Rotationally driven gas of inelastic rough spheres

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We study a two-dimensional gas of inelastic rough spheres, driven on the rotational degrees of freedom. Numerical simulations are compared to mean-field (MF) predictions with surprisingly good agreement for strong coupling of rotational and translational degrees of freedom – even for very strong dissipation in the translational degrees. Although the system is spatially homogeneous, the rotational velocity distribution is essentially Maxwellian. Surprisingly, the distribution of tangential velocities is strongly deviating from a Maxwellian. An interpretation of these results is proposed, as well as a setup for an experiment.

PACS: 45.70, 47.50+d, 51.10.+y, 47.11.+j

Systems of hard spheres have a long-standing history as a basic model for gases, liquids, and e.g. glasses. When dissipation is added, one has the minimal model for granular materials and it is only a small step to include also the rotational degrees of freedom via a tangential interaction at contact. Granular materials belong to the fascinating world of non-linear, dissipative, non-equilibrium systems, whose interest is due to their practical importance and due to the theoretical challenges they represent. Granular media are collections of macroscopic particles with rough surfaces and dissipative, frictional interactions. Numerical simulations are an established tool to complement advanced theoretical approaches and difficult experimental studies.

In order to study systems of rough spheres, kinetic theories have been extended to (weak) dissipation and friction. Alternative, more recent approaches are based on a pseudo-Liouville operator formalism and are less general in the sense that they assume homogeneity and Maxwellian velocity distributions in order to arrive at a mean field (MF) description of systems with rotational degrees of freedom. Either the system is left undisturbed and thus cools continuously, or a “driving” can be applied, i.e. energy is fed into the system in order to reach a steady-state situation.

The typical driving of a granular material, in both experiment and simulation, can be realized by moving walls which lead to rather localized input of energy. Alternatively, the system can be driven by a global homogeneous, random energy source in different variations. Depending on the experimental setup, energy can be given either to translational degrees of freedom or to the rotational ones, or to both. The first case caught most of the attention – reason enough to change the focus and feed rotational energy instead of translational. In the experiment, translational energy input was applied for special boundary conditions and a variety of interesting experimental results were obtained just recently. One can obtain a gas and a liquid state, together with dense, solid-like clusters which form due to dissipation.

The dynamics of the system is usually assumed to be dominated by two-particle collisions which are modeled by their asymptotic states: A collision is characterized by the velocities before and after the contact, and the contact is assumed to be instantaneous. In the simplest model, one describes inelastic collisions by a normal restitution coefficient $r$ only, i.e. the negative ratio between the normal velocities after and before the collision. However, since surface roughness and friction are important, one should allow for an exchange of translational and rotational energy. In the simplest approach, surface roughness is accounted for by a constant tangential restitution coefficient $r_t$, which is defined in analogy to $r$ in the tangential direction. A more realistic friction law involves the Coulomb friction coefficient, so that the tangential restitution will depend on the collision angle. Constant tangential restitution is recovered in the limit of perfect friction.

In this Letter, we will focus on a system of such perfectly rough particles, where only the rotational degrees of freedom are coupled to a homogeneous driving. Such a situation could correspond, for example, to a gas of rough magnetic particles subject to a rapidly varying, homogeneous, magnetic field. Besides a possible experimental application, we believe that this study is interesting in itself, since a correct modeling of the driving mechanism is of great importance for a theory of granular gases to describe realistic experimental situations.

The model consists of $N$ three-dimensional spheres with radius $a$ and mass $M$, interacting via a hard-core potential and confined to a 2D plane of linear extension $L$, with periodic boundary conditions. The degrees of freedom are the positions $r_i(t)$ the translational velocities $v_i(t)$ and the rotational velocities $\omega_i(t)$ for each sphere numbered by $i = 1, \ldots, N$. When two particles 1 and 2 collide, their velocities after collision are related to the velocities before collision, through a collision matrix which is derived from the linear and angular momentum conservation laws, energy/dissipation balance. The magnitude of dissipation is proportional to the quantities $1 - r^2$ and...
1 − \( r_g^2 \), while the strength of the coupling between rotational and translational motion is connected to \( 1 + r_t \), where the normal restitution \( r \) varies between 1 (elastic) and 0 (inelastic) and the tangential restitution \( r_t \) varies between −1 (smooth) and +1 (rough), corresponding to zero and maximum coupling, respectively [7, 22]. For a typical steady-state configuration (energy input is specified below), see Fig. 1.

In order to feed energy, the system is agitated each time interval \( \Delta t = f_{\text{dr}}^{-1} \), with a driving rate \( f_{\text{dr}} \). Here, we will not apply driving frequencies much higher than the collision rate \( \Omega \), but will use driving frequencies around 100 s\(^{-1} \), comparable to \( \Omega \). This is rectified, since numerical checks with strongly different values of \( f_{\text{dr}} \) lead to a similar behavior of the system even for driving frequencies lower than, but of the same order as \( \Omega \), provided that a stationary state is reached. The translational velocity remains unchanged, but the angular velocity \( \omega_i \) of particle \( i \) is modified at each time of agitation \( t \) so that

\[
\omega'_i(t) = \omega_i(t) + r_i \omega_i,
\]

where the prime on the left hand side indicates the value after the driving event. Due to the two-dimensionality of the system, we apply the driving force only to the \( z \)-direction, so that the scalar \( \omega \) is to be understood as the \( z \)-component of \( \omega \). \( \omega_0 \) is a reference angular velocity (in this study we use \( \omega_0 = 2.4 \times 10^{-4} \text{s}^{-1} \)) which allows, with \( v_0 = a \omega_0 = 2.4 \times 10^{-7} \text{m s}^{-1} \), where \( a = 10^{-3} \text{m} \), to define the dimensionless translational and rotational particle temperatures \( T_{\text{tr}} = E_{\text{tr}}/(N T_0) \) and \( T_{\text{rot}} = 2 E_{\text{rot}}/(N T_0) \), with the translational energy \( E_{\text{tr}} = (M/2) \sum_{i=1}^{N} v_i^2 \), the rotational energy \( E_{\text{rot}} = (q M a^2/2) \sum_{i=1}^{N} \omega_i^2 \), and the reference temperature \( T_0 = M v_0^2 \). The variance of the uncorrelated Gaussian random numbers \( r_i \) (with zero mean) can now be interpreted as a dimensionless driving temperature \( T_{\text{dr}} \) [21]. The stochastic driving leads thus to an average rate of change of temperature

\[
\Delta T_{\text{rot}}/\Delta t = H_{\text{dr}}, \quad \text{with} \quad H_{\text{dr}} = f_{\text{dr}} T_{\text{dr}}.
\]

The starting point for our mean-field analysis is the theory of Huthmann and Zippelius [3], for a freely cooling gas of infinitely rough particles, which was recently complemented by numerical simulations in 2D and 3D [8] and by studies of driven systems as well [11]. The main outcome of this approach is a set of coupled evolution equations for the translational and rotational MF temperatures \( T_{\text{tr}} \) and \( T_{\text{rot}} \) which can be extended to describe arbitrary energy input (driving) [8]. In the present study, given the random driving temperature \( T_{\text{dr}} \) and an energy input rate \( f_{\text{dr}} \), as defined above, one just has to add the positive rate of change of rotational energy \( H_{\text{dr}} \) to the system of equations:

\[
\frac{d}{dt} T_{\text{tr}}(t) = \left[ -G B T_{\text{tr}}^{3/2} + G B T_{\text{tr}}^{1/2} T_{\text{rot}} \right],
\]

\[
\frac{d}{dt} T_{\text{rot}}(t) = 2 \left[ G B T_{\text{tr}}^{3/2} - G C T_{\text{tr}}^{1/2} T_{\text{rot}} \right] + H_{\text{dr}},
\]

where the positive terms are

\[
G = 8/(\sqrt{\pi M a}) \nu q_{2a}(\nu),
\]

and the pair correlation function at contact \( q_{2a}(\nu) = (1 - 7 \nu/16)/(1 - \nu)^2 \) in the approximation proposed by Henderson [24, 25], dependent only on the volume fraction of the granular gas \( \nu = \pi a^2 N/V \). The constant coefficients in Eqs. (3) and (4) are \( A = (1 - r^2)/4 + \eta (1 - \eta)/2, \quad B = \eta^2/(2q), \quad C = \eta (1 - \eta)/2q, \) with the abbreviation \( \eta = \eta (r_i) = \eta (1 + r_i)/(2q + 2), \) as derived in Ref. [8].

FIG. 1. Snapshot of the particle distribution in the steady state for a system of \( N = 11025 \) particles, \( \nu = 0.34, \quad r_t = 1 \), and \( r_n = 0.1 \).

FIG. 2. Simulation (points) and theory (lines) for the parameters \( \nu = 0.34, \quad N = 11025, \quad r_t = 1 \), plotted against \( r \). (a) Equilibrium rotational temperature \( T_{\text{rot}} \), normalized by the MF value \( T_{\text{rot}}^\text{eq}(r = 0) \) at \( r = 0 \). (b) Ratio of equilibrium rotational and translational temperature \( R = T_{\text{rot}}/T_{\text{tr}} \) with \( \Gamma = 2(B/A)^{1/2}(C - B^2/A) \), and \( R = A/B \).
In Fig. 2, we present equilibrium values of $T_{rot}$, normalized by the MF value $T_{rot}^{eq}(r = 0)$ at $r = 0$, and of the ratio $R = T_{rot}^{eq}/T_{rot}$, as obtained from numerical simulations of a system of $N = 11025$ particles, with volume fraction $\nu = 0.34$, $r_t = 1$, and $r$ ranging from 0.99 to $10^{-4}$. Surprisingly, the agreement with the MF prediction is very good, even for the lowest value $r = 10^{-4}$ of the normal restitution, which corresponds to very strong dissipation, were the deviation from MF theory is of the order of only 10%.

Rotational velocities are then characterized by good homogeneization at low $r$, while the translational velocity distribution shows strong deviations from a Maxwellian. This deviation is due to the high dissipation. Numerical simulations with $r = 0.99$ give a Maxwellian distribution for both rotational and translational velocities.

In order to check the role of the tangential restitution, we show in Fig. 3 the equilibrium values of $R$ with $r = 0.1$ and $r_t \in [-1,1]$. While for positive $r_t$ there is still good agreement with MF theory, strong deviations appear as $r_t \to -1$. Note that many realistic materials obey the relation $r_t \approx 0.4$ [24], what renders our mean field approach still acceptable.

To give an example, if the system is driven on the translational degrees of freedom, the equilibrium temperatures show deviations of 30–40% from MF predictions already for $r = 0.6$, see [22]. The snapshot in Fig. 2 shows the equilibrium particle distribution for $r = 0.1$ and appears spatially homogeneous – apart from small density fluctuations not quantified here.

In Fig. 3 we show the equilibrium rotational and translational velocity distributions for $r = 0.1$, with the other parameters as above. The rotational velocity distribution is very near to a Maxwellian. A three parameter fit $f(x) = A \exp(-B/(x - \langle x \rangle)/\sigma^\alpha)$, where $\sigma = ((x - \langle x \rangle)^2)^{1/2}$, and $x$ either equals $\omega$ or $v$, is plotted as dashed line in Fig. 3. The parameters $\langle \omega \rangle$ and $\sigma$ are taken from the simulations, and the fit gives $\alpha = 1.92(6)$ for $\omega$, while we obtain $\alpha = 1.41(6)$ for $v$.

![Fig. 3](image-url) Steady state rotational (a) and translational (b) velocity distributions for $N = 11025$, $\nu = 0.34$, $r_t = 1.0$ and $r = 0.1$. A power law fit (dashed line) gives an exponent $\alpha = 1.92(6)$ for the rotational distribution and $\alpha = 1.41(6)$ for the translational distribution (see text for details). For comparison, a Maxwellian (full line) is plotted in (b).

![Fig. 4](image-url) Simulation (points) and theory (lines) results for $R = T_{rot}/T_{trans}$, with parameters $\nu = 0.34$, $N = 11025$, and $r = 0.1$, plotted against $r_t$.

The conclusions of our study are that the driving on the rotational degrees of freedom is able to keep the spatial homogeneity of the system up to very high dissipation rates, for positive values of $r_t$. This leads to a very good agreement of the equilibrium temperatures with the MF predictions. There are two possible reasons for this. From one side, the driving acts on rotations. Then, it cannot favorise collisions, since it does not increase the normal component of the relative velocity of the colliding particles. From the other side, the increase of rotational energy triggered by the driving leads to a shearing force between particles, which reduces density fluctuations and destroys velocity correlations. When $r_t \to -1$, the agreement with MF is lost. To explain this result one has to remember that $1 + r_t$ is a measure for the strength of the coupling. Not enough rotational energy is transferred to the translational degree, so that the randomization on the coupling. 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with a non Maxwellian velocity distribution. This poses a theoretical challenge, since recently proposed theories for horizontally driven granular gases assume that clustering is responsible for fat tails in the velocity distribution. Apparently the temperature of the system depends mainly on the energy balance relations, which depends indirectly on density fluctuations (density fluctuations influence strongly both the frequency of collision and the rate of dissipated energy per collision) while higher moments, and the overall shape of the velocity distributions are more sensible to other details.

A difficult to realize, but probably good, experimental setup is the following. Each, extremely rough, granular sphere, contains a small (to reduce the effect of dipole-dipole interaction at collision) magnetic bar. The plane on which the spheres move should be extremely smooth, in order to avoid energy dissipation. Then, a spatially homogeneous magnetic pulses periodically spaced in time can be applied in the horizontal directions. This would be the magnetic analogon of the oscillating plane. If the magnetic field is really spatially homogeneous, the magnetic dipoles of the spheres will receive angular momentum from the field, so only rotations are driven, and this angular momentum will be “randomized” by the collisions, if they are frequent enough, exactly like it happens for the kinetic energy coming from the oscillating plane usually employed in experiments. To reach an equilibrium, it is necessary to give an initial translational velocity to the particles. We are aware that such an experiment is extremely difficult to realize, but we hope there will be some experimentalist willing to try it.

Summarizing, the main discovery of this work is that a dissipative gas has strongly anomalous velocity distributions even in the absence of large-scale inhomogeneities. This is achieved by injecting the energy into rotational motion and allowing for a transfer to translations through strong friction. The system acts like a “transformer” converting Maxwellian degrees of freedom into distributions with fat tails.

R. C. and H. J. H. acknowledge financial support under the European network project FMRXCT980183; S. L. and H. J. H. acknowledge funding from the Deutsche Forschungsgemeinschaft (DFG). We thank E. Clément for helpful discussions.

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