Simulation study on kinetic temperatures of vibrated binary granular mixtures

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We study the unequal kinetic temperatures in two-dimensional binary granular mixtures heated by vertical vibrations under gravity by molecular dynamics simulations. By introducing several variable parameters describing particle and composition properties of mixtures, the coexistence of two different kinetic temperatures for the two components is exhibited. In dilute situations, our numerical results confirm the overall experimental measurements by Feitosa and Menon recently [Phys. Rev. Lett. **88**, 198301 (2002)]. For example, the temperature ratio along the vertical direction is constant in the bulk of a system, and is insensitive to external driving or relative concentration of the two components, but mainly influenced by their masses. However, outside of the dilute situations, especially as the number density becomes high enough where the spatial and momentum correlations become salient, the ratio profiles show some different characteristics. Generally, the plateau shape along the vertical direction is broken, and instead, a saddlelike shape appears. Furthermore, the physical implications are discussed.

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I. INTRODUCTION

Granular materials are large conglomerations of macroscopic particles. If they are noncohesive, then particles can move free of interparticle forces except for isolated collisions where they suffer repulsive forces in contact. After each collision a little kinetic energy is dissipated. If we continuously inject power into such a system to keep particles in motion, dynamics of a granular system will resemble that of fluids, wherever the particles move seemingly randomly. Depending on the energy injection and dissipation rates a nonequilibrium steady state can be obtained. However, due to the dissipative nature of the interactions between particles, granular media are commonly induced to show correlated collective behaviors in contrast to classical elastic particle systems. Clustering, surface waves, and convection rolls are some examples of strong collective correlation behaviors [1]. Even for a system in a dilute and nearly elastic regime, where the correlation is small, differences from ordinary molecular fluids are also obvious, such as the appearance of non-Gaussian velocity distributions [2,3].

Recently, the violation of energy equipartition among granular media has attracted particular interest [4–13]. Similar to elastic gases, the kinetic theory for granular systems usually defines an average kinetic energy of particles as the granular temperature. In a mixture of two or more kinds of particles, each species will attain a different granular temperature, depending on the balance of external power injection and internal energy dissipation by inelastic collisions. A theoretical investigation [4] using the Enskog kinetic theory to the homogeneous cooling process for a binary mixture shows that the two species have different temperatures throughout the cooling process while their cooling rates are equal. This result was verified by detailed Monte Carlo simulations using the Boltzmann equation [5]. In fact, the coexistence of different temperatures in a binary mixture has been studied by analytical works [6,7], numerical simulations [8–10], and experiments [11–13]. Although the mechanisms of energy feeding in analytical studies and experiments are different, i.e., theoreticians favor a uniform thermal Gaussian bath while in experiments the energy was injected by a vibrating wall, the qualitative results are similar. In both cases systems can all achieve a nonequilibrium steady state where the temperatures of different species are different, depending on material properties (mass, sizes, and inelasticity), compositional parameters (average number density and number fraction of each component), and driving strengths. Such a temperature difference cannot be attributed to segregation or insufficient mixture of components in a system, due to the assumptions that particles are spatially homogeneously distributed in analytical works and violently vibrated in experiments and simulations. Even the temperature of a single tracer particle in an equilibrium fluid was found to be different from the surrounding bath [14]. These findings demonstrate that a long preserved assumption in previous theoretical development [15,16] of the kinetic theory for binary mixtures (i.e., a single temperature is used to characterize a system) is not justified, and suggest a challenge for the understanding of granular mixtures.

The aim of this paper is to explore the breakdown of energy equipartition in strongly vibrated two-dimensional binary granular systems over broader parameter selection ranges by molecular dynamics simulations. The advantage for the present study is that by molecular dynamics simulation, we can provide a macroscopic description by averaging over microscopic details of motions and interactions between individual particles, and avoid the assumptions inherent in the kinetic theory or approximations made in solving the kinetic equations, and difficulties of tuning parameters widely used in experiments. Therefore, with computer simulations we are allowed to tune system parameters such as particle properties and compositional parameters in a systematical manner to gain a more thorough study on the breakdown of energy equipartition in a vibrated granular mixture and find some different characteristics.

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II. MODEL AND METHOD

The simulation cell is assumed to be a vertical rectangular container with dimensions $L_y \times L_z$. Its upside and bottom plates are required to vibrate synchronously. Periodic boundaries are used to eliminate the side-wall effects, such as convection [17] and inhomogeneous particle distribution along the horizontal direction that may cause cluster formation near side walls [8]. The particles receive energy by colliding with the two horizontal walls, harmonically vibrated at a frequency f. The gravitational force acts along the negative z direction.

The simulated particles are homogeneous and inelastic circular disks which are free to rotate around an axis normal to the y-z plane. These disks can be categorized into two species by different diameters d_i, masses m_i, or normal restitution coefficients α_{ij}. All these parameters are variable. In addition, the two compositional parameters are tunable: they are the number fraction of each species (x), and the average number density ρ_a, specified in terms of the occupied area divided by the total area of the container. The collision rule includes a reduction of the relative normal velocity V_n, a reduction of the relative tangential velocity V_r, and an exchange of energy between those two degrees of freedom for any two particles [18]. After a particle-particle collision, we have

$$V_n' = -\alpha_{ij} V_n, \tag{1}$$

where V_n and V_n' are the relative radial velocities of two particles i, j before and after a collision. The normal restitution coefficients α_{ij} is not a constant. It depends on the relative normal velocity in the form [19]

$$\alpha_{ij}(V_n) = \begin{cases} 1-(1-e_{ij})(|V_n|/V_0)^{3/4} & \text{for} \quad V_n < V_0, \\ e_{ij} & \text{for} \quad V_n > V_0, \end{cases} \tag{2}$$

where the normal elastic coefficients e_{ij} are constants related to three types of colliding pairs. $V_0 = \sqrt{gd}$, where d is the average diameter of all particles and g the gravitational acceleration. The interaction along the tangential direction can be distinguished into two types, i.e., sliding and sticking. If the condition

$$\frac{|V_r|}{|V_n|} \geqslant 3\mu(1+\alpha_{ij}) \tag{3}$$

is satisfied, the collision is in the sliding fashion, otherwise it is in the sticking fashion [20]. Here μ is the friction coefficient reflecting the surface roughness of particles, and is assumed to remain unchanged. Thus, after a collision, the total angular momentum and translational momentum are conserved while the energy is dissipated through the reduction of the relative normal velocity and relative tangential velocity. Particle-wall collisions obey the same rule while the mass of walls is taken as infinite. Between two collisions a particle moves along a parabolic trajectory due to the gravitational field.

For the convenience of simulation, we would prescribe some basic parameters. At first, we choose $d = 1.6$ mm, $m = 5$ mg, and the box dimensions are $L_y = 96d$ and $L_z = 64d$, respectively. Then driving frequency is varied from 40 Hz to 80 Hz, and the amplitude A is mostly of $2.4d$, corresponding to a maximum acceleration $\Gamma = A(2\pi f)^2$ and a maximum velocity of the cell $v_0 = A(2\pi f)$, which are about $99g$ and 1.9 m/s, respectively. Finally, the friction coefficient $\mu = 0.1$, while the normal elastic coefficient is chosen to be 0.9, representing a moderately strong dissipation.

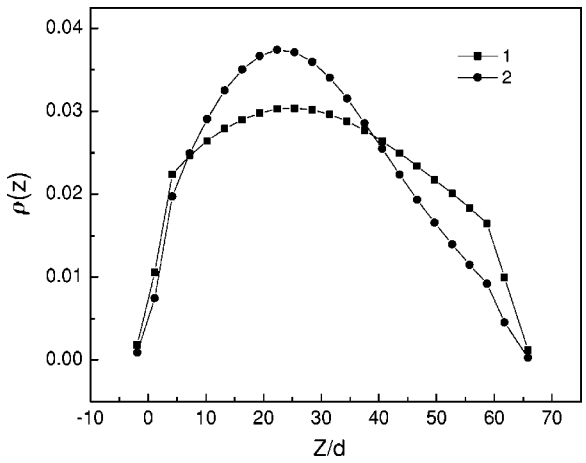

FIG. 1. Vertical number density ρ versus height z/d. $m_1 = m$, $m_2 = 3m$, $d_1 = d_2 = d$, $e_{11} = e_{22} = e_{12} = 0.9$, and particle numbers $N_1 = N_2 = 150$.

An efficient hard sphere molecular dynamics simulation [21], also known as event driven algorithm, is employed to evolve a system. In all of our simulations the external vibration is so strong that the two species of particles are well mixed locally. All the quantities reported in the following have been obtained by averaging the sampling over more than 10^5 vibration cycles.

III. DILUTE SITUATIONS

There are quite a few parameters giving influences on the kinetic temperatures of a granular mixture and their ratios. We will first present some general profiles of those characteristic quantities by simulations with $N = 300$ particles of two species and the number fraction $x = 1/2$ to get some general perception of the present dynamical system. The two kinds of particles have the same properties except $m_1 = m$ and $m_2 = 3m$. The cell vibrates sinusoidally at the frequency 60 Hz and the amplitude $2.4d$. According to the data analysis, the mean free path is of the order $6.2d$ for species 1 and $4.8d$ for species 2. Because particles are mostly concentrated in the center of the cell, generally, collisions take place more frequently than in a uniform distribution system. The typical particle-particle collision rates are of the orders 150 Hz for species 1 and 120 Hz for species 2, which are quite higher than the particle-wall collision rates of the orders 12 Hz and 6 Hz, respectively.

The density profiles along the vertical direction are shown in Fig. 1. It is obvious that the heavier particles have a higher

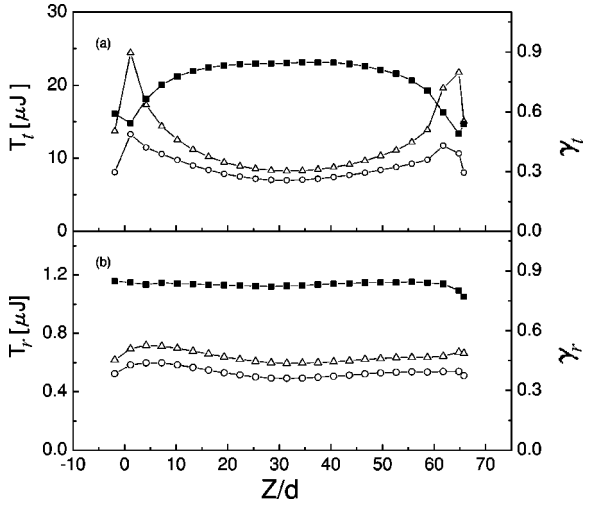

FIG. 2. (a) Translational temperatures T_t (left scale) for species 1 (○) and species 2 (△), and their ratio γ_t (■, right scale) versus height z/d. (b) Rotational temperatures T_r (left scale) for species 1 (○) and species 2 (△), and their ratio γ_r (■, right scale) versus z/d. All the system parameters are the same as those in Fig. 1.

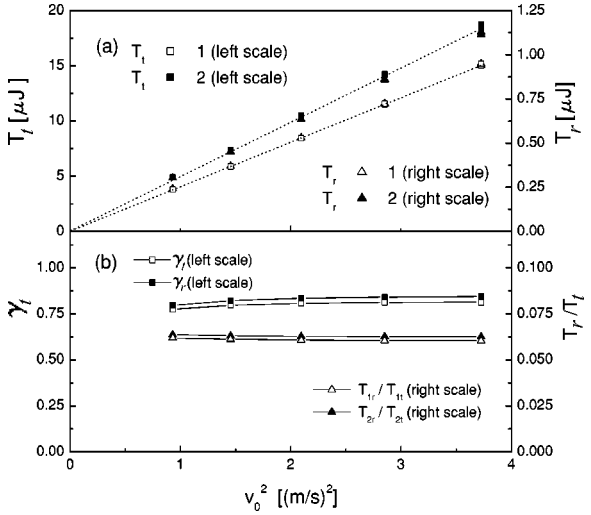

FIG. 3. Translational and rotational temperatures (a) and temperature ratios (b) of two species plotted against the square of vibration velocity v_0^2. All other parameters are the same as those in Fig. 1.

concentration in the center of the cell, while the lighter ones tend to spread out. However, particles of two species are locally mixed well and there is no apparent cluster formation observed in such a dilute and strongly vibrated state [13]. It is required that the local density of two species will attain maximum at roughly the same height near the center of the cell, and in such a well-mixed state particle-particle collision frequencies among the same and different components are of the same order. Incidentally, due to the periodic boundary conditions, the density and temperature distributions are verified to be uniform along the horizontal direction over long time sampling for both species.

Figure 2 shows the translational and rotational temperatures for both species and the temperature ratios along the vertical direction. It can be seen that the two components of a binary mixture do not equilibrate to the same kinetic temperature, but heavier species retains a higher temperature. Similar to the density profiles, the temperature profiles along the horizontal direction are uniform, while in the vertical direction things become different. Both species tend to cool down as the distance from two moving walls increases, however, their temperature ratio reaches a plateau in the interior of the cell over a broad region. This fact has been observed by the previous experiment [13] and simulation [8], and indicates that although the number density ratio varies with the height, the temperature ratio remains nearly constant in the bulk. It can be further verified below by tuning some parameters of two species if the number density is in the dilute case. We also notice that the rotational temperature ratio remains constant over the entire cell, and in the interior of the cell, the two kinds of temperature ratios, i.e., the translational temperature ratio of two kinds of particles and the rotational temperature ratio of two kinds of particles, will approach the same value.

Generally, after colliding with a moving wall both kinds of particles gain a velocity $\propto v_0$ on average, thus the temperature ratio of two species $\gamma = T_1/T_2$ is proportional to m_1/m_2 near the wall, which implies that the heavier particles gain higher kinetic energy from this energy injection source. Bounced off the wall, a particle moves into the interior of the cell and carries the kinetic energy to the bulk granular gas. Due to the higher concentration of particles in the interior, the particle-particle collision rates increase correspondingly. The energy exchanges between the same kind and different kind of particles drive their temperatures to approach each other. However, due to the combination of external energy injections and dissipative collisions among particles in the present nonequilibrium system, ordinary thermodynamic arguments become useless. Therefore, the zeroth law of thermodynamics is unapplicable, i.e., particles of different species will not relax to the same kinetic temperature, like that in an equilibrium system.

To make clear the influence of external driving, we plot Fig. 3 to show the temperatures and their ratio profiles averaging over the entire cell. These results verify that the translational temperature T_t and rotational temperature T_r are both proportional to v_0^2 in the mixture of both species. Here the driving frequency varies from 50 Hz to 80 Hz, and maximum acceleration varies from $39g$ to $99g$. Under these strong agitations, it is found that although their respective average temperatures increase with v_0^2, the temperature ratio profiles are independent of the variation of driving frequency or amplitude. This relation was also observed in the previous experiment [13].

From the simulation results obtained, it can be concluded that a steady state is achieved in dilute granular gases under strong agitation. Based on the energy exchanges between particle-particle and particle-wall by inelastic collisions, a kind of energy balance is established, i.e., the ratio of the kinetic energies for two species remains constant with varying external power injection.

We can take into account the influences of particle properties including the normal elastic coefficient e_{ij}, particle

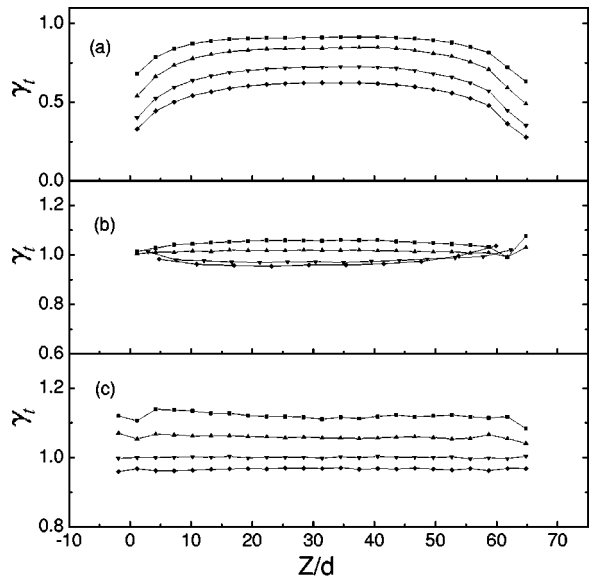

FIG. 4. Vertical profiles of the translational temperature ratios γ_t for a binary mixture with different material properties. For this system there are totally 300 particles with the number fraction $x=1/2$ for both species and $\Gamma=56g$. (a) Two species with the same diameter d, the same normal elastic coefficients $e_{11}=e_{22}=e_{12}=0.9$, but different masses, $m_1=m$, $m_2=2m$ (■), $3m$ (▲), $5m$ (▼), and $7m$ (♦). (b) Two species with the same mass m, the same normal elastic coefficient $e_{11}=e_{22}=e_{12}=0.9$, but different diameters, $d_2=d$, $d_1=0.5d$ (■), $0.8d$ (▲), $1.5d$ (▼), and $2d$ (♦), (c) Two species with the same mass m, the same diameter d, but different normal elastic coefficients, $e_{11}=0.9$, $e_{22}=0.7$ (■). $e_{22}=0.8$(▲), $e_{22}=0.9$ (▼), $e_{22}=0.96$ (♦), and $e_{12}=(e_{11}+e_{22})/2$.

mass m, and diameter d. We keep the tangential friction coefficient μ as a constant, because the rotational kinetic energy is much smaller than the translational one.

The mass difference is an important factor to determine the temperature difference. We perform several simulations with two kinds of particles distinguished only by their masses. The result is plotted in Fig. 4(a). It is obvious that the heavier species gains a higher temperature, and the temperature difference increases as the mass difference increases. On the other hand, for a binary mixture with the same mass but different diameters as shown in Fig. 4(b), we found that although the temperature ratio is only slightly influenced by the size difference in contrast to the mass difference, the variation trend is rather apparent, i.e., particles with larger sizes tend to gain a lower temperature. This result is not difficult to understand. In fact, particles with a larger diameter have a larger cross section and generally have more chances to collide with other particles. As we know, after each collision, part of the particle's energy will be lost. Therefore, the more the collision times, the more the energy dissipated, and, on average, the larger particles tend to be cooler than smaller ones. But the influence of size difference on temperature difference is much smaller than that of mass difference. This result is in qualitative agreement with the theory obtained in a homogeneous binary heated mixture [6]. We also analyze the influence of the normal elastic coefficient on γ by tuning the elastic coefficient of one species. It is apparent to see from Fig. 4(c) that the particles with a higher elastic coefficient achieve a higher temperature. In fact, the elastic coefficient determines the fraction of the total kinetic energy lost after a collision. Thus the particles with a lower elastic coefficient tend to lose more kinetic energy on average. In addition to test the effects of these material properties separately, another interesting question would be what is the cross effect of these factors, e.g., what happens if the more massive particles are also more inelastic in a real granular mixture. We have also taken some simulations to investigate this cross effect, and find that the temperature ratio will depend on the competition between them. The sensitivity of temperature ratio on mass and elasticity differences is still marked, and temperatures of two species will approach each other if the more massive particles are also more inelastic. This result agrees well with the simulations by Paolotti *et al.* [8].

We also test the influence of different number fractions of one component x for the same total number of particles on the temperature ratios. For strongly agitated dilute systems, it is found in our simulations that the temperature ratio γ is insensitive to x when the lighter particles are more elastic than the heavier particles. This fact is also in agreement with the experiment [13].

IV. HIGHER DENSITY SITUATIONS

When we change the number density, there is something different. In the previous cases, the granular systems are in dilute and strongly agitated states where the density and momentum correlations are small, and the collision rate of particle-particle is quite higher than that of particle-wall. If we tune the number density down to the limit of a dilute case, then the collision rate of particle-wall is comparable or even higher than that of particle-particle, a particle exchanges little energy with other particles between successive collisions with vibrating walls. It is obvious that the granular temperature of each component on average would be close to its kinetic energy obtained from the vibrated wall, and then the temperature ratio is equal to the mass ratio of two species.

On the other hand, as the number density is increased, the collision rate between particles is also increased, which is more frequent than the rate of collision with the two moving walls. So the kinetic energy of particles is dissipated more quickly, and then little by little a strong density and momentum correlation will be established. In other words, granular materials will induce a correlated collective motion which severely influences the temperature ratio of two species. In the following, we will consider these higher density situations.

In order to keep the average height of all particles still near the center of the cell and avoid global particle segregation in the vertical direction when the number density becomes higher, we increase the normal elastic coefficients of both species to $e_{11}=e_{22}=e_{12}=0.96$. The two species have the same diameter $d_1=d_2=d$, but different masses $m_1=m, m_2=3m$; external sinusoidal driving $f=60$ Hz, $\Gamma=56g$. Figure 5 shows the temperature ratio profiles of two

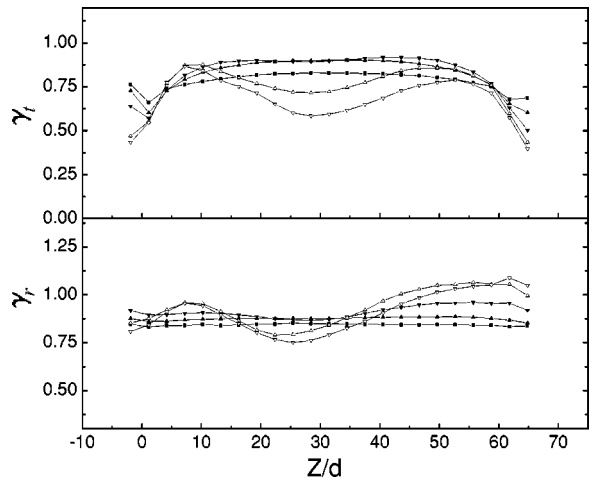

FIG. 5. Translational temperature ratio γ_t (a) and rotational temperature ratio γ_r (b) in the vertical direction for the total particle number $N=100$ (■), 300 (▲), 500 (▼), 1000 (△), 1200 (▽), and the number fraction $x=1/2$.

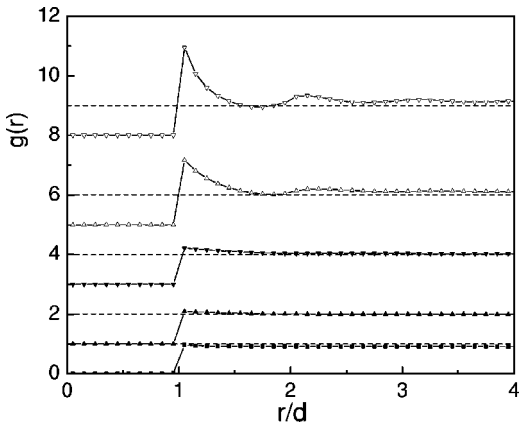

FIG. 6. The radial distribution function $g(r)$ for total particle number $N=100$ (■), 300 (▲), 500 (▼), 1000 (△), 1200 (▽), and the number fraction $x=1/2$. Other parameters are $f=60$ Hz and $\Gamma=56g$. The plots of $g(r)$ have been shifted for the sake of clarity, and the dashed lines show $g(r)=1$.

species with the total number of particles varying from 100 to 1200 but the number fraction $x=1/2$.

We can find that in the most dilute case $N=100$, the temperature profile is still a plateau while γ_t is slightly lower than those of a little denser cases. The collision rates at this density are 86 Hz and 55 Hz for particle-particle, and 20 Hz and 11 Hz for particle-wall of species 1 and species 2, respectively. When the total number of particles varies from 300 to 500, the temperature ratio profile remains constant in the interior region of the cell and seems to be insensitive to the average number density ρ_a. As N is further increased, the ratio plateau is replaced by a saddlelike profile with a dent appearing in the interior; and the rotational temperature profile behaves similar to the translational one. Such a newly explored behavior can only arise from correlated collective motion as will be exposed in detail below.

As has been mentioned above, in the vicinity of a moving wall, particles gain kinetic energy proportional to mv_0^2 on average. Thus the translational temperature ratio of two species approaches their mass ratio near the wall. Then, as particles leave from the wall into the interior, the collision rate between particles increases correspondingly with increasing local particle number density. The energy is exchanged between the same and different kinds of particles, and the granular temperatures of two species approach each other but are usually not equal. As the distance from the bottom increases, the particles number density increases, and the system continuously cools down. Then a transition from a gaslike state to a liquidlike state may appear, corresponding to strong density and momentum correlations of particles. Finally, near the center of the interior both species tend to be trapped together and form a strongly correlated granular liquid. Particles in this liquidlike state tend to move coherently, i.e., heavier particles and lighter particles tend to gain the same velocity. Therefore, the temperature ratio goes down and approaches the mass ratio again, and a dent appears in the center of the vertical temperature ratio profile. This is the reason why the temperature ratio of two species first increases, and then decreases with increasing height. In the present case, it is the dissipative nature of granular collisions which may induce density and momentum correlations to make the process quite complicated.

To characterize the transition from the gaslike to the liquidlike states, we show the radial particle-particle correlation function $g(r)=\langle\rho(0)\rho(r)\rangle/\langle\rho\rangle^2$ normalized by the particle diameter d in Fig. 6. Here ρ is the particle density and the sampling is taken in a rectangular $96d\times38.4d$ window centered in the geometrical center of the cell. It is clear to see that with an increase of number density, the oscillations of $g(r)$ became more and more marked. Figure 6 clearly demonstrates the transition from a gaslike state to a liquidlike state as the number density increases. With the injection of continuous energy flux, particles behave as a correlated bulk and move like a liquid. Interestingly, contrary to the gaslike case, if we apply a strong external driving in the liquidlike state, the temperature ratio can even surpass 1, i.e., the lighter particles can gain higher temperature than the heavier ones in some local regions. We ascribe this to the fact that in this region, the heavier particles have formed some clusters (dissipate more energy) while the lighter ones relatively still move freely. This will cause the heavier particles become cooler, and hence the temperature ratio increases further. Therefore the sensitivity of external vibration on temperature ratio in the dense system is quite different from that in the dilute one.

Based on the present simulations and analyses, it seems valid that the independence of temperature ratios on the average number density ρ_a can only appear in the range of some dilute and moderate number densities under an external driving. In Feitosa and Menon's experiment [13], their measurement was averaged over a rectangular region in the cell; this may smear out the details of a temperature ratio profile which is more possibly not a plateau in the cell center as number density becomes higher.

Finally, we would like to point out that although our simulation results agree with Feitosa and Menon's experiment qualitatively, there exist some difficulties to obtain a

precise numerical agreement between simulations and the experiment. The possible explanations are the following: First, in our simulations the system is a strictly two-dimensional (2D) one, while in Feitosa and Menon's experiment the spheres are confined in a quasi-2D cage ($32d$ high $\times 48d$ wide $\times 1.1d$ thick). In a quasi-2D system, particles move with higher freedom than in a strict 2D system. Second, in our simulations, we use a periodic boundary condition in the horizontal direction, while in the experiment particles can collide with four side walls. With the periodic boundaries, the kinetic temperatures and number densities of particles are homogeneous along the horizontal direction, but with fixed boundaries, the temperatures are lower and number densities are higher in the vicinity of the boundaries than in the bulk. Third, there are some other causes that may influence the precise numerical comparisons between our simulations and the experiment. For example, in our simulations, we have not considered the deformation of particles and the duration of collisions. Besides we do not know the experimental value of friction coefficients, while the tangential friction surely has an influence on the system [22].

V. SUMMARY

We have systematically investigated the spatial distributions of densities and temperatures in a vertically vibrated binary granular mixture over broad ranges of parameters by using molecular dynamics simulations. Our numerical simulations include both translational and rotational kinetic energies, and show that both the translational and rotational temperature ratios of two kinds of particles are similar in the interior of the container, although the energy for two kinds of motion differ by an order of magnitude. The breakdown of energy equipartition among different species of a binary granular mixture was verified, and the reasonable physical discussions were given.

It has been found that as particles are confined in a vibrating container and the average number density is not too high, a plateau of the temperature ratio of two components along vertical direction is established in the interior of the system and is independent of the external driving frequency and amplitude. The material properties of particles do influence the temperature ratio, and particles which are heavier, smaller, and more elastic, tend to gain a higher temperature. By tuning these material parameters separately, we have found that the enhancement of the temperature difference depends much more on mass differences than on size differences, and the influence of elasticity is also quite marked. The cross effect of these material properties will depend on the competitions among them. These results are quite consistent with recent experimental and theoretical studies.

The insensitivity of the temperature ratio on average number density is verified in some moderate range, however, at relatively high densities things become complicated. As the number density increases, a transition from a gaslike state to a liquidlike state is observed and the temperature ratio plateau along the vertical direction is violated with a dent appearing in the center of the profile. At very high densities, a strong momentum correlation is established and the temperature ratio approaches mass ratio of two species since particles move with roughly the same velocities. Furthermore, the correlation makes the binary mixture so complicated that the lighter component could gain a higher temperature than the heavier one in some conditions.

ACKNOWLEDGMENTS

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