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Granular gases: dynamics and collective effects

A Barrat¹, E Trizac² and M H Ernst³

¹ Laboratoire de Physique Théorique (UMR 8627 du CNRS), Bâtiment 210,
Université Paris-Sud, 91405 Orsay, France

² Laboratoire de Physique Théorique et Modèles Statistiques (UMR 8626 du CNRS),
Bâtiment 100, Université Paris-Sud, 91405 Orsay, France

³ Instituut voor Theoretische Fysica, Universiteit Utrecht, Postbus 80.195, 3508 TA Utrecht,
The Netherlands

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Abstract

We present a biased review of some of the most ‘spectacular’ effects appearing in the dynamics of granular gases where the dissipative nature of the collisions leads to a rich phenomenology, exhibiting striking differences with equilibrium gases. Among these differences, the focus here is on the illustrative examples of the ‘Maxwell demon’-like experiment, modification of Fourier’s law, non-equipartition of energy and non-Gaussianity of the velocity distributions. The presentation remains as non-technical as possible.

1. Introduction

Coulomb, Faraday, Huygens and Reynolds are among the prominent founding fathers of the study of granular materials. Subsequently, this field has mostly been investigated by engineers. During the last 15 years, however, physicists seem to have rediscovered the field and have gradually become more involved again, partly due to the increase of computer resources [1, 2]. Beyond fashion effects and important industrial stakes, the behaviour of granular matter in its own right is remarkably rich, and often resists understanding [3].

The corresponding systems are nevertheless simple to define. Broadly speaking, they are composed of macroscopic compounds (with sizes larger than a fraction of millimetre). Two crucial properties of granular matter directly follow from this size constraint: first, ordinary temperature is irrelevant, as may be appreciated by comparing the typical gravitational energy of a grain to the thermal agitation energy. Second, the interactions between grains are dissipative. They involve complex macroscopic processes such as fracture, friction, and internal vibrations, which contribute to dissipate kinetic energy. The mechanisms for exploring configuration space are therefore unusual and any dynamics results from an external drive. The resulting stationary states often differ from those observed in conservative systems (such as molecular gases, ordinary liquids, or colloidal suspensions) with sometimes spectacular or unexpected effects. The purpose of the present paper is to present in a concise and non-technical manner four manifestations of those differences. We will restrict the discussion to

the so-called gaseous state of granular matter, where a rapid flow is obtained by a violent and sustained excitation. This does not necessarily mean that the total density has to be small. In this regime (as opposed to the quasi-static limit which has been the object of intense research and where solid or liquid-like behaviour may be observed), the only contacts between grains occur during collisions. The corresponding ‘gases’ have been studied experimentally, but also with numerical and analytical tools, and they provide an ideal situation for comparison between the various approaches [1, 2].

This paper is organized as follows. Section 2 describes the general experimental and theoretical framework of granular gases. Sections 3–6 then present four striking consequences of the dissipative nature of collisions in granular gases. For more details, the interested reader is referred to comprehensive books, such as [1, 2], to reviews [4–6], and to the references provided therein.

2. Experiments, models and theoretical approaches

2.1. Experiments

A granular gas is typically obtained by enclosing sand or balls made of glass, steel, brass, ceramic beads, etc in a container, which is subsequently vigorously shaken. The energy injected at the boundaries compensates for the dissipative collisions [7], and allows the grains (particles) to follow ballistic trajectories between collisions. The experimentally challenging aspects deal with measurements of different relevant quantities (e.g. local density, velocity distribution from which the velocity field may be extracted, etc). This requires sophisticated detection devices (such as ultra-fast cameras, diffusive wave spectroscopy, magnetic resonance, and positron-based techniques) [9–11, 8]. The most frequently employed experimental set-ups are made up either of cylindrical containers [10] (which may block direct visualization), or of thin cages with transparent boundaries [9], which make the system quasi-two-dimensional. In order to obtain reproducible and reliable results, much effort has been paid to control the size distribution, with spherical beads of typical millimetric size.

2.2. Modelling

Two features are essential to capture the behaviour of granular gases: the excluded volume on the one hand (hard core effect), and the dissipative nature of collisions on the other hand. The simplest approach incorporating these two aspects is the paradigmatic inelastic hard sphere model [12, 13]. In this modelling, spherical grains that do not interact at distances larger than their diameter (with forbidden overlaps) undergo momentum-conserving but dissipative (inelastic) collisions. These collisions are assumed instantaneous so that events involving more than two partners may be neglected. Suppose we have a binary mixture, where i labels both the particle and the species in the mixture, and where $m_i = \{m_1, m_2\}$. For two grains i and j belonging to species i and j respectively, the post-collision velocities (denoted with primes) read

$$\mathbf{v}'_i = \mathbf{v}_i - \frac{m_j}{m_i + m_j} (1 + \alpha_{ij}) (\hat{\boldsymbol{\sigma}} \cdot \mathbf{v}_{ij}) \hat{\boldsymbol{\sigma}} \quad (1)$$

where i and j take the values 1 or 2. Here $\hat{\boldsymbol{\sigma}}$ is the centre-to-centre unit vector (oriented $i \rightarrow j$ or $j \rightarrow i$) and $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$ is the pre-collision value of the relative velocity. In equation (1), α_{ij} is the coefficient of normal restitution associated with the pair (ij) . The collision dissipates kinetic energy for $\alpha_{ij} < 1$, whereas $\alpha_{ij} = 1$ corresponds to the elastic (conservative) case. For the sake of simplicity, the latter coefficient is taken independent of \mathbf{v}_{ij} or of the impact

parameter of the collisions. While this is certainly an oversimplification of the experimental reality, it appears that thorough measurements of the restitution coefficient are scarce under conditions relevant for the study of bulk properties [14–17]. Bearing these limitations in mind, the inelastic hard sphere model with a constant coefficient of normal restitution is useful as a minimal approach to understand the rich phenomenology of granular gases, since it not only facilitates numerical investigations but also allows for analytical studies. In particular, the next sections will show how the striking effects of inelasticity are captured by this simple model.

More realistic models have also been proposed, where the particles have rotational degrees of freedom, and where there is also, in addition to normal restitution, tangential restitution [18], with sticking and sliding friction, the restitution coefficients depending on the velocities or visco-elastic interactions [1, 2, 14, 19–22].

2.3. Analytical approaches

From the theoretical point of view, the methods range from a microscopic description using kinetic theory, to continuum mechanics-like approaches (hydrodynamics), aiming at establishing the evolution equations governing the dynamics of suitably defined coarse-grained fields (density, momentum, kinetic energy, etc) [5]. In a molecular gas or an ordinary liquid, the validity of the hydrodynamic approach relies on the existence of conserved quantities (collisional invariants) among which the kinetic energy plays a key role. In a granular gas, this approach seems *a priori* questionable, due to dissipation. In addition, new length and timescales emerge, that may equally well interfere with the microscopic and macroscopic scales [23].

3. From the Maxwell demon . . .

In a celebrated thought experiment, James Clerk Maxwell described in 1871 a demon capable of separating slow from fast molecules in a gas, in order to create a ‘hot’ compartment and a ‘cold’ one. Many physicists—among which Brillouin—have contributed to exorcize this demon: in an equilibrium gas, such a spontaneous separation is impossible. However, a granular gas is not an equilibrium system, but is driven by a continuous supply of energy. Several groups have shown that under those circumstances, a spontaneous separation reminiscent of that put forward by Maxwell could be realized [24].

The required experimental set-up is simple: the confining box is divided into two identical compartments that may communicate through a hole. The box is then filled with particles of a granular material and brought into a gas-like state by vertical shaking. With strong shaking, the grains fill the two halves of the box symmetrically, but upon decreasing the agitation, a critical threshold is met below which the above symmetry is broken. One compartment becomes more populated than the other; the grains suffer more collisions there and dissipate more kinetic energy. Identifying the mean kinetic energy and the temperature by analogy with the terminology of molecular gases (see section 4), one then obtains a rather dense and ‘cold’ compartment, coexisting with a more dilute and ‘hot’ counterpart. This phenomenon explains the name ‘Maxwell demon’, often used to refer to the previous situation [25] and [26]. The second law of thermodynamics is nevertheless not violated! In contradistinction with the molecules Maxwell had in mind, the grains are here macroscopic and may absorb and dissipate energy.

The left/right asymmetry may be anticipated on simple grounds. Due to the inelasticity of collisions, a dense region in which more collisions occur will see its mean kinetic energy decrease. If such a fluctuation leads to an increase of density in one of the compartments,

the grains will subsequently escape at a lower rate. Conversely, in the other compartment, the mean energy will increase, which facilitates the escape. The fluctuation is amplified and may overcome the energy input from the base if the shaking is not strong enough, leading to a breakdown of symmetry. Translating the above heuristic argument into a more quantitative theory is, however, not an easy task. Phenomenological approaches have been proposed to refine the argument, with simplifying assumptions [25, 27, 28]. Equating left–right and right–left fluxes of grains leads to qualitative agreement with the experimental observation. The situation where the hole is of large size (e.g. when the aperture between the two compartments typically extends over half the box height [29, 30]) seems more amenable to analytic treatment. When the external forcing is sufficiently strong to allow the neglect of the gravitation force, a hydrodynamic-like description may be put forward, leading to excellent agreement with molecular dynamics simulations of inelastic hard spheres [29, 31]. At constant forcing, the symmetric non-equilibrium steady state becomes unstable when the number of grains exceeds a critical threshold. One of the compartments then becomes ‘colder’ and denser than the other one [32].

4. . . . to Fourier’s law

The hydrodynamic approach, based on a Chapman–Enskog expansion procedure starting from the relevant Boltzmann equation (see e.g. [31, 33, 34]), specifies the form of the constitutive relations between fluxes and gradients. A striking result derived along these lines is that Fourier’s law (relating the heat flux \mathbf{q} to the temperature gradient) is modified with respect to conservative systems. A new term proportional to the density gradient must be added to obtain the heat flux, and one has

$$\mathbf{q} = -\kappa \nabla T - \mu \nabla n, \quad (2)$$

where n denotes the local density of grains. The new transport coefficient μ is positive, whereas it vanishes in a conservative system, as required by the second law of thermodynamics to guarantee that heat flows from hot to cold. On the other hand, the collisions induce a ‘heating’ of the internal degrees of freedom of the grains, which is neglected in modelling of granular systems. So, there is no reason to expect a positive entropy production.

In equation (2), the so-called ‘granular temperature’ T has no thermodynamic foundation, but only a kinetic status. This quantity has no relation with the usual temperature (irrelevant at the grain scale as emphasized in the introduction), but is defined as the variance of the velocity distribution at a given point. The quantity nT is therefore the local kinetic energy density in the local centre-of-mass frame. This definition allows for a direct measurement in an experimental system. Furthermore, it coincides with the thermodynamic definition for a system in equilibrium. The coefficient κ is therefore the counterpart of the thermal conductivity, whereas μ has no analogue in a molecular system and is intrinsically related to the dissipative nature of collisions. The latter quantity has profound consequences on the behaviour of the system, among which is a possible inversion of the granular temperature profile [35–38], a phenomenon that has been observed experimentally [39–41] and may be understood from a hydrodynamic argument [36, 37]. Consider a granular gas driven by an oscillating piston located (on average) at height $z = 0$. The energy flux is clearly directed toward positive z since no energy comes from the empty region at large height. Starting from the base where energy is injected, and increasing z , the temperature first decreases since the energy is dissipated in the bulk. The density of grains may conversely increase or decrease, depending on parameters (gravity and inelasticity). However, the temperature T is not a monotonically decreasing function of height, but passes through a minimum before increasing. This behaviour is at first

sight inconsistent with the dissipative nature of collisions, and indicates that heat flows from ‘cold’ to ‘hot’! It is a direct consequence of the fact that $\mu \neq 0$ in a granular system: in the region where $dT/dz > 0$, the density decays very rapidly, which constitutes the dominant contribution to \mathbf{q} (see equation (2)). The resulting heat flux has therefore a positive projection onto the z -axis, as it should. Note also that this constraint implies that the density is either a decreasing function of z [37] or may reach a maximum at a smaller altitude than that where T is minimum [38].

5. Velocity distribution

Another important characteristic of *molecular gases* lies in the velocity distribution of the molecules. There collisions do not dissipate energy, and the distribution is a Gaussian. One can naturally expect this property to break down for granular gases with dissipative collisions. The first experimental measurements, however, were not precise enough to show deviations from a Gaussian. It was only recently that experimental techniques became available to determine distributions with pronounced differences from Maxwell–Boltzmann statistics, especially in the high-velocity tails of the distributions [42, 11, 9, 43, 8]. Several authors reported a stretched exponential law (on the whole range of velocities available, which covers an accuracy of four to five orders of magnitude for $P(v)$):

$$P(v) \propto \exp[-(v/v_0)^\nu], \quad (3)$$

with various exponents (here v_0 is the ‘thermal’ rms velocity). In particular, an exponent ν close to $3/2$ was found in various experiments [11, 9, 8]. This behaviour was observed for the horizontal velocity components of a vertically vibrated 2D system of steel beads in a wide range of driving frequencies and densities [9], but also in a 3D electrostatically driven granular gas [8]. A question that naturally arises concerns the possible universality of this distribution.

On a theoretical level, a delicate point concerns the supply of energy to the inelastic hard sphere system, which compensates for the dissipation caused by inelastic collisions. The description of driven experiments indeed requires a forcing mechanism allowing the system to reach a steady state. This task is difficult, but the heating process and resulting fluidization described by a ‘stochastic thermostat’ [44–50] has attracted attention, in particular because it has been shown analytically that $P(v)$ exhibits a high-energy tail of the form of equation (3) with $\nu = 3/2$, independent of dimension and restitution coefficient [46], in apparent agreement with the experiments. The above model, where an external spatially homogeneous white-noise driving force acts on the particles and thus injects energy through random ‘kicks’ between the collisions, is therefore considered to provide a relevant theoretical framework to quantify the non-Gaussian form of velocity distributions.

The experimental and theoretical conditions are quite different: in the experiments, the energy is injected at the boundaries, and the system is not homogeneous; the theoretical model on the other hand considers a homogeneous driving by a white noise, acting in the bulk of a homogeneous system. It turns out, however, that the agreement between experiment and theory for the exponent ν is somewhat misleading. For realistic values of the inelasticity ($\alpha > 0.7$), and at the level of the spatially homogeneous Boltzmann equation, the predicted high-velocity tails for $P(v)$, decaying as $\exp(-Av^{3/2})$, are only reached for velocities far beyond the experimentally accessible ones [51]. At ‘thermal’ velocities, $P(v)$ is in fact close to a Gaussian. Of course this does not correspond to a failure of kinetic theory, but is most likely caused by a too simple model for forcing.

Various groups have subsequently tackled the problem by numerical simulations of molecular dynamics [52–57]: such simulations of inelastic hard discs in a two-dimensional box

allow the use of a reasonably realistic energy injection through vibrating walls at the boundaries of the box, and a study of the effect of the various parameters (inelasticities, average density). The parameters can be adjusted to obtain velocity distributions close to their experimental counterparts, and a very good precision can be reached. The simulations lead to the conclusions that the distributions display generically overpopulated tails with respect to a Gaussian; moreover, the details of the distributions depend on the various parameters (density, inelasticity, energy injection . . .) and even on the part of the system where the distribution is measured (i.e. it depends slightly for example on the distance from the boundaries injecting energy).

From the kinetic theory point of view, numerous works have also been devoted to the understanding of the velocity distributions emerging from the inelastic Boltzmann equation. Simplified models such as the Maxwell model may allow for analytical solutions [58–60], while numerical resolution is often used in addition to partial solutions which allow for the prediction for example of the high-velocity tail behaviour [48, 61]. These high-velocity tails generically display stretched exponential behaviours with an exponent depending on the details of the model, while power-law velocity distributions may also be obtained in marginal situations [58–61].

The present consensus emerging from these various studies tends to the conclusion of the absence of universality in the velocity distributions: various experimental conditions and various energy injection modes lead to different distributions. Of course, these conclusions are based on numerical studies of simplified models, so the question of universality can still be considered as open from an experimental point of view. The only common point seem to concern the overpopulation of the high-velocity tails with respect to a Gaussian. To our knowledge, no simple argument, however, exists to justify this phenomenon.

6. Breakdown of equipartition in mixtures

Before concluding, let us briefly turn our attention to mixtures. For a mixture of molecular gases in equilibrium, all species have the same temperature, irrespective of their mass, size, or density. One may wonder if such an equipartition still holds in a granular gas. Two groups have addressed this question experimentally [10, 62], and their results for binary mixtures clearly demonstrate that equipartition does not hold. The mean kinetic energy of heavy grains is larger than that of the light component. These studies have stimulated numerical and analytical investigations, mostly centred on the kinetic theory of inelastic hard spheres [63–65, 53, 66–68].

In simplified situations of homogeneous systems (with no forcing [69] or white-noise driving [65], as well as in shear flows [70]), analytical progress is possible. The distinction between collisions of particles of the same species or of different species leads to closed equations for the granular temperatures of the two components. Solving these equations allows us then to investigate the dependence of the non-equipartition of temperature on the various parameters of the problem (mass ratio, size ratio, densities, inelasticities, etc), which can be varied more easily than in experiments. More realistic molecular dynamics simulations with, for example, energy injection at the boundaries have also been carried out [64, 53, 66, 68, 54]. The results of these various investigations are in qualitative agreement with the experiments, despite the simplifications implied by the modelization. In particular, the heavier particles carry typically more kinetic energy (even if this is not always the case). Moreover, the violation of equipartition increases with the mass ratio, but depends only weakly on the relative densities.

7. Conclusion

Because of the dissipative nature of the collisions, granular gases are inherently out of equilibrium. They are subject to continuous injection and dissipation of energy. An analogy

with molecular gases is usually drawn because of their dilution and incessant collisions. However, this analogy breaks down as soon as the phenomenology is studied: numerous effects forbidden by thermodynamics in equilibrium gases appear (the ‘Maxwell demon’ experiment, modification of Fourier’s law, non-equipartition of energy) as complex consequences of an apparent simple ingredient, the inelasticity of collisions.

In this short review, we have arbitrarily chosen to present some aspects of the rich phenomenology of granular gases, leaving aside many questions worth attention. Among these, we can cite the problem of inelastic collapse [71], the propagation of shock waves [72], possible phase transitions [73], the formation of clusters [74], the long-range correlations of hydrodynamic fields [47], and thermal convection [75–80].

In conclusion, in spite of impressive recent advances in the comprehension of its phenomenology, the field of granular gases still poses serious experimental and theoretical challenges. In particular, independently of its successes and the technical difficulties, the hydrodynamic approach is still a controversial issue. In view of the lack of scale separation and neglect of certain correlations, its efficiency seems to go (far) beyond what one could have expected *a priori*.

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