Heating mechanism affects equipartition in a binary granular system

Hong-Qiang Wan and Narayanan Menon

Department of Physics, University of Massachusetts, Amherst, Massachusetts 01003-3720

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Two species of particles in a binary granular system typically do not have the same mean kinetic energy, in contrast to the equipartition of energy required in equilibrium. We investigate the role of the heating mechanism in determining the extent of non-equipartition of kinetic energy. In most experiments, different species are unequally heated at the boundaries. We show by event-driven simulations that differential boundary heating affects non-equipartition even in the bulk of the system. This conclusion is fortified by studying numerical and solvable stochastic models without spatial degrees of freedom. In both cases, even in the limit where heating events are rare compared to collisions, the effect of the heating mechanism persists.

An issue of broad generality for nonequilibrium physics is the assignment of intensive temperature variables to steady states of driven systems. A widely-studied example of practical importance is a dilute system of macroscopic grains. A granular gas of this kind is different from an equilibrium gas in that a continuous supply of energy from an external source is necessary to maintain a steady state and balance dissipation due to inelastic collisions between particles. The energy source determines typical scales of the dynamics in the system, but is presumed not to affect the microscopic constitutive laws such as the equation of state or expressions for transport coefficients. In this Letter we study an externally fluidised granular gas and find that the details of the energising mechanism affect relations between intensive quantities even in the bulk of the system.

In a typical real-world situation, energy is delivered at the boundaries of a granular system by vibration, shear or other mechanical means. In equilibrium, a gas placed in contact with a heat bath acquires a uniform temperature and density. However, in the case of a granular system, there are gradients in density and particle motions as a function of distance from the energising boundary. For dilute gases of inelastic particles there has been considerable progress in describing this inhomogeneous steady state in terms of density and “temperature” fields, where the temperature is a purely kinetic construct, defined as the mean kinetic energy per degree of freedom, analogy to kinetic theory of a molecular gas.

An important conceptual tool in validating the use of nonequilibrium temperatures involves thermal contact between systems. One can ask whether a candidate definition for the temperature governs the direction of energy flow and whether the temperatures equalise or evolve to bear a fixed relationship. In this spirit, we consider a granular system with two species of particles. There is no requirement that the species acquire the same kinetic temperature; indeed, experiments document a violation of equipartition. It is observed that two species \(a\) and \(b\) acquire temperatures whose ratio \(\gamma \equiv T_a/T_b\) is affected strongly by the ratio of particle masses, \(m_a/m_b\), and weakly by their inelasticity. The temperature ratio \(\gamma\) is observed to be only weakly affected by the composition - the number density and stoichiometry - of the mixture. These observations have been reproduced and more comprehensively explored by event-driven simulations of vibration-fluidised systems.

This raises the question of whether the extent of departure from equipartition can be predicted, that is, can the temperature ratio \(\gamma\), be expressed in terms of specified properties of the two types of particles in the mixture. If so, it would not be necessary to introduce independent temperature fields to describe each species in the mixture. Following early work that addresses this question within the framework of kinetic theory, there have been several theoretical treatments of this issue in spatially homogeneous models. Garzó and Dufty studied theoretically the homogeneous cooling of a binary granular mixture and found that cooling rates of the two species are the same while their temperatures remain different, thus maintaining a time-independent \(\gamma\). These predictions have been compared against MD simulations. Likewise, kinetic theory treatments of homogeneously heated steady-states of mixtures have been successfully compared to event-driven simulations in which particles get occasional velocity boosts from an external noise source. Other treatments of the homogeneously heated case have been advanced by Langevin-like models and by mean-field solutions of the Boltzmann equation. All of these theoretical results have been compared to the \(\gamma\) found in spatially inhomogeneous vibration-fluidised steady states, and while some qualitative agreement has been found, it is appropriate to be cautious in comparing these situations.

A further, and often-neglected ingredient in this problem is that in a typical experiment, the driving mechanism couples differently to different species of particles. For instance, in a vibration-fluidized system, the vibrating boundaries may be treated as infinitely massive, and therefore, impart a characteristic velocity scale (rather than an energy scale) to the particles. If the particles in the system are of different mass, then they are differentially heated at the boundary. This is not an is-
sue in an equilibrium system, where equipartition holds even if the two species are coupled differently to a heat bath. In the granular systems under consideration, the temperature ratio $\gamma$ is experimentally observed to be close to the mass ratio of the two species of particles near the boundary, and then attain an apparently constant value after a few mean free paths. The question remains whether this apparently constant bulk value depends on the boundary condition. A similar issue has previously been commented on in the context of a homogeneously heated system with both species coupled to different heat baths and in comparing homogeneously heated systems to boundary-driven systems.

In this Letter, we address by molecular dynamics simulations the effect of this differential boundary heating on the extent of nonequipartition of energy in the bulk of the system for a binary granular mixture. We find that the level of differential heating affects nonequipartition in the bulk, and that the effect of the boundary is never forgotten. These results are strengthened by consideration of a numerical simulation model without spatial degrees of freedom, and of a stochastic model.

In our event-driven simulations, two types of smooth discs (labelled a and b), both of diameter d, but with different masses, are fluidized inside a rectangle of dimensions $48 \times 32d$. These simulation parameters are chosen to mimic an experimental geometry previously studied by us. For the simulations reported here, the ratio of particle masses $m_b/m_a$ is 5, the restitution coefficient of both species is 0.93 and an equal number of both species are used with the total number of particles $2N=200$ corresponding to area fraction 10.2%. We set $g=0$ and employ periodic boundary conditions in the horizontal ($xz$) direction. In order to isolate the effects we are concerned with, we choose to heat the particles using fixed"thermal" walls rather than with the additional space- and time-dependence introduced by oscillating walls. Following a collision with the top or bottom boundary, a particle is reflected with normal and tangential velocity components independently drawn from gaussian distributions. The width of the gaussian is chosen to be $v_x^2 = v_y^2 = 2E_{a,b}/m_{a,b}$ for the two types of particles, thus allowing us to control the differential heating at the boundary.

In Fig.1 we show three choices of differential heating: $E_b/E_a = 1$ where equal amounts of energy are fed to two types of particles at the boundaries, $E_b/E_a = 5$ where the energy fed is proportional to the mass ratio as in the vibrational experiments, and $E_b/E_a = 25$ which even more disproportionately emphasizes the heavier particles. Fig.1 displays (a) the average temperature ratio $\gamma = T_a(z)/T_b(z)$ and (b) number density ratio $n_a(z)/n_b(z)$ profiles along the direction perpendicular to the top and bottom boundaries. Comparing any single pair of curves, say the case $E_b/E_a = 5$ - with experimental data - we find similar profiles of $\gamma$ and number density ratio, although the energy-supplying boundaries are fixed and gaussian. In each of the three cases, the value of $\gamma$ at the boundaries is determined by the heating mechanism, as expected, but changes to a nearly constant value in the bulk. However, taken together, the three cases show clearly that the bulk value of $\gamma$ depends on the choice of differential heating at the boundary. Thus shows that the value of $\gamma$ is not an intrinsic property of the pair of particle species and that the effect of the boundary permeates the bulk of the system.

We further check whether the persistence of the boundary condition into the bulk is a finite size effect by doubling the height of the system to $64d$ while holding fixed the total area fraction. The three heating schemes shown in Fig.1 are once again employed, and the temperature ratio and number density ratio as a function of $z$ are shown in Fig.2. Clearly, the temperature ratio $\gamma$ is still affected by the value of $E_b/E_a$ specified at the boundary.

It is straightforward to simulate substantially taller systems, however, the increasing segregation of the heavier particles to the middle of the system presents a new complication. We thus address the issue of whether the data in Fig.1 and 2 are still affected by finite-size limitations by considering the number of collisions $q$ suffered by a particle since it has collided with a boundary. Each time a particle $i$ collides with another particle, $q_i$ is incremented by 1, and after it collides with either heating boundary, $q_i$ is set to zero. The probability distribution of the vertical distance $l$ of a particle from the wall it last collided with, is shown in the inset of Fig.3 for various values of $q$. As expected, P(l) broadens and shifts.

![FIG. 1: (a) Temperature ratio profile and (b) number density ratio profile for two species of particles along the vertical (z) direction. The particles differ only in their masses with $m_b = 5m_a$. There are 100 particles of each species in a rectangle of size $48 \times 32d$, corresponding to an area fraction of 10.2%. Three levels of differential heating are shown: $E_a = E_a\langle \text{dotted line} \rangle$, $E_a = E_a/5\langle \text{solid line} \rangle$, $E_a = E_a/25\langle \text{dashed line} \rangle$.]

![FIG. 2: Density Ratio vs. z/d for three levels of differential heating: $E_a = E_a\langle \text{dotted line} \rangle$, $E_a = E_a/5\langle \text{solid line} \rangle$, $E_a = E_a/25\langle \text{dashed line} \rangle$.]
monotonically to larger \( l \), for larger \( q \), saturating at the half-height of the system 16\( d \) for large \( q \). Next, statistics for the kinetic energy of the two types of particles as a function of \( q \) are sampled at fixed time intervals during a long simulation time and the temperature ratio \( \gamma \) is obtained as a function of \( q \). As shown in Fig.3, each curve of \( \gamma(q) \) reaches a plateau after a small number of collisions. This is consistent with MD simulations of bidisperse systems\[13\] where it was found that after about 10 collisions the temperature ratio \( \gamma \) reached a steady-state value from arbitrary initial conditions. However, as can be seen in Fig.3, the asymptotic value of \( \gamma \) at large \( q \) remains a function of \( E_b/E_a \). Therefore, details of the driving mechanism at the boundary appear not to be erased by interparticle collisions. To ensure that this conclusion is not dominated by particles that suffered many collisions but happened to remain close to a boundary, we also plot in Fig.3 \( \gamma \) for the subset of particle trajectories that start at one heating wall and terminate at the other. The plateau values of \( \gamma \) of these trajectories coincide with those from the entire set of particles.

It may still be argued that a finite-size effect persists since particles with large \( q \) suffer collisions with particles that have recently collided with the boundary. In order to further confirm the persistent effect of the differential heating mechanism we turn to a numerical model without spatial degrees of freedom, based on that introduced by van Zon and MacKintosh\[13\] to simulate a monodisperse system. A system of 2N(N=100) inelastic particles is initialized with gaussian-distributed initial velocities, and in each time step, \( C \) pairs of particles are randomly selected to collide in a 2-dimensional inelastic collision, and \( H \) particles are selected for heating. The impact parameters for the collisions are chosen from a uniform random distribution. For each heating event, velocities are selected randomly from Gaussian distributions with average energy \( E_a \) and \( E_b \), depending on the species of particle selected. Once again, the three cases of differential heating used in the spatial event-driven simulations can also be implemented here. For each of these three cases, statistics for the temperature ratio \( \gamma \) are accrued for many values of \( q_{\text{avg}} = 2C/H \), the ratio of the frequency of collisions to heating events. (The large \( q_{\text{avg}} \) limit corresponds to a boundary driven system in which the inter-particle collisions are much more frequent than heating events, and corresponds to large \( q \) in Fig.3 without the complications introduced by spatial gradients). As shown by the three sets of data symbols in Fig.4, the temperature ratio \( \gamma \) as a function of \( q_{\text{avg}} \) is different for the three heating mechanisms even for large \( q_{\text{avg}} \), where the heating events are rare relative to the collisions that one might intuitively expect to erase details of the heating mechanism.

The numerical model discussed above can be described in terms of an exactly solvable stochastic model\[19\]. We have adapted the model of Shokef and Levine\[19\] to incorporate equal numbers of two types of particles \( a \) and \( b \). The time evolution of the energy \( E^i(t) \) of a particle \( i \) of either species during an infinitesimal time step \( dt \) is
expressed by a stochastic equation,

\[
E^i(t + dt) = \begin{cases} 
E^i(t), & \text{probability: } 1 - Pdt, \\
\frac{\lambda_{ij}(1-\eta)^2}{2(1+\lambda_{ij})}E^j(t) - \frac{\lambda_{ij}(1+\lambda_{ij})^2}{2(1+\lambda_{ij})^2}E^i(t) + \frac{(1-\eta^2) + \frac{1}{2}}{4}E^i(t), & \text{probability: } (1-f)Pdt,
\end{cases}
\]

\[E^a_i \text{ or } E^b_i, \quad fPdt,\]

where \(E^{(j)}(t)\) is the instantaneous energy of the particle \(j\) at time \(t\), \(P\) is the interaction rate per particle per unit time, \(f\) is the fraction selected for external heating, \(\lambda_{ij} = m_i/m_j\), \(\eta\) is the restitution coefficient, \(E^a_i, b\) is the external energy given to particle \(i\) for a heating event with an input energy \(E^a_i\) or \(E^b_i\) depending on the species of particle \(i\). Therefore, the first line on the RHS of Eq.\[1\] corresponds to particle \(i\) not undergoing interaction, the second line corresponds to particle \(i\) being selected for collision with another particle \(j\) (averaged over collisions with species \(a\) and \(b\)) and the third line corresponds to particle \(i\) being selected for heating. For the second line, we use a simple one-dimensional collision model with uncorrelated pre-collisional velocities. In steady state, the ensemble averages obey \(<E^i(t + dt)> = <E^i(t)>\). By solving this stochastic equation, we determine the dependence of the temperature ratio \(\gamma\) on \(q_{avg}\) as shown in Fig.\[4\]. To make comparison to the numerical simulations of the random heating model, we make the correspondence \(f = H/(H + 2C) = 1/(1 + q_{avg})\). Once again, three different values of \(E_b/E_a\) are shown. Despite the simplified treatment of collisions within our adaptation of the Shokef-Levine model, we obtain reasonable agreement between the numerical model and this stochastic model. Qualitatively, the dependence on \(E_b/E_a\) follows the same trend, and the smooth curves in Fig.\[4\] for the three heating conditions do not converge at large \(q_{avg}\).

In summary, we have demonstrated by three independent means, the persistent effect of the boundary heating mechanism on the extent of nonequipartition in a binary granular system. The specific context for studying the effect of differential heating come from studies of vibration-fluidized granular systems, however, this type of differential heating should be generic to other forms of driving: in shear, for example, particles will be differentially excited depending on their frictional properties, shape, or size relative to the features of the shearing surface. Similar effects may be anticipated even in monodisperse systems where the equipartition between rotational and translational degrees of freedom may not be determined purely by particle properties but by the degree to which each degree of freedom is pumped by the driving mechanism. More generally, details of the boundary heating mechanism can not be ignored in describing inelastic gases, leading to concerns about quantitative comparisons between theories of homogeneously excited granular systems and boundary-driven experiments.

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* Electronic address: hqwang@physics.umass.edu
† Electronic address: menon@physics.umass.edu

[1] C.Bizon, M.D.Shattuck, J.B.Swift, and H.L.Swinney, Phys. Rev. E, 60, 4343(1999); E.L.Grossman, T.Zhou, and E.Ben-Naim, Phys. Rev. E, 55, 4200(1997).
[2] I.Goldhirsch, Annu. Rev. Fluid Mech. 35, 267(2003).
[3] E.Bertin, K.Martens, O.Dauchot, and M.Droz, Phys. Rev. E 75, 031120(2007).
[4] Y.Shokef, G.Shult and D.Levine, Phys. Rev. E, 76,030101(2007).
[5] W.Losert et al., Chaos 9, 682(1999).
[6] K. Feitosa and N.Menon, Phys. Rev. Lett., 88, 198301(2002).
[7] R.D.Wildman and D.J.Parker, Phys. Rev. Lett. 88, 064301(2002).
[8] A.Barrat and E.Trizac, Phys. Rev. E 66, 051303(2002).
[9] D.Paolotti, C.Cattuto, U.Marinelli Bettolo Marconi, A.Puglisi, Granular Matter 5(2), 75(2003).
[10] H.-Q. Wang, G.-J. Jin, and Y.-Q. Ma, Phys. Rev. E 68, 031301(2003).
[11] J.T. Jenkins and F. Mancini, J. Appl. Mech, 54, 27(1987).
[12] V.Garzó and J.Dufty, Phys. Rev. E 60, 5706(1999).
[13] S.R.Dahl, C.M.Hrenya, V.Garzó and J.W.Dufty, Phys. Rev. E 66, 041301(2002).
[14] A.Barrat, E.Trizac, Granular Matter 4(2), 57(2002).
[15] R.Pagnani, U.Marinelli Bettolo Marconi and A.Puglisi.
[16] W.A.M. Morgado, Physica A 320, 60 (2003).
[17] U. Marini Bettolo Marconi and A. Puglisi, Phys. Rev. E 66, 011301 (2002).
[18] J. S. van Zon and F. C. MacKintosh, Phys. Rev. Lett. 93, 038001 (2004); Phys. Rev. E 72, 051301 (2005).
[19] Y. Shokef, D. Levine, Phys. Rev. E 74, 051111 (2006); Y. Srebro and D. Levine, Phys. Rev. Lett., 93, 240601 (2004).