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Dynamics of inelastically colliding rough spheres: Relaxation of translational and rotational energy

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We study the exchange of kinetic energy between translational and rotational degrees of freedom for inelastic collisions of rough spheres. Even if equipartition holds in the initial state it is immediately destroyed by collisions. The simplest generalization of the homogeneous cooling state allows for two temperatures, characterizing translational and rotational degrees of freedom separately. For times larger than a crossover frequency, which is determined by the Enskog frequency and the initial temperature, both energies decay algebraically like t^{-2} with a fixed ratio of amplitudes, different from 1. [S1063-651X(97)51112-3]

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Kinetic theory of inelastically colliding particles has become a subject of growing research activity, motivated partly by renewed interest in granular materials. A Boltzmann equation and the Enskog variant of it have been formulated for inelastically colliding particles with normal and tangential restitution [1–6]. Whereas the derivation of the kinetic equation is relatively straightforward, the methods of solution which were developed for elastic collisions cannot be taken over to the inelastic case because there is no simple stationary or local equilibrium distribution, around which one could expand the nonlinear kinetic equation. One simple distribution is the homogeneous cooling state (HCS) [7,8], which depends on time only implicitly via the average kinetic energy $T(t)$. The latter is predicted to decay like t^{-2} for large times. The homogeneity assumption is certainly violated when clustering occurs and, in particular, if inelastic collapse happens. Nevertheless we have found recently [9] in a model of inelastically colliding rods that the kinetic energy follows *on average* a t^{-2} behavior, even if clustering occurs. This suggests that the above scaling law may be a useful approximate description, even when the assumptions of HCS break down.

In this paper we show that rotational and translational energy relax with different rates in general. Once friction is included, HCS with a single time dependent temperature is no longer consistent with the time evolution of translational and rotational energy separately. Instead, one has to introduce two temperatures that characterize translational and rotational degrees of freedom separately. Both are found to fall off like t^{-2} with the ratio approaching a constant value, which is determined by the coefficients of normal and tangential restitution.

We briefly recall the collision dynamics of hard spheres with normal and tangential restitution. These results can, for example, be found in Cerginani [6]. We consider two spheres of equal diameter a, mass M, and moment of inertia I. The unit vector from the center of the first sphere to the center of the second is denoted by $\hat{\boldsymbol{n}}$ and velocities and angular velocities before collision by $\boldsymbol{v}_1$, $\boldsymbol{v}_2$, $\boldsymbol{\omega}_1$, and $\boldsymbol{\omega}_2$. The relative velocity of the contact point before collision is given by $\boldsymbol{V}=\boldsymbol{v}_2+a/2\,\hat{\boldsymbol{n}}\times\boldsymbol{\omega}_2-\boldsymbol{v}_1+a/2\,\hat{\boldsymbol{n}}\times\boldsymbol{\omega}_1$. Normal and tangential restitution determine the relative velocity after collision according to

$$\hat{\boldsymbol{n}}\cdot\boldsymbol{V}'=-\epsilon(\hat{\boldsymbol{n}}\cdot\boldsymbol{V}),\quad \text{with}\ \ \epsilon\in[0,1], \tag{1}$$

$$\hat{\boldsymbol{n}}\times\boldsymbol{V}'=-\beta(\hat{\boldsymbol{n}}\times\boldsymbol{V}),\quad \text{with}\ \ \beta\in[-1,1]. \tag{2}$$

Using the property of conserved linear and angular momenta one obtains for the velocities after collision

$$\begin{aligned}
\boldsymbol{v}_1'&=\boldsymbol{v}_1-\eta_t\boldsymbol{v}_{12}-(\eta_n-\eta_t)(\hat{\boldsymbol{n}}\cdot\boldsymbol{v}_{12})\hat{\boldsymbol{n}}+\eta_t\frac{a}{2}\,\hat{\boldsymbol{n}}\times(\boldsymbol{\omega}_1+\boldsymbol{\omega}_2),\\
\boldsymbol{v}_2'&=\boldsymbol{v}_2+\eta_t\boldsymbol{v}_{12}+(\eta_n-\eta_t)(\hat{\boldsymbol{n}}\cdot\boldsymbol{v}_{12})\hat{\boldsymbol{n}}-\eta_t\frac{a}{2}\,\hat{\boldsymbol{n}}\times(\boldsymbol{\omega}_1+\boldsymbol{\omega}_2),\\
\boldsymbol{\omega}_1'&=\boldsymbol{\omega}_1-\frac{2}{ak}\,\eta_t\hat{\boldsymbol{n}}\times\boldsymbol{v}_{12}+\frac{\eta_t}{k}\,\hat{\boldsymbol{n}}\times[\hat{\boldsymbol{n}}\times(\boldsymbol{\omega}_1+\boldsymbol{\omega}_2)],\\
\boldsymbol{\omega}_2'&=\boldsymbol{\omega}_2-\frac{2}{ak}\,\eta_t\hat{\boldsymbol{n}}\times\boldsymbol{v}_{12}+\frac{\eta_t}{k}\,\hat{\boldsymbol{n}}\times[\hat{\boldsymbol{n}}\times(\boldsymbol{\omega}_1+\boldsymbol{\omega}_2)],
\end{aligned} \tag{3}$$

with $\boldsymbol{v}_{12}=\boldsymbol{v}_1-\boldsymbol{v}_2$ and parameters $k:=4I/Ma^2$ ($k=0.4$ for homogeneous spheres), $\eta_n:=(1+\epsilon)/2$, and $\eta_t:=k(1+\beta)/[2(1+k)]$.

We consider a system of N classical particles, confined to a three-dimensional volume V and interacting via a hard-core potential. Each particle is characterized by its position $\boldsymbol{r}_i(t)$, its linear momentum $\boldsymbol{p}_i(t)=M\boldsymbol{v}_i(t)$, and angular velocity $\boldsymbol{\omega}_i(t)$. The time development of a dynamical variable $A=A(\{\mathbf{r}_i(t),\mathbf{p}_i(t),\boldsymbol{\omega}_i(t)\})$ is determined by a pseudo-Liouville-operator $\mathcal{L}_+$

$$A(\{\boldsymbol{r}_i,\boldsymbol{p}_i,\boldsymbol{\omega}_i\},t)=\exp(i\mathcal{L}_+t)A(\{\boldsymbol{r}_i,\boldsymbol{p}_i,\boldsymbol{\omega}_i\},0)\quad\text{for}\quad t>0. \tag{4}$$

Such a pseudo-Liouville-operator was first introduced for hard (perfectly smooth) spheres by Ernst *et al.* [10] and subsequently applied to the calculation of transport coefficients of a hard sphere fluid (see, e.g., [11] and references therein). Van Noije and Ernst [12] have generalized the formalism to inelastic collisions with normal restitution. Here we extend these results to rough spheres with normal and tangential restitution.

The pseudo-Liouville-operators $\mathcal{L}_+$ consist of two parts, $\mathcal{L}_+ = \mathcal{L}_0 + \mathcal{L}'_+$. The first one, $\mathcal{L}_0$, describes free streaming of particles

$$\mathcal{L}_0 = -\frac{i}{M}\sum_n \boldsymbol{p}_n \cdot \boldsymbol{\nabla}_{\boldsymbol{r}_n} \tag{5}$$

and the second one, $\mathcal{L}'_+ = \frac{1}{2}\Sigma_{n\neq m} T_+(nm)$, describes hard-core collisions of two particles by

$$T_+(nm) = \frac{i}{M}(\boldsymbol{p}_{nm}\cdot\hat{\boldsymbol{r}}_{nm})\Theta(-\boldsymbol{p}_{nm}\cdot\hat{\boldsymbol{r}}_{nm}) \times \delta(|\boldsymbol{r}_{nm}|-a)(b^+_{nm}-1). \tag{6}$$

The operator b^+_{nm} replaces the linear and angular momenta of two particles n and m before collision by the corresponding ones after collision. $\Theta(x)$ is the Heaviside step-function and we have introduced the notation $\boldsymbol{p}_{nm} = \boldsymbol{p}_n - \boldsymbol{p}_m$, $\boldsymbol{r}_{nm} = \boldsymbol{r}_n - \boldsymbol{r}_m$ and $\hat{\boldsymbol{r}} = \boldsymbol{r}/|\boldsymbol{r}|$.

Equation (6) has a simple interpretation. The factor $(\boldsymbol{p}_{nm}\cdot\hat{\boldsymbol{r}}_{nm})/M$ gives the flux of incoming particles. The Θ and δ functions specify the conditions for a collision to take place. A collision between particles n and m happens only if the two particles are approaching each other, which is taken into account by $\Theta(-\boldsymbol{p}_{nm}\cdot\hat{\boldsymbol{r}}_{nm})$. At the instant of a collision the distance between the two particles has to vanish, as expressed by $\delta(|\boldsymbol{r}_{nm}|-a)$. Finally $(b_{nm}-1)$ generates the change of linear and angular momenta [13].

The ensemble average of a dynamical variable is defined by

$$\langle A\rangle_t = \int d\Gamma\, \rho(0)A(t) = \int d\Gamma\, \rho(t)A(0) = \int \prod_i (d\boldsymbol{r}_i d\boldsymbol{p}_i d\boldsymbol{\omega}_i) \prod_{i<j} \Theta(|\boldsymbol{r}_{ij}|-a)\rho(t)A(0). \tag{7}$$

Here $\rho(t) = \exp(-i\mathcal{L}^\dagger_+ t)\rho(0)$ is the N-particle distribution function, whose time evolution is governed by the adjoint $\mathcal{L}^\dagger_+$ of the time evolution operator $\mathcal{L}_+$. The quantities of interest are the translational and rotational energies per particle

$$E_{\rm tr} = \frac{1}{N}\sum_i \frac{M}{2}\boldsymbol{v}_i^2, \tag{8}$$

$$E_{\rm rot} = \frac{1}{N}\sum_i \frac{I}{2}\boldsymbol{\omega}_i^2, \tag{9}$$

as well as the total kinetic energy $E = E_{\rm tr} + E_{\rm rot}$.

As a first step we compute the initial decay rates

$$\frac{d}{dt}\langle E_{\rm tr}\rangle_{t=0} = \langle i\mathcal{L}_+ E_{\rm tr}\rangle_{t=0} = \nu_{\rm tr}, \tag{10}$$

$$\frac{d}{dt}\langle E_{\rm rot}\rangle_{t=0} = \langle i\mathcal{L}_+ E_{\rm rot}\rangle_{t=0} = \nu_{\rm rot}, \tag{11}$$

assuming that the system has been prepared in a thermal equilibrium state $\rho(0)\propto\exp(-E/T)$, which is characterized by the temperature $3T/2 = \langle E\rangle_{t=0}$. The changes of translational and rotational energy are given by

$$\nu_{\rm tr} = -\frac{2\pi a^2 T^{3/2} n_0 g(a)}{(\pi M)^{1/2}}\left((1-\epsilon^2) + \frac{k}{1+k}(1-\beta^2)\right), \tag{12}$$

$$\nu_{\rm rot} = -\frac{2\pi a^2 T^{3/2} n_0 g(a)}{(\pi M)^{1/2}}\left(\frac{1}{1+k}(1-\beta^2)\right). \tag{13}$$

Here $g(a)$ denotes the pair correlation at contact and $n_0 = N/V$. Rotational energy is conserved in two cases, for either perfectly smooth spheres ($\beta = -1$) or perfectly rough spheres ($\beta = +1$). Translational energy is only conserved if in addition $\epsilon = 1$. For all other values of the parameters ϵ and β the translational and rotational energy decrease linearly with time but with *different* rates. This implies that after a small time interval Δt equipartition among rotational and translational degrees of freedom no longer holds,

$$\langle E_{\rm tr}\rangle_{\Delta t} = \langle E_{\rm tr}\rangle_0 - \nu_{\rm tr}\Delta t, \qquad \langle E_{\rm rot}\rangle_{\Delta t} = \langle E_{\rm rot}\rangle_0 - \nu_{\rm rot}\Delta t. \tag{14}$$

Hence for collisions with friction ($\beta \neq -1$) the homogeneous cooling state is not consistent with the time evolution of translational and rotational energy separately. To generalize the concept of a homogeneous cooling state to collisions with friction we introduce two temperatures $T_{\rm tr}(t) = 2/3\langle E_{\rm tr}\rangle_t$ and $T_{\rm rot}(t) = 2/3\langle E_{\rm rot}\rangle_t$. We keep the assumption of spatial homogeneity and assume that both linear and angular momenta are normally distributed with in general different time dependent widths or temperatures

$$\rho(t) \propto \exp -\frac{1}{2}\sum_{i=1}^N [M\boldsymbol{v}_i^2/T_{\rm tr}(t) + I\boldsymbol{\omega}_i^2/T_{\rm rot}(t)]. \tag{15}$$

The above distribution allows for a calculation of the decay rates of $T_{\rm tr}(t)$ and $T_{\rm rot}(t)$ for arbitrary times, resulting in two coupled differential equations,

$$\frac{d}{dt}T_{\rm tr} = -(1-\epsilon^2)\frac{\gamma}{4}T_{\rm tr}^{3/2} - \gamma\eta_t(1-\eta_t)T_{\rm tr}^{3/2} + \frac{\gamma}{k}\eta_t^2 T_{\rm tr}^{1/2}T_{\rm rot}, \tag{16}$$

$$\frac{d}{dt}T_{\rm rot} = \frac{\gamma}{k}\eta_t^2 T_{\rm tr}^{3/2} - \gamma\frac{\eta_t}{k}\left(1-\frac{\eta_t}{k}\right)T_{\rm rot}T_{\rm tr}^{1/2}, \tag{17}$$

with $\gamma = (16/3)a^2 n_0 g(a)\sqrt{\pi/M}$.

As we have seen above the energies decrease linearly for short times. For large times both, translational and rotational energy fall off algebraically like t^{-2} with, however, different amplitudes. The amplitudes can be determined analytically, e.g., by solving the differential equation for

$$\frac{dT_{\rm tr}}{dT_{\rm rot}} = \frac{-T_{\rm tr}[(1-\epsilon^2)/4 + \eta_t(1-\eta_t)] + T_{\rm rot}\eta_t^2/k}{T_{\rm tr}\eta_t^2/k - T_{\rm rot}(1-\eta_t/k)\eta_t/k}. \tag{18}$$

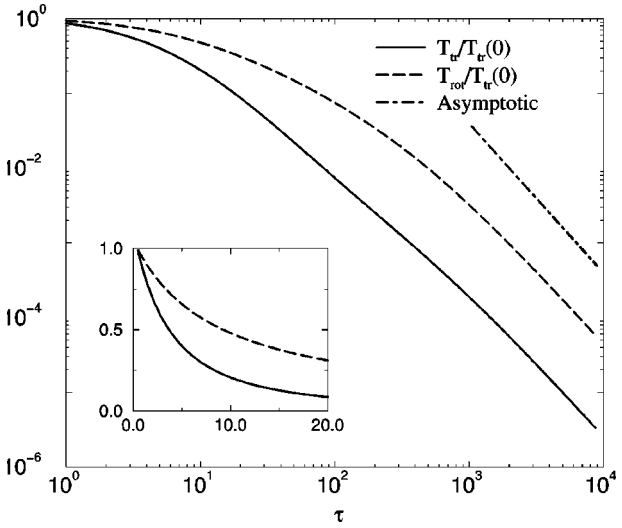

FIG. 1. Time decay of the translational and rotational energy. Parameters were chosen according to: $k=0.4$, $\epsilon=0.4$, $\beta=-0.6$, and $T_{tr}(0)=T_{rot}(0)=20$. We have introduced a dimensionless time argument $\tau=t\gamma\sqrt{T_{tr}(0)}$. The dashed–dotted line indicates the asymptotics.

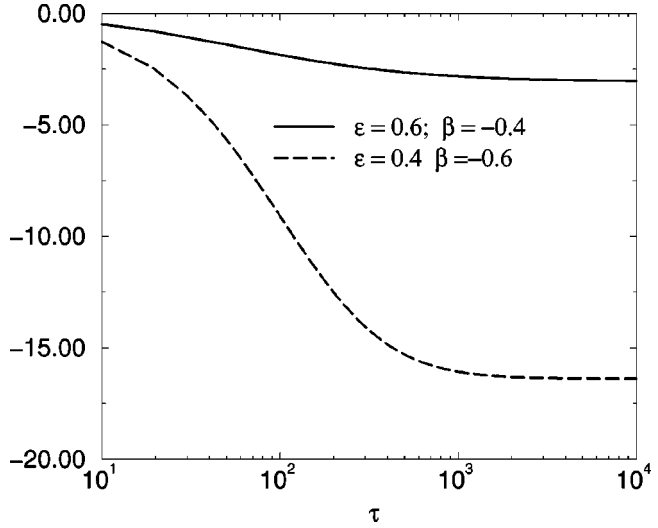

FIG. 2. Ratio $1-T_{rot}/T_{tr}$ as a function of time with $k=0.4$, $\gamma=1$, $T_{tr}(0)=T_{rot}(0)=100$, $\epsilon=0.6$, $\beta=-0.4$, and $\epsilon=0.4$, $\beta=-0.6$. Unit of time was chosen as in Fig. 1.

This equation is solved by a constant ratio $T_{tr}/T_{rot}=-c_1/c_2+\sqrt{1+(c_1/c_2)^2}$ with c_1, c_2 given in terms of ϵ, β and k by $c_1=(1-\epsilon^2)/4+(1-\beta^2)(k-1)/(4k+4)$ and $c_2=2k(1+\beta)^2/(2+2k)^2$, in agreement with Ref. [5]. The crossover time t_0 between the linear regime and the algebraic decay is determined by γ and $T_{tr}(0)$ according to $t_0^{-1}\propto\gamma\sqrt{T_{tr}(0)}$. The full solution [14] has been obtained by numerical integration of Eqs. (16,17) and is shown in Fig. 1 for $k=0.4$, $\gamma=1$, $\epsilon=0.4$, $\beta=-0.6$, and $T_{tr}(0)=T_{rot}(0)=20$. The asymptotics is indicated by a dashed-dotted line and the inset is a blowup of the short time behavior. The deviation of the ratio of rotational and translational energy from 1, i.e., $1-T_{rot}/T_{tr}$, is shown in Fig. 2 for two different values of β and ϵ.

Cooling of a granular gas has been investigated by several groups [15,16] modeling collisions with a normal coefficient of restitution. The t^{-2} behavior of the total energy has been confirmed for a wide range of parameters such that the system is stable to shear fluctuations [16] and inelastic collapse. Luding [17] has considered a more detailed model of inelastic collisions, including tangential restitution and Coulomb's law of friction. It is straightforward to generalize the model to include Coulomb friction; one just has to modify the updating rules [Eq. (3)] accordingly. Driving the system with a vibrating wall is an open problem so far. One may also generalize the approach to nonspherical objects, e.g., hard rods or needles [18], for which elastic collisions have been analyzed by Frenkel and Maguire [19].

Note added. After this paper was completed we learned about related work by S. McNamara and S. Luding who also studied the ratio of translational and rotational energy in the HCS.

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[13] In some calculations it is helpful to know the evolution backwards in time. In that case the momenta after collision are given and one wants to know the momenta before collision. These are obtained by replacing the parameters in Eq. (3) according to $\beta\rightarrow 1/\beta$ and $\epsilon\rightarrow 1/\epsilon$. With this replacement the momenta before collision are given by the right hand side of Eq. (3) in terms of the momenta after collision. These collision rules can then be used to construct an operator $\mathcal{L}_-$, which describes the evolution backwards in time, but in general $\mathcal{L}_-$ is not the adjoint of $\mathcal{L}_+$ (see also [12]).
[14] With the substitution $T_{tr}=z^2$ the two coupled differential equations can be reduced to a single second order equation

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