to the γ found in spatially inhomogeneous systems and while some qualitative agreement has been found. In a real world, granular systems often contain continuous distributions of particle sizes, whereas the majority of previous efforts for mixtures have been focused on binary systems. The granular energy and segregation properties of granular gases with continuous size distributions have been seldom reported.

In experiments[4–6] the driving mechanism couples differently to different species of particles. A characteristic velocity scale rather than an energy scale is imparted to the particles. Therefore, the particles of different mass are differentially heated at the boundary. Feitosa and Menon[5] found that the temperature ratio γ is close to the mass ratio of the two species of particles near the boundary and reaches a constant value in the bulk. This raises the question of whether the bulk value of γ and the segregation behavior for a continuous size system depend on the differetial heating mechanism.

In this Letter, molecular dynamics simulations are employed to study the effect of the differential boundary heating on the granular energy and segregation behaviors in a granular gas with a Gaussian particle size distribution. It is found that nonequipartition in the bulk depends on the choice of differential boundary heating, while a change in the heating mechanism does not change the segregation behavior of the system. By considering a numerical simulation model[17] without spatial degrees of freedom, we confirmed that nonequipartition is sensitive to the differential heating mechanism.

We use an event-driven algorithm to simulate N particles with identical material to motion in a two-dimensional circular box with radius R in the absence of gravity. A symmetrical container has the advantage that we can examine density and granular temperature gradients along a single coordinate r, the distance from the center of the box. Collisions between particles are dissipated and treated as hard-sphere collisions (instantaneous, binary and momentum conserving). When two particles i and j collide, their post-collisional velocities are related to their pre-collisional velocities through the rules:

$$\boldsymbol{v}_{i,\mathrm{post}} = \boldsymbol{v}_{i,\mathrm{pre}} - (1+\eta)\frac{m_j}{m_i+m_j}[(\boldsymbol{v}_{i,\mathrm{pre}} - \boldsymbol{v}_{j,\mathrm{pre}}) \cdot \boldsymbol{n}]\boldsymbol{n}, \quad (1)$$

$$\boldsymbol{v}_{j,\mathrm{post}} = \boldsymbol{v}_{j,\mathrm{pre}} + (1+\eta)\frac{m_i}{m_i+m_j}[(\boldsymbol{v}_{i,\mathrm{pre}} - \boldsymbol{v}_{j,\mathrm{pre}}) \cdot \boldsymbol{n}]\boldsymbol{n}, \quad (2)$$

where $0 \leq \eta < 1$ is the coefficient of restitution

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and $\eta = -[(\boldsymbol{v}_{i,\text{post}} - \boldsymbol{v}_{j,\text{post}}) \cdot \boldsymbol{n}]/[(\boldsymbol{v}_{i,\text{pre}} - \boldsymbol{v}_{j,\text{pre}}) \cdot \boldsymbol{n}]$, $\boldsymbol{v}_{\text{pre}}$ is the pre-collisional velocity, $\boldsymbol{v}_{\text{post}}$ is the post-collisional velocity, $\boldsymbol{n}$ is the unit vector connecting the centers of particles i and j.

For the current effort, the particles are in assigned diameters consistent with a Gaussian distribution. In particular, the particle diameters are assigned using the Box–Muller[18] method and the L'Ecuyer[18] random number generator. Once generated, the particle size distribution is then validated using the Kolmogorov–Smirnov test.[19] For the purpose of data presentation, the particles are assigned to "families" based on their diameter. Each simulation includes 10 families. Particles are first ordered according to increasing size. An equal number of particles are then placed in each family, with the smallest particles placed in the first family and the largest particles placed in the last family. The total number of particles is $N = 500$. The mass of the particles can be described as $m_\alpha = \pi\rho_{\text{P}}(d_\alpha/2)^2$, where α ($\alpha = 1, 2, \ldots, 10$) is family (species) index, ρ_{P} is the mass density and d_α is the diameter of the particle in family α. It is worth noting that Gaussian particle size distributions with values of $\sigma/d_{\text{ave}} \gg 0.3$ (σ/d_{ave}, the ratio of the standard deviation of the particle size distribution σ to the mean particle diameter d_{ave}) are not physically plausible, as they require particles of negative diameter. Hence, the width of Gaussian particle distributions up to $\sigma/d_{\text{ave}} = 0.3$ was studied. The total area fraction ϕ_{total} of the particles in all simulations is fixed and $\phi_{\text{total}} = 0.1$.

When heating through the fixed thermal wall at the boundary, particles gain velocity with normal and tangential velocity components independently draw from Gaussian distributions. The width of the Gaussian is chosen to be $\langle v_x^2\rangle = \langle v_y^2\rangle = 2E_\alpha/m_\alpha$ for the particles allowing us to control the differential heating at the boundary, where E_α is the energy fed to the particles in family α.

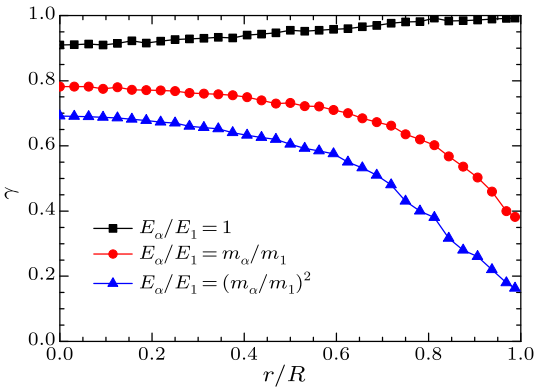

Fig. 1. Temperature ratio as a function of distance r to the center of the box with $\phi_{\text{total}} = 0.1$, $\sigma/d_{\text{ave}} = 0.3$, $\eta = 0.9$. The container has radius R. Three levels of differential heating are shown: $E_\alpha/E_1 = 1$, $E_\alpha/E_1 = m_\alpha/m_1$, $E_\alpha/E_1 = (m_\alpha/m_1)^2$ ($\alpha = 2, 3, \ldots, 10$).

Figure 1 shows the average temperature ratio $\gamma = T_1/T_{10}$ (ratio of the partial granular temperature of the smallest particles in family 1 to the partial granular temperature of the largest particles in family 10) as a function of distance r to the center of the box. Three levels of differential heating are inserted to the system: $E_\alpha/E_1 = 1$ ($\alpha = 2, 3, \ldots, 10$), where equal amounts of energy are fed to 10 types of particles at the boundaries, $E_\alpha/E_1 = m_\alpha/m_1$ ($\alpha = 2, 3, \ldots, 10$), where the energy fed is proportional to the mass ratio, and $E_\alpha/E_1 = (m_\alpha/m_1)^2$ ($\alpha = 2, 3, \ldots, 10$), where the energy fed is proportional to the square of the mass ratio. The bulk value of γ is different when exposed to differetial heating mechanism. This indicates that the bulk value of γ depends on the choice of differential heating at the boundary. The granular temperature ratio is not an intrinsic property of particle species. The effect of the boundary heating permeates the bulk of the system. It is worth noting that the temperature ratio profiles of the system with a Gaussian particle size distribution follow the same trend, though the results presented here are limited to $\gamma = T_1/T_{10}$ for the sake of brevity.

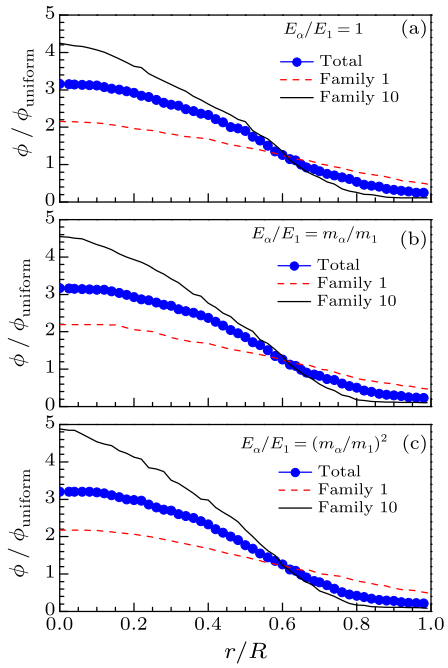

Fig. 2. Behavior of $\phi/\phi_{\text{uniform}}$ as a function of distance r to the center of the box under three levels of differential heating: (a) $E_\alpha/E_1 = 1$, (b) $E_\alpha/E_1 = m_\alpha/m_1$, (c) $E_\alpha/E_1 = (m_\alpha/m_1)^2$, with $\phi_{\text{total}} = 0.1$, $\sigma/d_{\text{ave}} = 0.3$, $\eta = 0.9$.

We further check whether the segregation profile is sensitive to the differential boundary heating. The segregation behavior of the system can be investigated by comparing the observed area fractions of each family to the area fractions that would be expected if all particles in a given family were uniformly distributed throughout the interior of the container (ϕ_{uniform}). Figure 2 shows the $\phi/\phi_{\text{uniform}}$ as a function of distance r from the center of the box. The three heating mechanisms used in Fig. 1 are again employed. The "total" curve in Fig. 2 represents the overall segregation within the mixture, while a comparison between

family 1 and family 10 curves indicates the species segregation of the particles in family 1 and family 10, respectively. In each of the three cases, all particles prefer regions of lower granular temperature, but large particles appear to have a higher affinity for cold regions than their smaller counterparts, as was reported in Ref. [20]. However, taken together, the three cases clearly reveal that the overall and the species segregation behaviors are not affected by the choice of differential heating at the boundary.

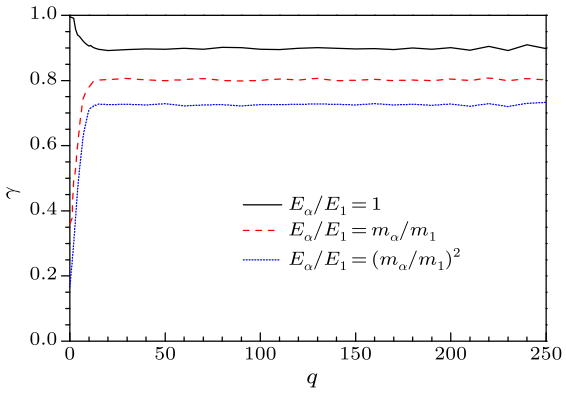

Fig. 3. The temperature ratio γ versus q under three levels of differential heating, with $\phi_{\rm total} = 0.1$, $\sigma/d_{\rm ave} = 0.3$, $\eta = 0.9$.

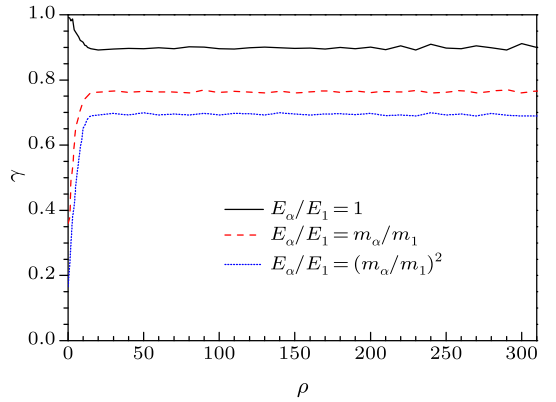

Fig. 4. The temperature ratio γ as a function of ρ under three levels of differential heating with $\phi_{\rm total} = 0.1$, $\sigma/d_{\rm ave} = 0.3$, $\eta = 0.9$.

Furthermore, we turn to consider the number of collisions q suffered by a particle since it has collided with the boundary. Each time a particle i collides with another particle, q_i is added by 1, and once it collides with heating boundary again, q_i is set to zero. During a long simulation time, after the system reaches a steady-state, the temperature ratio γ reaches a steady-state value from initial conditions after about 12 collisions, which is shown in Figure 3. However, the asymptotic value of γ at large q remains a function of E_α/E_1. Hence, details of the driving mechanism at the boundary persist in the bulk of the system.

In order to further confirm the persistent effect of the differential heating on the bulk value of γ, we turn to a numerical model without spatial gradient.[15] In this numerical model, N particles of a two-dimensional inelastic gas with a Gaussian particle size distribution are initialized with Gaussian-distributed velocities. In every time step, C pairs of particles are selected at random and collide using Eq. (1) with uniform random impact parameters. At the same time, H particles are selected at random to be heated. For each heating event, velocities are selected randomly from Gaussian distributions with average energy E_α, depending on the types of the particle selected. This gives us a dissipation-heating ratio $\rho = 2C/H$, the ratio of the frequency of collisions to heating events. The three differential heating used in Fig. 1 are employed again here. The large ρ limit represents a boundary heating (the collisions between particles are much more frequent than the heatings) and corresponds to large q in Fig. 3 without the complications introduced by spatial gradients. The temperature ratio γ for a Gaussian system as a function of ρ is shown in Fig. 4. It illustrates that the values of γ for the three differential heating events are different even where the heating events are rare relative to the collisions.

In conclusion, molecular dynamics simulations of a granular mixture with a Gaussian particle size distribution are employed to elucidate the effect of the differential boundary heating on the temperature and segregation properties of the mixture. The differential boundary heating affects nonequipartition in the bulk of the system and the effect of the boundary is never erased, while the segregation behavior of the mixture is insensitive to the differetial heating. Furthermore, a numerical model without spatial degrees of freedom is presented to confirm the results obtained by the event-driven simulations with spatial degrees of freedom.

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