Inelastic hard spheres with random restitution coefficient: a new model for heated granular fluids

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We consider a vertically shaken granular system interacting elastically with the vibrating boundary, so that the energy injected vertically is transferred to the horizontal degrees of freedom through inter-particle collisions only. This leads to collisions which, once projected onto the horizontal plane, become essentially stochastic and may have an effective restitution coefficient larger than 1. We therefore introduce the model of inelastic hard spheres with random restitution coefficient α (larger or smaller than 1) to describe granular systems heated by vibrations. In the non-equilibrium steady state, we focus in particular on the single particle velocity distribution $f(v)$ in the horizontal plane, and on its deviation from a Maxwellian. We use Molecular Dynamics simulations and Direct Simulation Monte Carlo (DSMC) to show that, depending on the distribution of α, different shapes of $f(v)$ can be obtained, with very different high energy tails. Moreover, the fourth cumulant of the velocity distribution (which quantifies the deviations from Gaussian statistics) is obtained analytically from the Boltzmann equation and successfully tested against the simulations.

I. INTRODUCTION

Granular matter can exist in many very different states, all of which are currently subject of a large interest [1]. On the one hand, dense granular matter can be studied at rest, and in particular many open problems concern the transmission of forces through a sandpile. On the other hand, since thermal energy is negligible with respect to gravitational or kinetic energy, any dynamical behaviour has to be a response to a certain external energy input: for example, tapping leads to compaction [2], while a strong, continuous energy input by vibrations produces granular gases in continuous motion, for which kinetic energy is much larger than the gravitational one [3–8]. These vibrated systems are out of equilibrium but the energy input can compensate the dissipation due to inelastic collisions between grains and therefore lead to stationarity. While many experiments study the appearance of patterns or inhomogeneities, others, on which we will here concentrate, focus on the velocity distributions and its deviations from the Maxwell-Boltzmann distribution (which would correspond to a system with neither dissipation -i.e. elastic collisions- nor energy injection).

II. SYSTEM STUDIED AND MODELISATION

We want to study a three-dimensional system of grains on a plate, which is shaken vertically (i.e. along the z direction): the energy is therefore injected by a vibrating elastic boundary only in the z direction (Figure 1). It is partly transferred to the other degrees of freedom, and also dissipated, through the inelastic collisions between grains. The velocities and their distribution are then studied in the horizontal (xy) plane.

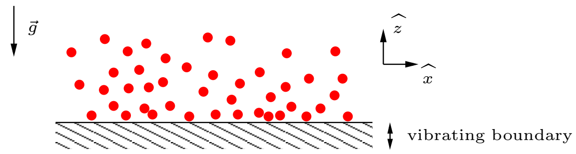

FIG. 1. Schematic view of the system under consideration: the grains are subject to gravity, and submitted to the vibration of an horizontal plate.

A. Usual theoretical approach

The grains are modeled as smooth inelastic hard spheres (IHS) undergoing binary momentum-conserving collisions with a constant normal restitution coefficient $\alpha < 1$: a collision between two spheres 1 and 2, with velocities $\mathbf{v}_1$ and

$\mathbf{v}_2$, dissipates a fraction $(1-\alpha)$ of the component of the relative velocity $\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2$ along the center-to-center direction $\hat{\boldsymbol{\sigma}}$. Once the dissipation has been described in this way, the problem is how to represent the energy injection. A possibility, used and studied by various authors [9–13], consists in submitting the spheres to a random force, i.e. to random "kicks" at a given frequency between collisions. Energy input then acts in all space directions.

B. A new model

However, as previously noted, the real energy input occurs only in the vertical direction, and is not transferred *between* but *through* collisions to the horizontal plane. Indeed, a three-dimensional inelastic collision between two spheres globally dissipates energy, but its projection onto the xy plane can in fact gain energy (see fig 2 for an example). Therefore, the *effective* restitution coefficient of the *projected* collision can be larger than 1. This observation leads to the following effective (projected) simple model [14]:

- two-dimensional hard spheres (of diameter σ) in the xy-plane
- binary momentum-conserving collisions
- *random* normal restitution coefficient α (< 1 or > 1) with distribution $\rho(\alpha)$ (the means over $\rho(\alpha)$ will be denoted by an overline), uncorrelated with the velocities of the particles.

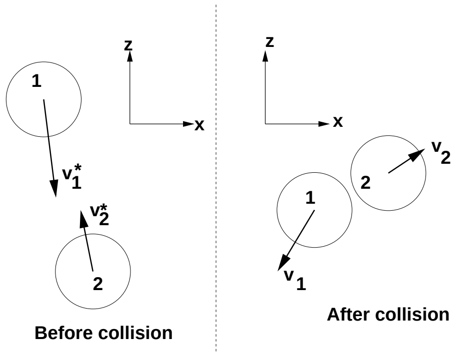

FIG. 2. Example of a globally dissipative collision leading to an energy increase in the horizontal plane.

Since, in a binary collision with restitution coefficient α, the energy change is proportional to $(\alpha^2 - 1)$, we shall consider distributions with $\overline{\alpha^2} = 1$ in order to ensure a stationary, constant temperature regime (at each collision, energy changes, but it is conserved on average). Since the average energy is constant, the granular temperature is also a constant determined by the initial velocity distribution. We will therefore study the distribution of *rescaled* velocities $\mathbf{c} = \mathbf{v}/v_0$, using analytical and numerical tools.

III. KINETIC THEORY

The Molecular chaos approximation factorizes the two-point distribution function:

$$f^{(2)}(\mathbf{v}_1, \mathbf{v}_2, \underbrace{|\mathbf{r}_{12}| = \sigma}_{\text{contact}}, t) \;=\; \chi\, f(\mathbf{v}_1, t) f(\mathbf{v}_2, t) \tag{1}$$

where χ accounts for excluded volume effects (for elastic hard spheres, χ coincides with the density dependent pair correlation function at contact). We are then able to write the (Enskog-)Boltzmann equation in the steady state, averaged over the distribution of restitution coefficients:

$$\int' d\mathbf{v}_2 d\hat{\boldsymbol{\sigma}} d\alpha (\mathbf{v}_{12}\cdot\hat{\boldsymbol{\sigma}})\rho(\alpha)\left\{\alpha^{-2} f(\mathbf{v}_1^*) f(\mathbf{v}_2^*) - f(\mathbf{v}_1) f(\mathbf{v}_2)\right\} = 0 \tag{2}$$

The prime on the integration symbol is a shortcut for $\int d\hat{\boldsymbol{\sigma}}\Theta(\mathbf{v}_{12}\cdot\hat{\boldsymbol{\sigma}})$ ($\hat{\boldsymbol{\sigma}}$ is the center-to-center direction and Θ is the Heavyside function), and we consider collisions which yield $(\mathbf{v}_1, \mathbf{v}_2)$ as postcollisional velocities, for precollisional velocities $(\mathbf{v}_1^*, \mathbf{v}_2^*)$:

$$\mathbf{v}_1^* = \mathbf{v}_1 - \frac{1}{2}\left(1+\frac{1}{\alpha}\right)(\mathbf{v}_{12}\cdot\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}$$
$$\mathbf{v}_2^* = \mathbf{v}_2 + \frac{1}{2}\left(1+\frac{1}{\alpha}\right)(\mathbf{v}_{12}\cdot\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}\ . \tag{3}$$

From now on, we will be concerned with the study of the rescaled velocities $\mathbf{c} = \mathbf{v}/v_0$ and of their distribution:

$$f(\mathbf{v},t) = \frac{n}{v_0^d(t)} P(c)\ , \tag{4}$$

where n is the density and the thermal velocity v_0 is by definition related to the temperature $T(t)$ through $\frac{m}{2}v_0^2(t) = T(t) \equiv \frac{2}{nd}\int d\mathbf{v}\frac{m}{2}v^2 f(\mathbf{v},t)$ (d is the space dimension).

It is usual to look for solutions in the form of a Sonine expansion [15] around the Maxwell-Boltzmann distribution $\Phi(c) = \pi^{-d/2}\exp(-c^2)$

$$P(c) = \Phi(c)\left[1 + \sum_{p=1}^{\infty} a_p\, S_p(c^2)\right] \tag{5}$$

where the polynomials $\{S_p\}$ are orthogonal for the Gaussian weight Φ.

Using the methods exposed in [11], we obtain the leading non Gaussian correction ($a_1 = 0$ from the definition of temperature) a_2, which is related to the fourth cumulant:

$$a_2 \equiv \frac{\langle c^4\rangle}{\langle c^4\rangle_\Phi} - 1 = \frac{16\left(1 - 3\,\overline{\alpha^2} + 2\,\overline{\alpha^4}\right)}{9\, +\, 24\,d\, +\, 32(d-1)\overline{\alpha}\, +\, (8\,d-11)\overline{\alpha^2}\, -\, 30\overline{\alpha^4}} \tag{6}$$

We will compare this result to numerical simulations in the next section, for $d = 2$. For the high energy tail, no analytical results have been obtained and we will investigate this issue numerically.

IV. NUMERICAL SIMULATIONS

A. Methods

We use two complementary approaches

- the Direct Monte Carlo Simulation method (DSMC) [16] generates a Markov chain with the same probabilities of transition as the Boltzmann equation: it produces therefore an "exact" numerical solution of the Boltzmann equation.
- Molecular Dynamics (MD) integrate the *exact* equations of motion of the hard spheres, with no reference to the Boltzmann equation: we consider N spheres of diameter σ, in a box of linear size L in dimension d (here $d = 2$), with periodic boundary conditions [17,18]; the comparison with DSMC allows to test the molecular chaos approximation.

B. Results

The first results show the validity of the Sonine expansion and of the theoretical values for a_2: figure 3 shows a comparison between DSMC results and the theoretical expansion: the agreement is perfect at small a_2, and satisfying at low velocities (note that the Sonine expansion is a low-velocities expansion) for larger a_2.

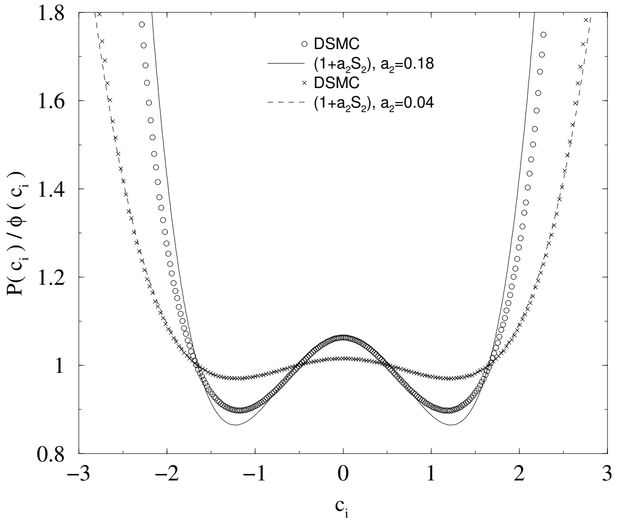

FIG. 3. Comparison of the $P(c)/\Phi(c)$ measured in DSMC (symbols) with the Sonine expansion with the calculated a_2 (lines), for two different $\rho(\alpha)$: flat distribution of $\alpha^2 \in [0.5, 1.5]$ ($a_2 = 0.04$), and flat distribution of $\alpha^2 \in [0, 2]$ ($a_2 = 0.18$).

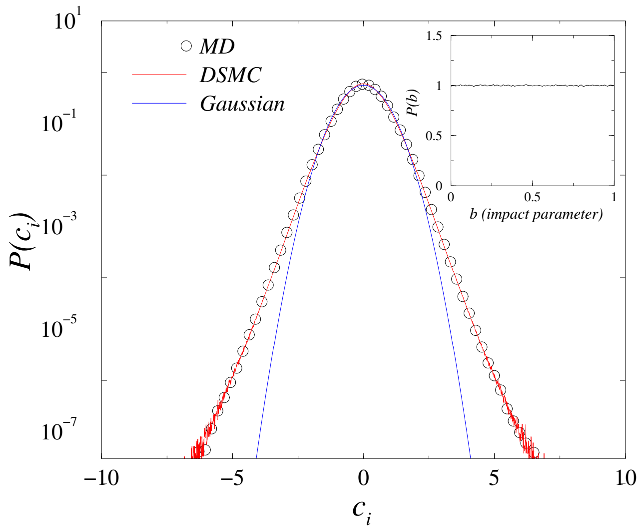

FIG. 4. Velocity distribution $P(c)$, for a flat distribution of $\alpha^2 \in [0, 2]$, for MD and DSMC. MD: $50\,10^3$ particles (30 % packing fraction); DSMC: $500\,10^3$ particles. A Gaussian is also shown for comparison. Inset: distribution of normalized impact parameters in MD

Moreover, figure 4 shows that MD and DSMC simulations are in perfect agreement (shown only for a particular choice of $\rho(\alpha)$, but checked for other choices of $\rho(\alpha)$). Moreover, the curves obtained in MD simulations with small or large packing fractions (up to 40%) are indistinguishable (not shown). Important deviations from the Maxwell-Boltzmann distribution are obtained, but the inset shows that the distribution of impact parameters in Molecular Dynamics simulations is flat: this is a hint that no violation of molecular chaos is observed and that the factorization of the 2-particle correlation function Eq. (1) holds. In MD simulations, inhomogeneities and/or violations of molecular chaos could a priori appear, contrarily to DSMC. The fact that no such phenomenon is observed is in contrast with the phenomenology at constant α [19] or with randomly driven IHS [20]: for a constant dissipative restitution parameter, colliding particles emerge with more parallel velocities than in the elastic case $\alpha = 1$ and, when they recollide, their velocities are still more parallel. The possibility of having $\alpha > 1$ seems to have removed this mechanism for the creation of velocity correlations violating molecular chaos, and to produce an efficient randomization of the velocities. This validates the theoretical approach based on the Boltzmann equation.

Let us now turn to the study of the large velocity tails: figure 5 shows fits to stretched exponentials (*over 6 orders* *of magnitude*)

$$P(c) \propto \exp(-c^B)$$

with a wide range of possible values for B. In particular, a convenient choice of $\rho(\alpha)$ is compatible with $B = 1.6$, which has been found in some experiments [6,7] (close to $B = 3/2$ obtained in [11] for randomly driven IHS fluids). The possibility to obtain such different values of B may question the relevance of this exponent as an intrinsic quantity for granular gases in steady states.

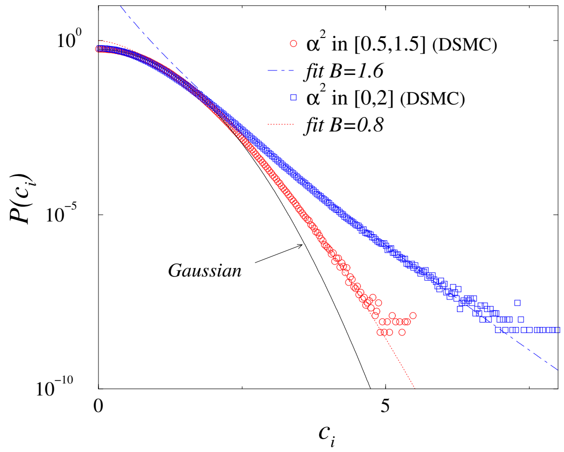

FIG. 5. Fits to stretched exponential forms $\exp(-c^B$ of the velocity distributions, for a flat distribution of $\alpha^2 \in [0, 2]$ and $\in [0.5, 1.5]$.

V. CONCLUSIONS AND PERSPECTIVES

We have introduced the idea of a random restitution coefficient in the IHS model, in order to account for the fact that, for a vertically vibrated layer of granular material, the energy is injected only along the vertical axis, and transferred through collisions in the horizontal directions: the projection in 2 dimensions of a 3-dimensional collision can correspond to a gain in the two-dimensional energy, and therefore to an effective restitution coefficient larger than 1, even if the genuine α is necessarily smaller than 1, i.e. corresponds to a dissipative collision.

We have subsequently studied this model in 2 dimensions, with a probability distribution $\rho(\alpha)$ for the restitution coefficient. We have focused on the velocity distributions, and in particular on the deviation from the Maxwellian:

- at low velocities, the Sonine expansion technique is used: we obtained analytically the expression of the fourth cumulant a_2 and tested it against Molecular Dynamics (MD) and Monte Carlo Direct Simulations (DSMC). The theoretical predictions for a_2 are quite accurate, with a slight overestimation for a_2 that probably corresponds to the approximations made during the calculation (nonlinear terms $\mathcal{O}(a_2^2)$ and higher order Sonine polynomials neglected); Moreover, the comparison between numerical data and the second order Sonine expansion shows a remarkable agreement for small values of a_2.

- the high energy tails, studied with DSMC simulations, can be fitted by functions of the form $\exp(-Ac^B)$, with $B < 2$ depending on $\rho(\alpha)$. It would certainly be interesting to have theoretical predictions concerning B. Note that once a functional form has been chosen for $\rho(\alpha)$, very different tails can be observed depending on the range of variation for α. This feature might question the relevance of the exponent B as an intrinsic quantity for granular gases in steady states.

The comparison of MD and DSMC results shows a remarkable agreement (even with a packing fraction as high as 40% in MD), and the study of the impact parameter in MD shows no violation of molecular chaos. This is to be compared with the situation of free cooling [19] but also with MD results on heated inelastic hard spheres with constant restitution coefficient [20], in which microscopic precollisional velocity correlations develop and molecular chaos is violated. A thorough investigation of short scale velocity correlations would require the computation of various precollisional averages involving moments of the relative velocities, and has not been performed. Our results however suggest that the dynamical correlations inducing recollisions [21] and responsible for the violation of molecular chaos may not be a generic feature of driven granular gases exhibiting a non equilibrium stationary state.

In the model introduced here, the random restitution coefficient is uncorrelated with the relative velocities of the particles; this somehow unrealistic feature could be improved in more refined models. Such correlations, which seem difficult to quantify from first principles, might affect the high energy tail or induce precollisional velocity correlations. It would be very interesting to be able to link a realistic energy injection mechanism with a precise distribution of restitution coefficients.

Finally, a hydrodynamic study of the present random α model, in which the conservation of the energy is valid on average only, while density and momentum are conserved locally, is left for future investigations.

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[1] See e.g. H.M. Jaeger, S.R. Nagel, Science **255**, 1523 (1992); *Granular Matter: An Interdisciplinary Approach*, A. Mehta, Ed. (Springer-Verlag, New York, 1994); H.M. Jaeger, S.R. Nagel, and R.P. Behringer, Rev. Mod. Phys 68, 1259 (1996); Proceedings of the NATO Advanced Study Institute on *Physics of Dry Granular Media*, Eds. H. J. Herrmann *et al*, Kluwer Academic Publishers, Netherlands (1998).

[2] Knight, J. B., Fandrich, C. G., Lau, C. N., Jaeger, H. M. and Nagel, S. R. Phys. Rev. E **51**, 3957 (1995); Nowak, E. R., Knight, J. B., Povinelli, M., Jaeger, H. M. and Nagel, S. R., Powder Technol. **94**, 79-83 (1997); Nowak, E. R., Knight, J. B., Ben-Naim, E., Jaeger, H. M. and Nagel, S. R., Phys. Rev. E **57**, 1971-1982 (1998); Jaeger, H. M. in Physics of Dry Granular Media (eds. Herrmann, H. J., Hovi, J.-P. and Luding, S.) 553-583 (Kluwer Academic, Dordrecht, The Netherlands, 1998).

[3] E. Clement and J. Rajchenbach, Europhys. Lett **16**, 133 (1991).

[4] S. Warr, G.T.H Jacques and J.M. Huntley, Powder Tech **81**, 41 (1994); S. Warr, J.M. Huntley and G.T.H Jacques, Phys. Rev. E **52** 5583 (1995).

[5] J.S. Olafsen and J.S. Urbach, Phys. Rev. Lett **81**, 4369 (1998); Phys. Rev. E **60**, R2468 (1999).

[6] W. Losert, D.G.W. Cooper, J. Delour, A. Kudrolli and J.P. Gollub, Chaos **9**, 682 (1999) and cond-mat/9901203.

[7] F. Rouyer and N. Menon, Phys. Rev. Lett. **85** 3676 (2000).

[8] A. Kudrolli and J. Henry, Phys. Rev. E **62** R1489 (2000).

[9] D.R. Williams and F.C. MacKintosh, Phys. Rev E **54**, R9 (1996).

[10] A. Puglisi, V. Loreto, U. Marini Bettolo Marconi and A. Vulpiani, Phys. Rev. E **59**, 5582 (1999).

[11] T.P.C. van Noije and M.H. Ernst, Gran. Matter **1**, 57 (1998).

[12] T.P.C. van Noije, M.H. Ernst, E. Trizac and I. Pagonabarraga, Phys. Rev. E **59**, 4326 (1999).

[13] R. Cafiero, S. Luding and H.J. Herrmann, Phys. Rev. Lett. **84**, 6014 (2000).

[14] A. Barrat, E. Trizac and J.N. Fuchs, cond-mat/0101158, Eur. Phys. J. E (2001).

[15] L. Landau and E. Lifshitz, *Physical Kinetics*, Pergamon Press (1981).

[16] G. Bird, "Molecular Gas Dynamics" (Oxford University Press, New York, 1976) and "Molecular Gas Dynamics and the Direct Simulation of Gas flows" (Clarendon Press, Oxford, 1994).

[17] See e.g. H.J. Herrmann, in "Disorder and granular media", edited by D. Bideau and A. Hansen (Elsevier Science Publisher, 1993).

[18] M.P. Allen and D.J. Tildesley "Computer simulations of liquids" (Clarendon Press, Oxford, 1987).

[19] S. Luding, GAMM 99 proceedings, June 1999.

[20] I. Pagonabarraga, E. Trizac, T.P.C. van Noije and M.H. Ernst, in preparation.

[21] J.R. Dorfman and H. van Beijeren, *The Kinetic Theory of Gases*, in *Statistical Mechanics, Part B: Time-Dependent Processes*, ed. B.J. Berne (Plenum Press, New York, 1977), ch. 3.