Rotationally driven gas of inelastic rough spheres

RAFFAELE CAFIERO[1], STEFAN LUDING[2,3], AND HANS JÜRGEN HERRMANN[1,2]
[1] *P.M.M.H., École Supérieure de Physique et de Chimie Industrielles (ESPCI) 10, rue Vauquelin, 75251 Paris CEDEX 05, FRANCE*
[2] *Institute for Computer Applications 1, Pfaffenwaldring 27, 70569 Stuttgart, GERMANY*
[3] *Particle Technology, DelftChemTech, TU Delft, Julianalaan 136, 2628 CJ Delft, The Netherlands*

Abstract. – We study a gas of inelastic rough spheres confined on a 2D plane, driven on the rotational degrees of freedom. Event driven molecular dynamics (MD) 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.
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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 [1–4], 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. Molecular dynamics (MD) 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 [5, 6]. Alternative, more recent approaches are based on a pseudo-Liouville operator formalism [7–10] 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 [7–9] 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 [11, 12, 18].

The typical driving of a granular material, in both experiment and simulation, can be realized by moving walls [2] which lead to rather localized input of energy. Alternatively, the system can be driven by a global homogeneous, random energy source in different variations [11, 13–18]. 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 catched 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 [19–24]. 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 [7–10, 25, 26], one should allow for an exchange of translational and rotational energy. In the simplest approach [5, 7, 26], 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 [9, 10, 27–29], so that the tangential restitution will depend on the collision angle. Constant tangential restitution is recovered in the limit of perfect friction.

In this Paper, 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. We examine the case of isolated rotational driving, since the 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 $\boldsymbol{r}_i(t)$ the translational velocities $\boldsymbol{v}_i(t)$ and the rotational velocities $\boldsymbol{\omega}_i(t)$ 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 $1 - r_t^2$, 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 [5, 7, 26].

In order to feed energy, the system is agitated each time interval $\Delta t = f_{\mathrm{dr}}^{-1}$, with a driving rate f_{dr}. Here, we will not apply driving frequencies much higher than the collision rate Ω, but will use driving frequencies around $100\,\mathrm{s}^{-1}$, comparable to Ω. This is rectified, since numerical checks with strongly different values of f_{dr} lead to a similar behavior of the system even for driving frequencies lower than, but of the same order as Ω, provided that a stationary state is reached. The translational velocity remains unchanged, but the angular velocity ω_i of particle i is modified at each time of agitation t so that $\omega_i'(t) = \omega_i(t) + r_i\,\omega_0$, 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 ω is to be understood as the z-component of $\boldsymbol{\omega}$. ω_0 is a reference angular velocity (in this study we use $\omega_0 = 2.4\ 10^{-4}\,\mathrm{s}^{-1}$) which allows, with $v_0 = a\omega_0 = 2.4\ 10^{-7}\,\mathrm{m\,s}^{-1}$, where $a = 10^{-3}\,\mathrm{m}$, to define the dimensionless translational and rotational particle temperatures $T_{\mathrm{tr}} = E_{\mathrm{tr}}/(NT_0)$ and $T_{\mathrm{rot}} = 2E_{\mathrm{rot}}/(NT_0)$, with the translational energy $E_{\mathrm{tr}} = (M/2)\sum_{i=1}^{N} \boldsymbol{v}_i^2$, the rotational

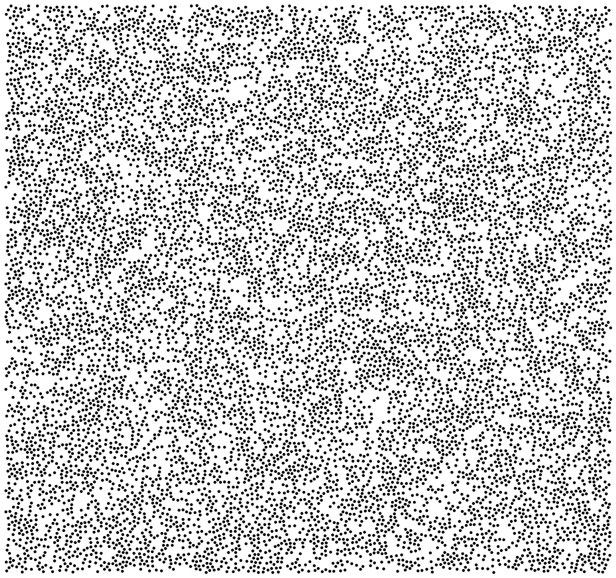

Fig. 1 – Snapshot of the particle distribution in the steady state for a system of $N = 11025$ particles, $\nu = 0.34$, $r_t = 1$, and $r = 0.1$.

energy $E_{\rm rot} = (qMa^2/2)\sum_{i=1}^{N} \omega_i^2$ ($q = 2/5$ for $3D$ spheres), and the reference temperature $T_0 = Mv_0^2$. The variance of the uncorrelated Gaussian random numbers r_i (with zero mean) can now be interpreted as a dimensionless driving temperature $T_{\rm dr}$ [11]. The stochastic driving leads thus to an average rate of change of temperature

$$\Delta T_{\rm rot}/\Delta t = H_{\rm dr} \ , \quad \text{with} \quad H_{\rm dr} = f_{\rm dr} T_{\rm dr} \ . \tag{1}$$

The starting point for our mean-field analysis is the theory of Huthmann and Zippelius [7], for a freely cooling gas of infinitely rough particles, which was recently complemented by event driven (ED) 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 $T_{\rm tr}$ and $T_{\rm rot}$ [7] which can be extended to describe arbitrary energy input (driving) [11]. In the present study, given the random driving temperature $T_{\rm dr}$ and an energy input rate $f_{\rm dr}$, as defined above, one just has to add the positive rate of change of rotational energy $H_{\rm dr}$ to the system of equations:

$$\frac{d}{dt}T_{\rm tr}(t) = \left[-GAT_{\rm tr}^{3/2} + GBT_{\rm tr}^{1/2}T_{\rm rot}\right] \tag{2}$$

$$\frac{d}{dt}T_{\rm rot}(t) = 2\left[GBT_{\rm tr}^{3/2} - GCT_{\rm tr}^{1/2}T_{\rm rot}\right] + H_{\rm dr} \ , \tag{3}$$

with $G = 8/(\sqrt{\pi}Ma)\nu g_{2a}(\nu)$, and the pair correlation function at contact $g_{2a}(\nu) = (1 - 7\nu/16)/(1-\nu)^2$ in the approximation proposed by Henderson [30, 31], dependent only on the volume fraction of the granular gas $\nu = \pi a^2 N/V$. The constant coefficients in Eqs. (2) and (3) are $A = (1-r^2)/4 + \eta(1-\eta)/2$, $B = \eta^2/(2q)$, and $C = \eta\,(1-\eta/q)\,/(2q)$, with the abbreviation $\eta = \eta(r_t) = q(1+r_t)/(2q+2)$, as derived in Ref. [7]. A typical steady-state configuration in shown in Fig. 1.

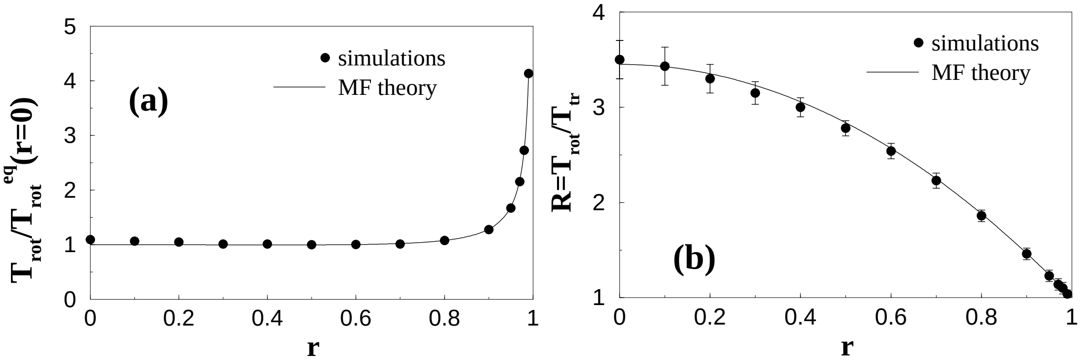

Fig. 2 – Simulation (points) and theory (lines) for the parameters $\nu = 0.34$, $N = 11025$, and $r_t = 1$, plotted against r. (a) Stationary rotational temperature $T_{\rm rot}$, normalized by the MF value $T_{\rm rot}^{\rm eq}(r=0)$ at $r = 0$. (b) Ratio of stationary rotational and translational temperature $R = T_{\rm rot}/T_{\rm tr}$.

Setting to zero the temporal derivatives in Eqs. (2) and (3), one obtains the steady state properties of the system:

$$T_{\rm rot}^{\rm eq} = \left(\frac{H_{\rm dr}}{G\Gamma}\right)^{2/3}, \quad \text{and} \quad T_{\rm tr}^{\rm eq} = T_{\rm rot}^{\rm eq}/R \;, \tag{4}$$

with $\Gamma = 2\,(B/A)^{1/2}\left(C - B^2/A\right)$, and $R = A/B$.

In Fig. 2 we present the stationary (steady-state) values of $T_{\rm rot}$, normalized by the MF value $T_{\rm rot}^{eq}(r=0)$, and of the ratio $R = T_{\rm rot}^{\rm eq}/T_{\rm tr}^{\rm eq}$, 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, where the deviation from MF theory is of the order of only 10%.

To give an example, if the system is driven on the translational degrees of freedom, the stationary temperatures show deviations of $30-40\%$ from MF predictions already for $r = 0.6$, see [11]. The snapshot in Fig. 1 shows the particle distribution for $r = 0.1$ and appears spatially homogeneous – apart from small density fluctuations not quantified here.

In Fig. 3, we show the stationary 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 $\sigma = \left(\langle(x-\langle x\rangle)^2\rangle\right)^{1/2}$, and x either equals ω or v, is plotted as dashed line in Fig. 3. The parameters $\langle\omega\rangle$, $\langle v\rangle$ and σ are taken from the simulations, and the fit gives $\alpha = 1.92(6)$ for ω, while we obtain $\alpha = 1.41(6)$ for v. This last value is quite near to the value $3/2$ obtained theoretically by T.P.C. van Noije et al. in [16]. The applicability of the approach of [16] to the present case, however, has to be discussed since in [16] a *translationally driven*, granular gas of *smooth* particles is considered. A generalization to arbitrary driving is a next possible step.

Rotational velocities are characterized by good homogenization at low r, while the translational velocity distribution shows strong deviations from a Maxwellian.

In order to check the role of the tangential restitution, we show in Fig. 4 the stationary 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 $r_t \approx 0.4$ [28], what renders our mean field approach still acceptable.

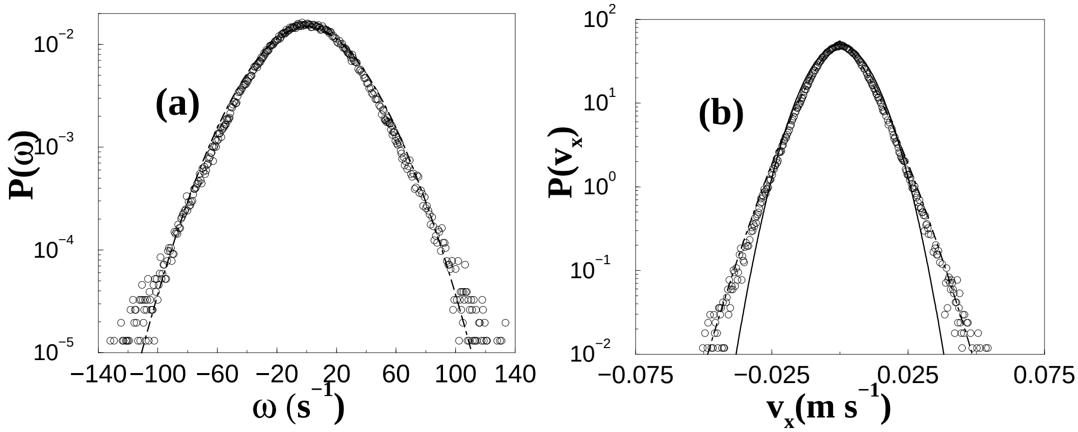

Fig. 3 – Steady state rotational (a) and translational (b) velocity distributions for $N = 11025$, $\nu = 0.34$, $r_t = 1.0$ and $r = 0.1$. A power law fit (dashed line) gives an exponent $\alpha = 1.92(6)$ for the rotational distribution and $\alpha = 1.41(6)$ for the translational distribution (see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

Our conclusions 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 stationary temperatures with the MF predictions. There are two possible reasons for this. From one side, the driving acts on rotations. Then, it cannot favorize 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 should destroy the translational velocity correlations - but astonishingly does not. 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

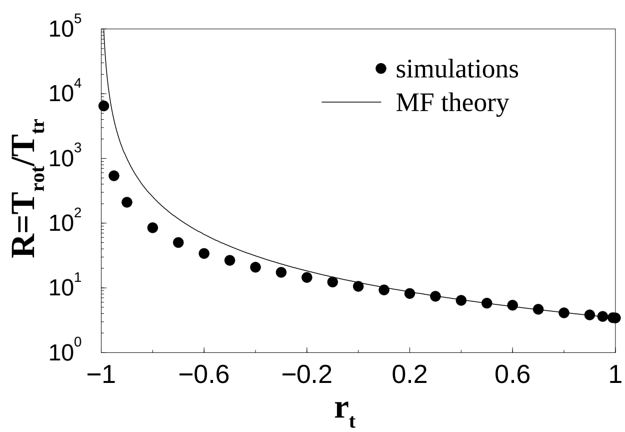

Fig. 4 – Simulation (points) and theory (lines) results for $R = T_{\rm rot}/T_{\rm tr}$, with parameters $\nu = 0.34$, $N = 11025$, and $r = 0.1$, plotted against r_t.

energy is transferred to the translational degree, so that the randomization on collisions does not take place. Thus, it is not surprising that MF is no more valid in this very singular limit. Snapshots of the particle distribution for $r = 0.1$ and r_t near to -1 (not displayed here) show indeed stronger density fluctuations in the system as reported in Fig. 1.

The translational velocity distribution exhibits strong deviations from MF prediction, in the *homogeneous* high dissipation regime, showing that deviations from a Maxwellian are not necessarily related to clustering. Moreover, one can have a good agreement of the second moment (the temperature) of the velocity distribution with MF theory *together with* non Maxwellian velocity distributions. This poses a theoretical challenge, since recently proposed theories for translationally driven granular gases [32], assume that clustering is responsible for fat tails in the velocity distribution. The reason why clusters do not to occur in our situation, possibly due to the fact that vortices in their early stage are destroyed by the rotational driving, is an issue for future studies.

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 possible setup for an experiment 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, 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. To reach a steady-state, 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 a similar setup seems already operational in Dortmund [34]. Another reason to look at rotational driving via magnetic forces is the recent interest in electrostatically driven granular media [33] and in magnetic particles with dipolar interactions [35, 36].

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.

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