

Energy nonequpartition in systems of inelastic, rough spheres

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We calculate and verify with simulations the ratio between the average translational and rotational energies of systems with rough, inelastic particles, either forced or freely cooling. The ratio shows a nonequpartition of energy. In stationary flows, this ratio depends mainly on the particle roughness, but in nonstationary flows, such as freely cooling granular media, it also depends strongly on the normal dissipation. The approach presented here unifies and simplifies different results obtained by more elaborate kinetic theories. We observe that the boundary induced energy flux plays an important role. [S1063-651X(98)11108-X]

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Granular materials are collections of macroscopic particles with rough surfaces and dissipative interactions. Although rotation and friction are often neglected, they play an active role for the dynamics of systems with rough or non-spherical constituents. In contrast to classical elastic systems, energy is not equipartitioned between the degrees of freedom in the system [1–5]. In order to examine this ratio, kinetic theories [1–4] and numerical simulations [5] were applied for special boundary conditions, and a variety of results was obtained. We unify these results in a single theory which also explains when each one is valid.

We consider a system of N particles. We define \bar{E} to be the average translational kinetic energy per degree of freedom, and E^o to be the rotational kinetic energy per degree of freedom, so that

$$\bar{E} \equiv \frac{1}{N\bar{n}} \sum_{i=1}^N \frac{m}{2} v_i^2 \quad \text{and} \quad E^o \equiv \frac{1}{Nn^o} \sum_{i=1}^N \frac{mq}{2} a^2 \omega_i^2. \quad (1)$$

Here, m is the mass and a the radius of a particle. v_i is the velocity of particle i , and ω_i is its angular velocity. \mathcal{D} is the number of dimensions (we restrict ourselves to $\mathcal{D}=2$ and 3 here), q is the dimensionless moment of inertia; $q=\frac{1}{2}$ for disks, and $q=\frac{2}{5}$ for spheres. The number of translational degrees of freedom per particle is $\bar{n}=\mathcal{D}$, and the number of rotational degrees of freedoms is $n^o=2\mathcal{D}-3$. \bar{E} and E^o are often referred to as ‘‘granular temperatures.’’ This terminology is not intended to suggest that a thermodynamic equilibrium exists in granular flows, but simply to draw an analogy with the temperature of an ideal gas, which is also the average energy per degree of freedom. \bar{E} and E^o in Eq. (1) are well defined whether or not the system is in equilibrium. In this paper, we consider all particles to be identical, however, the above definitions can easily be extended to different types of particles.

We quantify the distribution of energy between the translational and rotational modes with the quantity $R \equiv E^o/(E^o + \bar{E})$. When there is no energy in the rotational mode, $R=0$. When energy is equally distributed between all the modes, $R=\frac{1}{2}$. If rotational energy dominates, then $R \rightarrow 1$. We will study how R depends on the particle properties and the

boundary conditions. This question has been addressed by several authors [1–4], but serious and unexplained conflicts exist between their results. For example, Ref. [4] claimed that R depends on the normal restitution, whereas [1–3] said that R is independent of this parameter.

We use the standard constant roughness model for the instantaneous collisions of rotating particles with radius a , mass m , and moment of inertia $I=qma^2$. This model accounts for dissipation, using the restitution coefficient r and the tangential restitution β . Since this has been extensively used and discussed [1–4], we include only the results here. The post-collisional velocities \mathbf{v}' and $\boldsymbol{\omega}'$ are given in terms of the precollisional velocities \mathbf{v} and $\boldsymbol{\omega}$ by

$$\begin{aligned} \mathbf{v}_{1,2}' &= \mathbf{v}_{1,2} + \frac{1+r}{2} \mathbf{v}_n + \frac{q(1+\beta)}{2q+2} (\mathbf{v}_t + \mathbf{v}_r), \\ a\boldsymbol{\omega}_{1,2}' &= a\boldsymbol{\omega}_{1,2} + \frac{1+\beta}{2q+2} [\hat{\mathbf{n}} \times (\mathbf{v}_t + \mathbf{v}_r)]. \end{aligned} \quad (2)$$

Here $\mathbf{v}_n \equiv [(\mathbf{v}_1 - \mathbf{v}_2) \cdot \hat{\mathbf{n}}] \cdot \hat{\mathbf{n}}$ is the component of $\mathbf{v}_1 - \mathbf{v}_2$ parallel to $\hat{\mathbf{n}}$, a unit vector pointing along the line connecting the centers of the colliding particles. The tangential component of $\mathbf{v}_1 - \mathbf{v}_2$ is $\mathbf{v}_t \equiv \mathbf{v}_1 - \mathbf{v}_2 - \mathbf{v}_n$, and $\mathbf{v}_r \equiv -a(\boldsymbol{\omega}_1 + \boldsymbol{\omega}_2) \times \hat{\mathbf{n}}$ is the tangential velocity due to particle rotation.

Later on, we will need expressions for the change in rotational and translational kinetic energy during a collision. The change in translational energy is

$$N\bar{n}\Delta\bar{E} \equiv -Qv_n^2 + S[-C_{t1}v_t^2 - C_{t2}(\mathbf{v}_t \cdot \mathbf{v}_r) + C_{t3}v_r^2], \quad (3)$$

with the positive prefactors $Q \equiv m(1-r^2)/4$, $S \equiv mq(1+\beta)/[4(1+q)^2]$, and the constants $C_{t1} \equiv 2+q(1-\beta)$, $C_{t2} \equiv 2-2q\beta$ and $C_{t3} \equiv q(1+\beta)$. Likewise, the change in rotational energy is

$$Nn^o\Delta E^o \equiv +S[C_{r1}v_t^2 - C_{r2}(\mathbf{v}_t \cdot \mathbf{v}_r) - C_{r3}v_r^2], \quad (4)$$

where the constants are $C_{r1} \equiv (1+\beta)$, $C_{r2} \equiv 2(q-\beta)$, and $C_{r3} \equiv 2q+1-\beta$. Note that the (constants) C are positive (except that C_{r2} can be negative) so that the signs in Eqs. (3) and (4) indicate the direction of energy transfer between the degrees of freedom.

The quantity R (or its equivalent) has been calculated by several authors. One result found by three different authors [1–3] for granular material undergoing uniform shear is

$$R = \frac{q(1+\beta)}{q(1+\beta) + (1+2q-\beta)}, \quad (5)$$

i.e., a function independent of r .

On the other hand, Goldshtein and Shapiro [4] found a much different expression (for $D=3$), involving r :

$$R = \frac{1}{2} \left(1 - \frac{a_G}{b_G + \sqrt{a_G^2 + b_G^2}} \right), \quad (6)$$

with the quantities $a_G \equiv (1-\beta^2)(1-q)/(1+q) - 1 + r^2$ and $b_G \equiv 2q(1+\beta)^2/(1+q)^2$. Equation (6) differs greatly from Eq. (5) when $r < 1$. In the following, we show that the differences between Eqs. (5) and (6) arise from the boundary conditions, i.e., from the existence of external forcing.

Consider a granular material with external forcing, where the particles interact only through collisions obeying Eq. (2). The change in E^o from time t_0 to t_1 is

$$E^o(t_1) - E^o(t_0) = \sum_{\text{coll.}} \Delta E^o(C_i) + \frac{1}{Nn^o} \int_{t_0}^{t_1} P^o(t) dt, \quad (7)$$

where P^o is the rotational energy added by the forcing. The sum is taken over all the collisions which take place between t_0 and t_1 , and $\Delta E^o(C_i)$ is the change in E^o for collision i . Now, consider a situation where the granular medium is maintained in a stationary state [$E^o(t_1) = E^o(t_0)$] by some kind of forcing, and that this forcing adds only translational kinetic energy [$P^o = 0$]. Equation (7) becomes $\sum_{\text{coll.}} \Delta E^o(C_i) = 0$, which states that collisions do not, on average, change the rotational energy. When the assumptions made above are satisfied, the dissipation of rotational energy is exactly balanced by the conversion of \bar{E} into E^o . Using Eq. (4), we obtain: $-C_{r1}\langle v_t^2 \rangle + C_{r2}\langle \mathbf{v}_t \cdot \mathbf{v}_r \rangle + C_{r3}\langle v_r^2 \rangle = 0$. Here the angle brackets $\langle \dots \rangle$ indicate an average taken over the collisions. We now consider how to calculate these averages.

If ψ is the quantity to be averaged, then

$$\langle \psi \rangle = \{ \psi P_{\text{coll}}(\mathbf{v}_1, \mathbf{v}_2, \boldsymbol{\omega}_1, \boldsymbol{\omega}_2, b) \}_{b,1,2}, \quad (8)$$

where P_{coll} gives the probability of a collision occurring between particles 1 and 2 with a normalized impact parameter $0 \leq b \leq 1$. The normalized impact parameter is the distance between particle centers at closest approach if the particles did not interact, normalized by the particle diameter. The subscripts on the curly brackets means we average over all values of b , and over all pairs of particles. We now make several simplifying assumptions about P_{coll} . First, we assume that the angular velocities have no effect on the probability of collision: $P_{\text{coll}} = P_{\text{coll}}(\mathbf{v}_1, \mathbf{v}_2, b)$. Next, we assume that $P_{\text{coll}} \sim v f(b)$, ($v \equiv |\mathbf{v}_1 - \mathbf{v}_2|$) because particles with large relative velocities are more likely to collide. Finally, the dependence of P_{coll} on b can be deduced from geometrical arguments: $P_{\text{coll}} \sim v$ for $D=2$ and $P_{\text{coll}} \sim vb$ for $D=3$. Thus we have

$$\langle \psi \rangle = \{ \psi v (2b)^{D-2} \}_{b,1,2} / \{ v \}_{b,1,2}, \quad (9)$$

with the factor of 2 and the denominator required for normalization.

Since the rotational and translational velocities are uncorrelated,

$$\langle v_r^2 \rangle = \{ v_r^2 \}_{1,2} = 2a^2 \{ (\boldsymbol{\omega}_1 \times \hat{\mathbf{n}})^2 \}_1 = \frac{4(D-1)}{qm} E^o, \quad (10)$$

where $\{ \}_1$ indicates an average over all particles. The factor of $D-1$ arises because, in $D=3$, one of the three rotational degrees of freedom is excluded by the cross product with $\hat{\mathbf{n}}$. In $D=2$, there is only one rotational degree of freedom, and it always participates in every collision.

To calculate $\langle v_n^2 \rangle$ and $\langle v_t^2 \rangle$, we use $v_t^2 = v^2 b^2$ and $v_n^2 = v^2 - v_t^2$. The average can be factored into two parts:

$$\begin{aligned} \langle v_t^2 \rangle &= \frac{\{ v^3 b^2 (2b)^{D-2} \}_{b,1,2}}{\{ v \}_{1,2}} \\ &= \{ b^2 (2b)^{D-2} \}_b \frac{\{ v^3 \}_{1,2}}{\{ v \}_{1,2}}. \end{aligned} \quad (11)$$

Evaluating the first factor gives $\{ b^2 (2b)^{D-2} \}_b = D/6$, where $\{ \}_b$ indicates an average over all possible values of b . The second factor will be proportional to \bar{E}/m , but calculating the coefficient requires a knowledge of the distribution of velocities. Assuming a Maxwellian velocity distribution gives $\{ v^3 \}_{1,2} / \{ v \}_{1,2} = 24(D-1)\bar{E}/(Dm)$. Then we have $\langle v_t^2 \rangle = 4(D-1)\bar{E}/m$ and $\langle v_n^2 \rangle = 8\bar{E}/m$.

All of the assumptions we have made up to now are equivalent to those made in the kinetic theories [1–4]. Thus it is not surprising that we recover some of their results. In particular, putting the averages into Eq. (7) gives $-C_{r1}\bar{E} + C_{r3}E^o/q = 0$, and, after using the definitions of C_{r1} and C_{r3} , we obtain R as in Eq. (5).

Equation (5) does not depend on r because R is fixed by a balance between the conversion of \bar{E} into E^o and the dissipation of E^o . Both of these processes depend only on β and q , but not on r . As soon as the dissipation of \bar{E} starts to play a role in determining R , then r will appear. We examine such a case next. Consider a granular medium in the absence of forcing. If $r \neq 1$ and $\beta \neq 1, -1$, then E^o and \bar{E} decrease toward 0, but R can approach a constant. This can be verified by simulations and a more elaborate calculation in the framework of the kinetic theory [4], or with a Liouville operator formalism [6,7].

In the following, we simplify the algebra by using $K = \bar{E}/E^o$ instead of R [$R = 1/(1+K)$]. During a collision, K changes by

$$\Delta K = \frac{\bar{E} + \Delta \bar{E}}{E^o + \Delta E^o} - K = \frac{\Delta \bar{E} - K \Delta E^o}{E^o + \Delta E^o}. \quad (12)$$

We look for a value of K such that $\Delta K = 0$. The denominator of this equation is always positive. Equating the numerator to

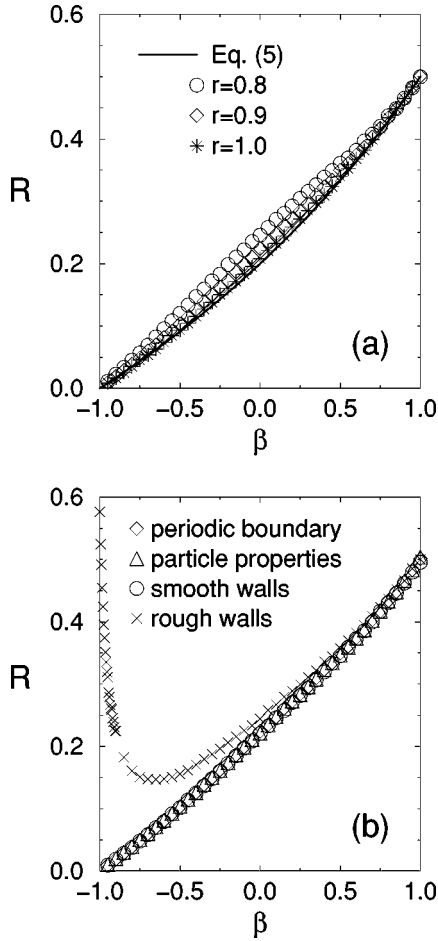


FIG. 1. Simulation results from a vertically vibrated system. (a) R is compared with the theoretical prediction in Eq. (5) for three values of r . (b) The data for $r=0.9$ from (a) are compared to simulations with different boundary conditions (see text for details).

0, we find that a collision leaves R unchanged if $K = \Delta \bar{E} / \Delta E^o$. This equation can be expanded in terms of $\langle v_n^2 \rangle$, $\langle v_t^2 \rangle$, and $\langle v_r^2 \rangle$ using Eqs. (3) and (4), to

$$K = \frac{A \langle v_n^2 \rangle + C_{t1} \langle v_t^2 \rangle - C_{t3} \langle v_r^2 \rangle}{-\alpha C_{r1} \langle v_t^2 \rangle + \alpha C_{r3} \langle v_r^2 \rangle}, \quad (13)$$

where $\alpha \equiv \bar{n}/n^o$, and $A \equiv Q/S$ [see Eq. (3)]. Because the energy decreases with every collision, the averages must be interpreted as taken over all possible collisions at a given time.

Using our previous expressions for the averages and reorganizing Eq. (13) as a quadratic equation for K yields

$$\alpha \frac{b_G}{2} K^2 - [\alpha a_G + (\alpha - 1) c_G] K - \frac{b_G}{2} = 0, \quad (14)$$

with the quantities a_G and b_G from Eq. (6), and $c_G \equiv (1 + \beta)(2q + q^2 - \beta q^2)/(1 + q)^2$. In deriving Eq. (14), we used $\alpha = 2/(\mathcal{D} - 1)$. For $\mathcal{D} = 3$, we have $\alpha = 1$, and the solution of Eq. (14) leads to Eq. (6).

Next we compare the theoretical results, derived above, with simulations in $\mathcal{D} = 2$. We examine three different simulation “experiments.” In the first case, energy is put into

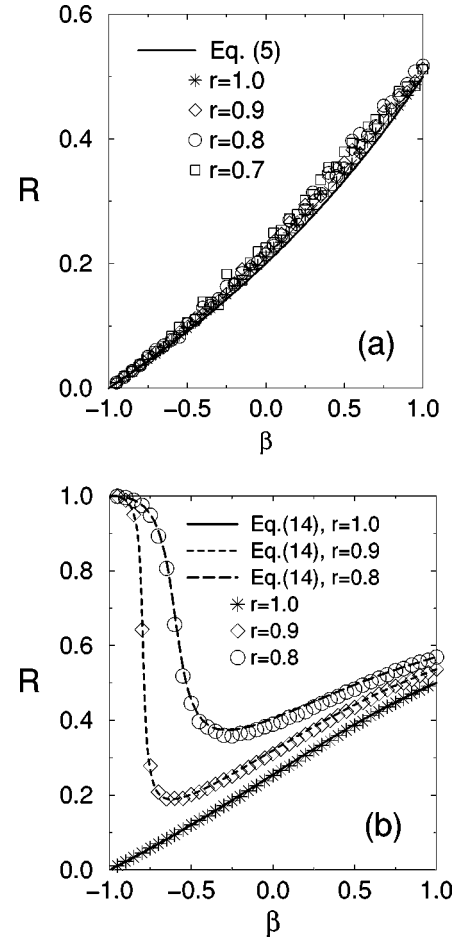


FIG. 2. (a) Results of the shearing experiment. The points show the results for different r , compared to the analytical result. (b) Results of the cooling experiment. The points show the results of simulations and the curves give $R = 1/(1 + K)$ with K from Eq. (14), with the appropriate value of r , and $\mathcal{D} = 2$.

one translational mode by a vibrating wall, and, in the second case, a granular material under sheared periodic boundary conditions is examined. Finally, a granular media is studied in the absence of any forcing whatsoever. On the basis of the theory presented above, we expect the first two cases to obey Eq. (5), and the last case to obey Eq. (6). In all cases, we perform the experiments with different r , and for each value of r , we vary β from -0.95 to 1 .

In the first experiment, $N = 160$ particles of radius a are placed on a vertically vibrating floor in the presence of gravity. The boundaries in the horizontal direction are periodic, the domain is 50 particle radii wide and infinitely high. The period of the floor vibration T and the gravitational acceleration are here related by $gT^2/a = 1$. The height of the floor varies periodically in time, following an asymmetric sawtooth wave form. (The choice of wave form is arbitrary; changing the wave form does not significantly change R .) The floor moves up a distance of $5a$, with an upwards velocity $5a/T$, and then returns instantly to its lowest position. In all cases, the simulations ran for $7000T$, with R being measured every $\Delta t = 0.25T$ for $5000T \leq t \leq 7000T$, and these values were averaged to give the points in Fig. 1(a). Since this experiment satisfies the assumption that energy is input into the translational modes only, we expect that the results will satisfy Eq. (5). Figure 1(a) confirms that this is indeed

the case, with some systematic underestimation of R by the theory when the dissipation is strong.

Since it is difficult to do experiments with periodic boundaries, we also examined the effect of stationary side-walls at the edges of the domain. We compare the results for $r=0.9$ from Fig. 1(a) with three different types of boundary conditions. (i) a perfectly rough wall with wall properties $r=\beta=1$, (ii) a wall where r and β have the same values for particle-particle and particle-wall collisions, and (iii) a perfectly elastic and smooth wall with $r=1$ and $\beta=-1$. The results presented in Fig. 1(b) show that only the first type of wall causes R to deviate significantly. We relate this to a competition between particle-particle and particle-wall collisions: The collisions with the wall in case (i) push R toward $R(\beta=1)=\frac{1}{2}$; i.e., equipartition holds, and the collision between particles push R toward a smaller value. (At $\beta=-1$, $R>\frac{1}{2}$ because the kinetic energy of the vertical velocities is greater than that of the horizontal, and the wall couples only to the vertical motions.) In case (ii), both types of collisions push R toward the same value, and in case (iii) the particle-wall collisions do not influence R , so that the results are not perturbed at all.

In the second experiment, we drive the granular material by shearing it, a case frequently considered in the literature [1–3]. $N=160$ particles are placed in a square domain whose sides are $L=50a$ in length. The boundaries are periodic in the x and y directions. A uniform shear is imposed by applying Lees-Edwards boundary conditions [8]: when a particle exits the domain at the bottom (top), its image enters at the top (bottom) of the domain, with its x velocity increased by a constant velocity U ($-U$), at its position shifted by a distance Ut ($-Ut$). These boundary conditions eliminate the need to specify wall properties, and make the system translationally invariant. In our simulations, $U=2a/T$, giving a shear rate of $\Gamma=U/L=0.04/T$. The time unit T is arbitrary.

A direct application of Eq. (5) will fail, because the boundary conditions generate both an average flow and an average rotation. However, if we interpret E^o and \bar{E} to be the energy which remains after removing the mean flow and rotation, the agreement between theory and simulation is good,

as shown in Fig. 2(a). The translational kinetic energy of the mean flow was calculated as $\bar{E}_{\text{mean}}=(m/2)\times\Gamma^2(1/N)\sum_{i=1}^N(y_i-L/2)^2$. The rotational energy of the mean flow was estimated by $E_{\text{mean}}^o=mqa^2\Omega^2/2$, where Ω is the observed average angular velocity. Even with longer averaging times ($5000T$ in our simulations), the data are considerably noisier than in Fig. 1.

In the last experiment, $N=160$ particles are placed in a periodic domain with $L=100a$, but no shear is applied. The initial condition is generated by setting $r=1$ and $\beta=-1$. The particles quickly attain a Maxwellian velocity distribution. Then dissipation is “switched on,” and the system evolves without any further input of energy. Although the energy decreases with every collision, R approaches the constant value shown in the graph. The results of many simulations were averaged together to reduce the fluctuations. In Fig. 2(b), we plot the results. The theoretical curves are the solutions of Eq. (14), with $\alpha=2$, and the three values of r shown in the plot.

In conclusion, we extend Eq. (6) to two dimensions and summarize the different results for R in the literature. Our method of calculation is simple enough to show why Eq. (5) applies to forced granular media, and Eq. (6) to cooling granular media. Equation (5) will apply whenever the forcing adds only translational energy. This is the case for both vibration and shear. We succeeded in formulating a procedure to calculate the ratio of tangential and rotational energy in homogeneously cooling systems. Our result replaces the value $K=1/2$ (in two dimensions when equipartition is true for elastic systems). We examined not only the limit of almost elastic particles, but also rather inelastic situations. For most boundary conditions used, the agreement between theory and simulations is encouraging. However, simulations in $\mathcal{D}=3$ are still needed to check the analytical expressions. Possible future work includes boundary conditions with non-zero rotational energy input, and calculating R for the more realistic interaction model that accounts also for Coulomb friction. [5,9,10]

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