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Fragmenting granular gases

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Abstract – We study the dynamics of granular gases which fragment due to their collisions. We have developed a kinetic model that accounts for the correlations between grains' size and velocity at collisions. We analyze how the fragmentation events taking place at collisions affect the growth in the number of grains, and also which distribution of grain' sizes they give rise to. We describe the effects that the mechanisms which control the fragmentation process have on the kinetics of the granular mixture, and have characterized the different kinetic regimes they give rise to, depending on the asymptotic behavior of the fragmentation probability. In these different scenarios the size and velocity distributions display also distinct features, and hence can be used to understand the physical processes in fragmenting systems.

Introduction. – Macroscopic objects are known to fragment when subject to external loads or impacts. In recent years, the understanding of fragmentation processes have attracted considerable interest [1–7], due to its scientifical and technological impact in a wide variety of situations. Granulate processing [8], particle comminution [9], collision-induced dissociation reactions [10], shattering of solid objects [11], and meteorite clouds [12] constitute relevant examples where fragmentation appears as a result of the dynamics of the grains and their interplay with energy injection.

In granular materials energy is dissipated at collisions through viscoelastic and plastic deformations; which are also responsible for grain damaging [13,14]. Collision-induced fragmentation is an intrinsically non-linear process because it arises only through grains' collisions. In granular gases grains' sizes and velocities become correlated at the collisions, and such correlations will affect which grains are more likely to break. Therefore, the properties of collision-induced fragmentation will differ qualitatively from linear fragmentation processes [1,15], where the properties or state of each object determine its likelihood to break up, as happens, *e.g.*, on polymer degradation [8].

Molecular Dynamics simulations of collision-induced fragmentation [5,6] have been carried out in dense granular media and have shown that the specific details of how fragmentation takes place does not significantly affect the basic features of the fragmentation process and generically both power law and log-normal fragment size distributions have been reported [6]. However, since such simulations have been carried out at high packing, they have focused on the development of force chain networks, their spatial distribution and its relevance in the efficiency of comminution, rather than in the kinetics of the fragmentation process or grain mass and size distributions.

Our work generalizes studies performed previously in which non-linear fragmentation is described in terms of kinetic equations with simple collision kernels [1,15]. Although for small grains dispersion interactions will lead to a combined action of coagulation and fragmentation [16], in this letter we will concentrate on the fragmentation process and will disregard this second effect to focus on the relevance that collision-induced fragmentation has on the kinetics and distributions of a granular gas. The present approach works at the level of the Boltzmann equation, disregarding the correlations built as a result of the collision process[1], although we will keep detailed account of correlations between size and velocity at the collision events.

Hard-sphere model. – We consider a fluid of D-dimensional inelastic hard spheres. They interact through a sequence of binary collisions and lose a fraction of their relative kinetic energy at each collision, $(1-\alpha^2)/(2D)$ (α is the restitution coefficient, $0<\alpha\leqslant 1$). We describe

[1]For elastic systems it becomes exact at high dilution; for inelastic fluids, one should be restricted to small inelasticities.

fragmentation as a stochastic process characterized by the probability that a grain breaks $P(L,E_p)$. It depends on the grain's size L and stored energy at the collision E_p. Extreme statistics [17] is usually used to characterize fragmentation, and assumes that the weakest defect in the particle is responsible for its failure. According to this approach, we will consider a family of breaking probabilities of the form, $P(L,E_p)=1-\exp\left[-(L/L_0)^\gamma(E_p/E_{p0})^\rho\right]$, where L_0 and E_{p0} stand for the corresponding characteristic scales. This general expression includes, as a particular case ($\gamma=D-1$), the well-known Weibull statistics [18]. The exponents ρ and γ are restricted to values which ensure a non-increasing product $L^\gamma E_p^\rho$ as a function of time.

This effective description disregards the details of how energy stored and lost at collisions is related to grain deformation and fracture [13]. Nonetheless, such simplified, effective modeling allows us to point out the basic effects associated to collision-induced fragmentation. For simplicity's sake we identify the energy stored at a collision, E_p, with the maximal potential energy stored by the grains, and which corresponds to the largest change in relative kinetic energy during grain collision. At fragmentation we enforce mass conservation and distribute the mass of the breaking grain uniformly into its offsprings; for simplicity's sake we will assume that two grains form out of the breaking parent.

We will analyze theoretically the kinetics and particle distribution of a homogeneous fluid of fragmenting grains. To this end, we will neglect grain correlations; in this case the dynamic state of the fluid is characterized by the one-particle distribution function, $f(\mathbf{v},\sigma,t)$, which depends on grain's velocity $\mathbf{v}$ and size σ. It obeys a Boltzmann equation which can be written as

$$\frac{\partial f}{\partial t}=-\mathcal{L}f+\mathcal{G}f+\mathcal{G}_b f+\mathcal{F}f, \qquad (1)$$

where the first term $\mathcal{L}f$ accounts for the disappearance of particles of a given velocity due to the collision process itself, while $\mathcal{G}f$ accounts for the production of new particles of a given species and velocity at the collision. These two terms are the usual gain and loss terms in the Boltzmann equation; they involve both pre-collision and post-collision velocities, $\mathbf{v}_i^*$ and $\mathbf{v}_i$, respectively, because we require that the out-coming velocity of the collision corresponds to the velocity $\mathbf{v}$. Moreover, it is through these relations, between post-collision and pre-collision velocities, that the inelastic character of the collision enters and intrinsic correlations are generated. The pre-collision velocities, in terms of the post-collisional ones, are given by

$$\mathbf{v}_{1,2}^*=\mathbf{v}_{1,2}\mp\frac{m_2}{m_1+m_2}\left(1+\alpha^{-1}\right)\left[\hat{\varepsilon}\cdot\mathbf{v}_{12}\right]\hat{\varepsilon}, \qquad (2)$$

where m_1 and m_2 represent the masses of the colliding particles and $\mathbf{v}_{12}=\mathbf{v}_1-\mathbf{v}_2$ accounts for their relative velocity. Finally, ε stands for the the unit vector joining the grains' center of mass. For a homogeneous system where the spatial dependence is irrelevant, ε can be understood as a uniformly distributed unit vector.

The third contribution in eq. (1), $\mathcal{G}_b f$, accounts for the fragmentation of the colliding grains for a prescribed fragmentation probability $P(L,E_p)$. This is the only non-standard term; it ensures mass and momentum conservation and can be written as

$$\mathcal{G}_b f(\mathbf{v},\sigma)=\int \mathrm{d}\mathcal{D}g(u)P(\sigma_1,E_p)f(\mathbf{v}_1,\sigma_1)f(\mathbf{v}_2,\sigma_2) \times\left[\delta(\sigma-\sigma_1 u^{\frac{1}{D}})+\delta(\sigma-\sigma_1(1-u)^{\frac{1}{D}})\right], \qquad (3)$$

where $g(u)$ is the probability density that one of the offsprings carries a fraction u of the parent's mass and $\mathrm{d}\mathcal{D}\equiv \mathrm{d}\hat{\epsilon}\mathrm{d}1\mathrm{d}2\delta(\mathbf{v}-\mathbf{v}_1^*)\sigma_{12}^{D-1}\theta(\hat{\epsilon}\cdot\mathbf{v}_{12})|\hat{\epsilon}\cdot\mathbf{v}_{12}|$. Here, $\mathrm{d}1=\mathrm{d}\mathbf{v}_1\mathrm{d}\sigma_1$, $\mathrm{d}2=\mathrm{d}\mathbf{v}_2\mathrm{d}\sigma_2$ and $\sigma_{12}^{D-1}\theta(\hat{\epsilon}\cdot\mathbf{v}_{12})|\hat{\epsilon}\cdot\mathbf{v}_{12}|$ corresponds to the collision cross-section with geometric radius $\sigma_{12}\equiv\sigma_1+\sigma_2$. Moreover, θ is the Heaviside function. The delta contributions within brackets enforce mass conservation when the two offsprings are produced. We will analyze the simplest case where mass is uniformly distributed ($g(u)=1$ with $0\leqslant u\leqslant 1$). Finally, $\mathcal{F}f(\mathbf{v},\sigma,t)$ represents the external forcing which injects energy into the system. Its form depends on the details of energy supply; several explicit forms are described, *e.g.*, in [19,20]. The increase in grain number as a result of fragmentation requires an equivalent increase in the frequency of energy injection to sustain a steady state. For ($\mathcal{F}f(\mathbf{v},\sigma,t)=0$), we recover a freely evolving fragmenting granular gas [21].

Kinetics. – The evolution of the hydrodynamic variables, which correspond to moments of $f(\mathbf{v},\sigma,t)$, are derived from the Boltzmann equation. Specifically, the number of grains, $n(t)=\int \mathrm{d}\mathbf{v}\mathrm{d}\sigma f(\mathbf{v},\sigma,t)$, can be expressed as

$$\frac{\mathrm{d}n}{\mathrm{d}t}=\tilde{\omega}n, \qquad (4)$$

where the fragmentation frequency, $\tilde{\omega}$, can be written as

$$\tilde{\omega}(t)=\frac{1}{n}\int \mathrm{d}\hat{\epsilon}\mathrm{d}1\mathrm{d}2\sigma_{12}^{D-1}\theta(\hat{\epsilon}\cdot\mathbf{v}_{12})|\hat{\epsilon}\cdot\mathbf{v}_{12}| \times f(\mathbf{v}_1,\sigma_1,t)f(\mathbf{v}_2,\sigma_2,t)P(\sigma_1,E_{p1}). \qquad (5)$$

The evolution equation for the kinetic energy is $E_c=(\rho/2)\int \mathrm{d}\mathbf{v}\mathrm{d}\sigma\sigma^D v^2 f(\mathbf{v},\sigma,t)$, with ρ the overall grain density. Therefore, it in turn obeys

$$\frac{\mathrm{d}E_c}{\mathrm{d}t}=-b_c\omega(1-\alpha^2)E_c+\psi, \qquad (6)$$

where the first term accounts for energy dissipation due to inelasticity, with b_c the dimensionless collisional average [22] and ω the collision frequency [21,22]. The second contribution describes the energy input and corresponds to the last term in eq. (1). Its specific form depends on energy injection, and $\psi=0$ for a freely evolving granular gas [21]. Subsequently, we discuss results corresponding to a steady state, where heating and collision frequencies are proportional to each other, *i.e.* $\psi\sim\omega$.

We will concentrate on the late-stage kinetics of the system, once transient effects from the initial conditions have vanished, and will assume that a scaling regime is achieved, consistent with numerical evidence as discussed below. In this regime, the distribution function reduces to $f(\mathbf{v},\sigma,t)=\frac{n}{\bar{v}^D\bar{\sigma}}\,\widetilde{f}(\mathbf{c},\bar{\sigma})$, where we have introduced the rescaled size and velocity as $\mathbf{c}=\frac{\mathbf{v}}{\bar{v}}$ and $\bar{\sigma}=\frac{\sigma}{\bar{\sigma}}$, respectively. A natural choice for size and velocity scales correspond to $\bar{v}^2=\langle v^2\rangle$ and $\bar{\sigma}=\langle\sigma\rangle$, where $\langle\ldots\rangle$ stands for an instantaneous particle average of the appropriate quantity.

Since the number of particles increases, mass conservation leads to a decrease of the grains' mean size; in the scaling regime it implies $\bar{\sigma}\propto n^{-1/D}$. In the late stage, the average velocity of the grains is also constant due to the thermostat. The latter implies that the total kinetic energy of the system also remains the same. As a result, the energy per particle decreases as the inverse of the number of grains.

We further assume that $\bar{\sigma}^\gamma E_p^\rho$ goes asymptotically to zero, then in the scaling regime the breaking probability vanishes asymptotically as $P(\bar{\sigma},\bar{E}_p)\propto\bar{\sigma}^\gamma\bar{E}_p^\rho\propto n^{-\frac{D\rho+\gamma}{D}}$. In this case, once the mean velocity has reached its asymptotic value (determined by the balance between the energy input per collision and the energy lost at every collision), the fragmentation frequency scales as $\tilde{\omega}\sim n^{\frac{1-\rho D-\gamma}{D}}$. This dependence determines the fragmentation kinetics,

$$\frac{\mathrm{d}n}{\mathrm{d}t}=n^{\frac{D(1-\rho)+1-\gamma}{D}} \tag{7}$$

which tells us that the number of grains increases with time as

$$n=\left[n_0^{\frac{D\rho-1+\gamma}{D}}+\frac{D\rho-1+\gamma}{D}(t-t_0)\right]^{\frac{D}{D\rho-1+\gamma}}, \tag{8}$$

assuming that scaling holds from a time t_0 when the fluid contains n_0 grains. We can identify three kinetic scenarios. If $D\rho-1+\gamma>0$, the number of grains increases with time algebraically, with exponents controlled by the breaking probability. On the contrary, for $D\rho-1+\gamma<0$, there exists a finite time singularity at which the number of grains diverges. $D\rho-1+\gamma=0$ corresponds to the limiting situation where there is no singularity but the number of grains increases exponentially. Equation (8) still holds for $\gamma=\rho=0$. The latter represents a heated granular gas with constant breaking probability, $P(L,E_p)=p$, and it leads to a finite time singularity. This case corresponds to materials whose fragmentation probability does not depend significantly on grains' size and energy as may happen for certain brittle materials [2]. The particular case of a Weibull type breaking probability ($\gamma=D-1$ and $\rho>0$) evolves as $n\propto t^{D/(D(\rho+1)-2)}$.

For elastic grains, $\alpha=1$, a steady velocity is reached in the absence of heating, and we predict that its kinetics is analogous to that of inelastic grains. The situation differs for freely evolving gases, where the elastic limit $\alpha=1$ is singular [21]. However, for $\alpha<1$ the kinetic scenarios for $\psi=0$ and $\psi\sim\omega$ do not differ qualitatively, although for freely evolving gases the exponents characterizing grains' particle number and kinetic energy depend also on the inelasticity coefficient α [23].

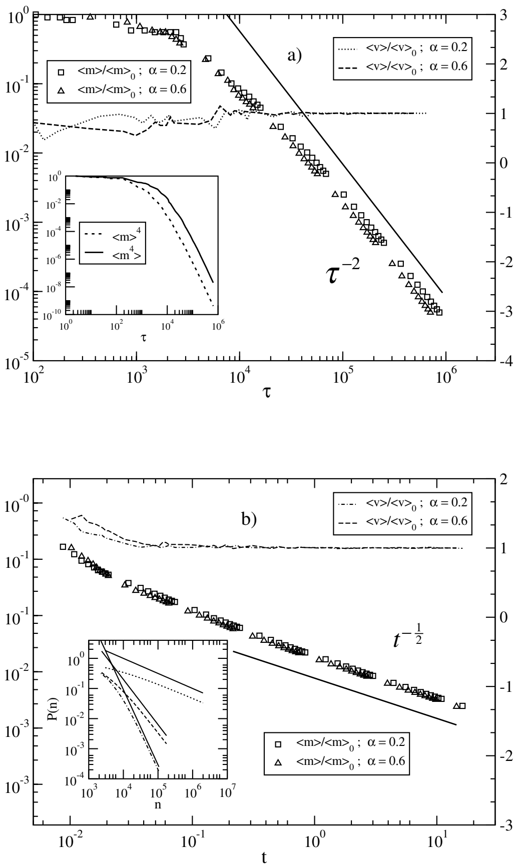

Fig. 1: Time evolution of the mean size (symbols; in log-log) and mean velocity (lines; in log-linear), normalized by their initial values, $\langle m\rangle_0$ and $\langle v\rangle_0$, for different inelasticities and fragmentation probabilities. a) $p=0.01$; b) Weibull fragmentation probability with $\rho=2$. The corresponding analytical power law decays for the mean mass are displayed as continuous lines. The insets show: a) different moments of the mass distribution; b) mean breaking probability as a function of the grain number. Used parameter, $\gamma=1$; $\rho=0$ (dotted line), $\gamma=1$; $\rho=1$ (dashed line) $\gamma=1$; $\rho=2$ (dot-dashed line). Straight lines show the corresponding theoretical predictions.

We have performed Direct Simulation Monte Carlo (DSMC) [19,24] simulations to validate the scaling hypothesis and to obtain the distribution functions in the scaling regime. We have considered only two-dimensional systems, $D=2$, and have started from a monodisperse initial condition. For all the fragmentation probabilities studied we have found no significant deviation from scaling. We will present results for fluids where the energy is injected homogeneously using the Andersen-Lowe thermostat [25] to ensure momentum conservation. However, our results for the grain mass distributions are generic and do not differ significantly if other mechanisms are used to supply energy. In fig. 1a we display the typical grain mass and velocity as a function of time for two inelasticities for a constant breaking probability. All other inelasticities analyzed give analogous results. For a constant breaking probability a finite-time singularity develops. To better appreciate the scaling approach to the singularity it is useful to study the time evolution in terms of a slower time scale, τ, such that $d\tau = n(t)dt$. In this time scale there is no singularity, and the scaling solution of eq. (7) reads $n \propto \tau^{\frac{D}{D-1}}$, and accordingly, $\langle m \rangle \sim \tau^{-\frac{D}{D-1}}$, for the mean mass. To validate further the scaling hypothesis, we have analyzed the decay of different moments of the mass distribution to check that $\langle m^n \rangle \propto \langle m \rangle^n$ (we show an example in the inset of fig. 1a). In fig. 1b we display the time evolution for the typical grain mass and velocity for a few examples where the breaking probability tends asymptotically to zero. As predicted theoretically, there is no finite time singularity for the parameters ρ and σ considered, and the typical mass decays algebraically with the expected exponent. The inset of fig. 1b shows the dependence of the breaking probability on grain size for different ρ values; agreement with the predicted behavior is achieved.

Grain distributions. – DSMC also allows us to analyze the grains' size and velocity distributions. Scaling implies that the distribution functions should collapse on a universal curve when mass and velocities are scaled by their characteristic mean values. We have numerically verified that such a collapse is fulfilled for values of α and p spanning at the range of allowed values. Figure 2a displays the scaled mass distributions corresponding to different restitution coefficients for a constant breaking probability. In all cases the mass distribution has an algebraic decay for small masses, and an asymptotic decay for large masses consistent with an exponential. The latter feature is clearly depicted in the inset, where the same mass distributions are shown in linear-log scale. The algebraic divergence at small masses has a characteristic exponent close to -0.75 ± 0.05. The algebraic divergence is consistent with theoretical predictions for a different family of collision-induced models [1], although with different exponents.

Freely evolving elastic grains show a qualitatively different behavior. Even if the kinetics for elastic and heated inelastic grains is the same, the mass distributions differ significantly for small masses, as depicted in fig. 2a. For elastic grains, $\alpha = 1$, a stronger divergence, controlled by the smallest grains, develops. This qualitative change appears also in the velocity distribution function (data not shown) [23]. Elastic grains develop a two-peak velocity distribution, indicating that the smallest particles have a larger kinetic energy. This behavior looks to be reminiscent of freely evolving fragmenting gases [24], where in the limit of nearly elastic grains a large asymmetry in the grain kinetic energy has been reported. On the contrary, for inelastic grains the velocity distributions decay monotonously with velocity. If one injects energy in an elastic granular gas while keeping its temperature constant, then the mass distribution is indistinguishable

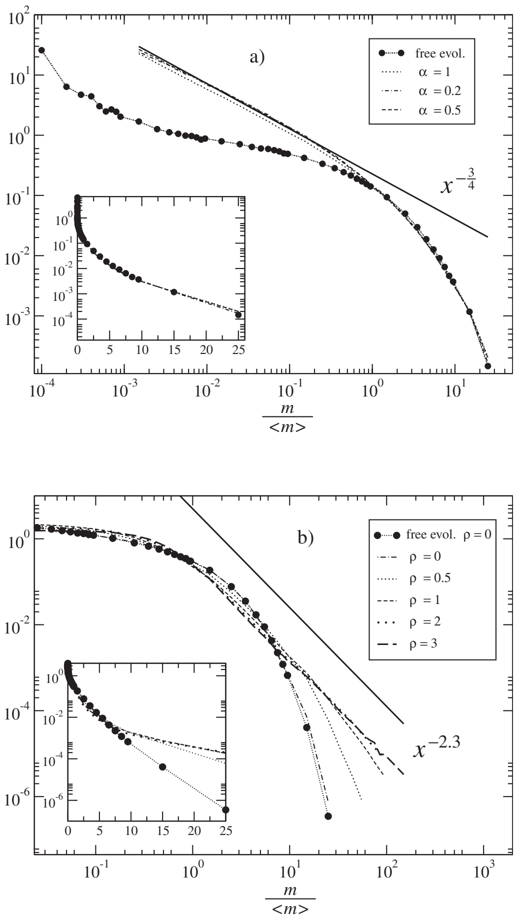

Fig. 2: The scaled mass distribution $f(\frac{m}{\langle em \rangle})$, obtained for fragmenting granular systems: a) constant breaking probability $p = 0.01$. b) Weibull breaking probability, several disorder values ρ are illustrated. In both figures, the dots corresponds to a freely evolving elastic system gas and the fitted power law decays are displayed as continuous lines. The insets show the same curves in linear-log scales, illustrating the distribution functions' large mass decay.

from that of inelastic grains, as shown also in fig. 2a. This indicates that the energy supply does not only serve to set the energy scale of the steady state; it deeply affects how grains break. Kinetic models that disregard the coupling between collisions and fragmentation will miss these qualitative effects on grains' mass and velocity distributions. Figure 2b displays mass distributions for fragmenting probabilities which vanish asymptotically where a plateau in the mass distribution, rather than a divergence, is observed for small grains. For large masses we see that the decay depends on ρ, and that as it increases the curves converge to an algebraic decay characterized by an exponent 2.30 ± 0.05 independent of ρ for the range of sizes sampled. As ρ increases, we observe an asymptotic decay, faster than algebraic, which sets in at larger scaled masses the larger ρ. One can conjecture that the algebraic decay observed does not correspond to the final asymptotic decay at large masses, although the crossover from one regime to the other as a function of ρ deserves a more careful analysis.

We have also analyzed the velocity distribution functions with DSMC. It is well known that inelasticity produces large deviations from Maxwellian behavior, and that the specific departure depends sensitively both on how energy is supplied [19] as well as on the details of grain interactions [20]. Generalized exponential tails are predicted for hard spheres and algebraic tails for Maxwell models. For fragmenting inelastic grains we have observed that the decay at long velocities is less sensitive to the energy injection mechanism than for their non-breaking counterparts and that, depending on the details of energy supply, the asymptotic decays are consistent with either simple exponential or Gaussian tails [23].

Conclusions. – We have studied the kinetics of fragmenting granular gases where fragmentation takes place as a result of their collisions. We have focused on heated systems, where a homogeneous steady state is reached as a balance between energy supply and energy lost through binary collisions, and where fragmentation depends on the energy stored by the grains during the collision. We have seen that the kinetics is essentially determined by the asymptotic behavior of the fragmentation probability, and have found two basic scenarios. If the fragmentation probability tends asymptotically to a finite value, a finite time singularity appears, when the number of grains diverge. On the contrary, if the breaking probability tends algebraically to zero, then the divergence is generically not present. Although we have considered a general family of breaking probabilities based on extreme statistics which generalize Weibull model, since the kinetics is controlled by the asymptotic algebraic decay of the fragmentation probability the results obtained apply to any fragmentation probability which vanishes analytically. Contrary to freely evolving gases, we have seen that the inelasticity does not play a role in the gas kinetics. Hence, the study of the kinetics in fragmenting system opens the possibility to gain insight in the details of how such a fragmentation takes place. The asymptotic behavior of the fragmentation probability also determines the form of the size distri bution functions. Hence, the study of such distributions can also help to identify relevant mechanisms in the fragmentation kinetics of these systems.

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