Mathematical Models and Methods in Applied Sciences
Vol. 12, No. 7 (2002) 1–19

KINETICS MODELS OF INELASTIC GASES

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Received 18 February 2002
Communicated by N. Bellomo and M. Pulvirenti

In the present paper we review some recent progresses in the study of the dynamics of cooling granular gases, obtained using idealized models to address different issues of their kinetics. The inelastic Maxwell gas is studied as an introductory mean field model that has the major advantage of being exactly resoluble in the case of scalar velocities, showing an asymptotic velocity distribution with power law tails $|v|^{-4}$. More realistic models can be obtained placing the same process on a spatial lattice. Two regimes are observed: an uncorrelated transient followed by a dynamical stage characterized by correlations in the velocity field in the form of shocks and vortices. The lattice models, in one and two dimensions, account for different numerical measurements: some of them agree with the already known results, while others have never been efficiently measured and shed light on the deviation from homogeneity. In particular in the velocity-correlated regime the computation of structure factors gives indication of a dynamics similar to that of a diffusion process on large scales with a more complex behavior at shorter scales.

Keywords:

AMS Subject Classification:

1. Introduction

Granular materials, a term often employed in physics, mathematics and engineering to classify collections of inelastic objects, subject to the laws of Newtonian Mechanics, have recently attracted the vivid attention of the scientific community and the field has been extensively studied. In fact, they not only pose novel questions to scientists, but also are of great technological and industrial importance.

These systems show rather peculiar and intriguing features both with respect to their static and dynamical properties. A dilute granular system, subject to tapping, shaking or some other kind of external driving, which supplies the energy dissipated by the inelastic collisions, may behave similarly to a fluid. On the contrary, in the absence of external forces it loses gradually its kinetic energy and comes to rest. In addition, it may become spontaneously inhomogeneous and form patterns. Such a behavior during the free cooling process displays interesting analogies and connections with other areas of non-equilibrium statistical mechanics such as ordering kinetics,[1] decaying turbulence[2] and diffusion.[1]

The statistical approach to the study of such subject seems to be one of the most promising tools to its comprehension. In fact, one deals with very large assemblies of particles so that it makes sense to measure only average properties and their fluctuations. On the other hand, it is not possible to apply the standard Gibbs Equilibrium Ensemble method, because these systems are intrinsically out of equilibrium. Hence, one is led to employ alternative statistical approaches such as kinetic theory or numerical simulations.

The Boltzmann equation plays a central role in non-equilibrium statistical mechanics of rarefied fluids and it has been applied to describe the behavior of dilute granular systems.[18] It governs the evolution of the one-particle distribution function taking into account only binary collisions. However, the solutions of the Boltzmann equation, being a nonlinear integro-differential equation, are not known for an arbitrary choice of the inter-particle potential and of the boundary conditions. Therefore, it is tempting to consider simplified models for which in some cases it is possible to obtain the solutions or at least the numerical effort is greatly reduced.

The first example of such an attitude is represented by the attention dedicated to the so-called Maxwell molecules. By an appropriate choice of the intermolecular potential the collision rate becomes a simple function of the energy and the resulting Boltzmann equation greatly simplifies. Several important studies have dealt, at the end of the 70s, with the treatment of the Boltzmann equation for Maxwell molecules (see review Ref. 4), i.e. of energy conserving systems. Among these perhaps the most influential has been the work of Bobylev and independently of Krook and Wu, who found exact similarity solutions for the model. After a period of relative calm, the advent of granular systems has revived the interest towards Maxwell models.[13] In the case of inelastic systems, in order to justify the major simplicity of the Boltzmann equation, one cannot invoke a particular form of the inter-particle potential, but has to assume its form as a definition. Nevertheless, the model displays a behavior which parallel that of more realistic systems, but also shows statistical features of great interest.

The present paper is organized as follows: in Sec. 2 we discuss the general issue of granular gas models, Sec. 3 describes the behavior of systems of particles mutually colliding with an energy-independent collision rate and disregarding their relative position: this system can be viewed as a Mean Field Model for granular gases, in the sense that all possible pairs may interact. In Sec. 4, instead, we place the particles on a regular lattice and assume that each particle can interact with its nearest neighbor only.

2. Granular Gases

Granular gases are defined, in the present paper, as assemblies of inelastic hard objects, i.e. particles that interact by means of instantaneous binary collisions. The inelasticity is accounted through the so-called normal restitution coefficient, α. If we model the grains as smooth spheres a collision between two particles i and j with precollisional velocities $\mathbf{v}_i$ and $\mathbf{v}_j$ and positions $\mathbf{r}_i$ and $\mathbf{r}_j$ has the effect of reversing and reducing the component of the relative velocity along the direction $\hat{\sigma} = (\mathbf{r}_i - \mathbf{r}_j)/|\mathbf{r}_i - \mathbf{r}_j|$ by a factor $(1-\alpha)$. This corresponds to the following relation between post-collisional velocities (primed) and pre-collisional velocities (not primed):

$$\mathbf{v}'_j = \mathbf{v}_j + \Theta(-(\mathbf{v}_i - \mathbf{v}_j)\cdot\hat{\sigma})\frac{1+\alpha}{2}((\mathbf{v}_i - \mathbf{v}_j)\cdot\hat{\sigma})\hat{\sigma}\,, \tag{2.1a}$$

$$\mathbf{v}'_i = \mathbf{v}_i - \Theta(-(\mathbf{v}_i - \mathbf{v}_j)\cdot\hat{\sigma})\frac{1+\alpha}{2}((\mathbf{v}_i - \mathbf{v}_j)\cdot\hat{\sigma})\hat{\sigma}\,. \tag{2.1b}$$

The Heaviside function Θ here represents the condition that colliding particles move against each other, a "kinematic constraint" to be satisfied at each collision. The restitution coefficient $\alpha \in [0,1]$ is usually considered not dependent on the relative velocity of the colliding particles. This is an important simplification which can lead to a dramatic instability in numerical simulations, called "inelastic collapse": the collision rate regarding a group of few particles may diverge; this can be avoided using velocity dependent restitution coefficients, in such a way that collisions among particles with a lower relative velocity have an higher restitution coefficient (i.e. are more elastic).

In the following we shall discuss the physics of cooling granular fluids by illustrating its rich phenomenology by means of a series of minimal models based on the simplest rule (2.1a) which ensures momentum conservation during inelastic collisions. We start from a mean field version with no positional degrees of freedom for the grains and successively we release such a constraint to consider one-dimensional and two-dimensional systems.

3. Mean Field Model

3.1. *Elastic models*

To appreciate the difference between an ordinary and a granular gas one can start with the following minimal model constituted by N particles without positional degrees of freedom and characterized only by d-dimensional velocities. The evolution of the system is driven by random selection of pairs of velocities $(\mathbf{v}_i, \mathbf{v}_j)$ which are updated according to Eq. (2.1). Since there is no true movement of the grains, the center-to-center direction $\hat{\sigma}$ is randomly chosen with a uniform distribution in the d-dimensional sphere (the "kinematic constraint" can be equivalently disregarded, as it would just randomly avoid half of the collisions to happen). A unit time corresponds to N collisions. This model, for two-dimensional velocities, has been put forward by Ulam[3] for elastic gases ($\alpha = 1$). He showed how the velocity distribution asymptotically converges to the Maxwell distribution, independently from the starting distribution.

The Master Equation for this stochastic model (including the "kinematic constraint") can be easily written down:

$$\frac{\partial}{\partial \tau} P(\mathbf{v}, \tau) = \int d\mathbf{v}_2 \int_{(\mathbf{v}-\mathbf{v}_2)\cdot\hat{\mathbf{n}}>0} d\hat{\mathbf{n}} [\mathbf{P}(\mathbf{v}', \tau)\mathbf{P}(\mathbf{v}'_2, \tau) - \mathbf{P}(\mathbf{v}, \tau)\mathbf{P}(\mathbf{v}_2, \tau)] , \qquad (3.2)$$

where the primed velocities are the pre-collisional velocity of an elastic collision and $\mathbf{v}_2$ is a generic post-collisional velocity vector.

Equation (3.2) is also well known in kinetic theory, as it belongs to the family of the nonlinear Model-Boltzmann equations[4]: in this context it can be justified in different ways, starting from the Boltzmann equation, e.g. in the following form:

$$\left(\frac{\partial}{\partial t} + v_i \frac{\partial}{\partial r_i}\right) P(\mathbf{r}, \mathbf{v}, \mathbf{t}) = \int d\mathbf{v}_2 \int d\hat{\mathbf{n}} \mathbf{g} \mathbf{I}(\mathbf{g}, \chi) [\mathbf{P}(\mathbf{r}, \mathbf{v}', \mathbf{t})\mathbf{P}(\mathbf{r}, \mathbf{v}'_2, \mathbf{t}) - \mathbf{P}(\mathbf{r}, \mathbf{v}, \mathbf{t})\mathbf{P}(\mathbf{r}, \mathbf{v}_2, \mathbf{t})] \qquad (3.3)$$

being $g = |\mathbf{v} - \mathbf{v}_2|$ and $I(g, \chi)$ the scattering cross-section which, for central interaction potentials, depends only upon the relative velocity g and the scattering angle χ.

If the particles of the gas interact via a power-law potential $V(r) \propto r^{-s}$, where $s = 2(d-1)$ and d is the space dimension, then the term $gI(g, \chi)$ becomes a function of only the scattering angle, obtaining the so-called Maxwell model kinetic equation; if the collisional kernel $gI(g, \chi)$ is approximated to not depend upon the scattering angle [eventually including the constraint $(\mathbf{v} - \mathbf{v}_2) \cdot \hat{\mathbf{n}} > 0$], then, in the spatially homogeneous case, Eq. (3.2) is obtained. This is sometimes referred to as Krook–Wu model.[4]

Another way to justify Eq. (3.2) is in the context of hard spheres: for hard spheres, in fact, $gI(g, \chi) \equiv |(\mathbf{v} - \mathbf{v}') \cdot \hat{\mathbf{n}}|$ and Eq. (3.2) can be immediately obtained, as an approximation, with the assumption:

$$|(\mathbf{v} - \mathbf{v}') \cdot \hat{\mathbf{n}}| \propto \sqrt{\mathbf{T}(\mathbf{r}, \mathbf{t})} , \qquad (3.4)$$

i.e. the relative velocities of the colliding particles are assumed to be of the order of the square-root of the local temperature of the gas. This leads to rewrite Eq. (3.3) as:

$$\left(\frac{\partial}{\partial t} + v_i \frac{\partial}{\partial r_i}\right) P(\mathbf{r}, \mathbf{v}, \mathbf{t}) = \mathbf{S}(\mathbf{r}, \mathbf{t}) \int d\mathbf{v}_2 \int_{(\mathbf{v}-\mathbf{v}_2)\cdot\hat{\mathbf{n}}>0} d\hat{\mathbf{n}} [\mathbf{P}(\mathbf{r}, \mathbf{v}', \mathbf{t})\mathbf{P}(\mathbf{r}, \mathbf{v}'_2, \mathbf{t}) - \mathbf{P}(\mathbf{r}, \mathbf{v}, \mathbf{t})\mathbf{P}(\mathbf{r}, \mathbf{v}_2, \mathbf{t})] . \qquad (3.5)$$

The pre-factor $S(\mathbf{r}, \mathbf{t})$ is proportional to $\sqrt{T(\mathbf{r}, \mathbf{t})}$. This derivation has been recently proposed by Bobylev *et al.*[17] The assumption of homogeneity changes the above equation in the following way:

$$\frac{\partial P(\mathbf{v},\mathbf{t})}{\partial t} = S(t)\int d\mathbf{v}_2 \int_{(\mathbf{v}-\mathbf{v}_2)\cdot\hat{\mathbf{n}}>0} d\hat{\mathbf{n}}[\mathbf{P}(\mathbf{v}',\mathbf{t})\mathbf{P}(\mathbf{v}'_2,\mathbf{t}) - \mathbf{P}(\mathbf{v},\mathbf{t})\mathbf{P}(\mathbf{v}_2,\mathbf{t})] \quad (3.6)$$

which reduces to (3.2) since the $S(t)$ dependence (e.g. the time dependence of the temperature) can be absorbed by a time reparametrization $t \to \tau$.

Note that the main physical property that distinguishes the nonlinear equation (3.2) among the family of nonlinear Boltzmann equations (3.3) is the fact that the collision rate is independent of the energy of the colliding particles. This introduces a dramatic simplification.

3.2. *Bobylev Fourier transforms and scaling solutions*

Equation (3.2) can be recast in a more convenient way by employing the characteristic function:

$$\tilde{P}(\mathbf{k},\tau) = \int d\mathbf{v}\exp\{-\mathbf{ikv}\}\mathbf{P}(\mathbf{v},\tau)\,, \quad (3.7)$$

that is the Fourier transform of $P(\mathbf{v})$, obtaining

$$\frac{\partial\tilde{P}(\mathbf{k},\tau)}{\partial\tau} = -\tilde{P}(\mathbf{k},\tau) + \frac{1}{\mathbf{\Omega}_d}\int d\hat{\mathbf{n}}\tilde{\mathbf{P}}\left(\frac{\mathbf{k}}{2}(\hat{\mathbf{k}}-\hat{\mathbf{n}}),\tau\right)\tilde{\mathbf{P}}\left(\frac{\mathbf{k}}{2}(\hat{\mathbf{k}}+\hat{\mathbf{n}}),\tau\right). \quad (3.8)$$

Here $\hat{\mathbf{n}}$ is a unit vector, and Ω_d is the d-dimensional solid angle. In the derivation of the last equation, we use the normalization condition, which reads for the characteristic function $\tilde{P}(\mathbf{0},\tau) = \mathbf{1}$. The conservatin laws to be imposed to the solutions are:

$$\nabla_{\mathbf{k}}\tilde{P}(\mathbf{k},\tau)\mid_{\mathbf{k}=\mathbf{0}} \equiv -i\langle\mathbf{v}\rangle = \mathbf{0}\,, \quad (3.9a)$$

$$\nabla^2_{\mathbf{k}}\tilde{P}(\mathbf{k},\tau)\mid_{\mathbf{k}=\mathbf{0}} \equiv -\langle v^2\rangle = -d\,, \quad (3.9b)$$

where we choose, without loss of generality, solutions with zero momentum and energy equal to d. Several studies have focused on the finding of families of self-similar solutions of this equation of the kind

$$\phi(\exp(-\lambda\tau)\mathbf{k})\,. \quad (3.10)$$

In fact such an expression violates the conservation law (3.9b). However exploiting the "Bobylev symmetry"[4] of the equation which makes $\Phi_s(\mathbf{k},\tau) = \exp(-\mathbf{sk}^2/2)\mathbf{\Phi}(\mathbf{k},\tau)$ a solution whenever $\Phi(\mathbf{k},\tau)$ is a solution, then a similarity solution can be found of the form

$$\Phi(\mathbf{k},\tau) = \exp(-\mathbf{k}^2)\phi(\mathbf{k}\exp(-\lambda\tau)) \quad (3.11)$$

with a proper choice of λ. Coming back to the velocity distribution, this accounts to finding a solution of the form

$$P(\mathbf{v},\tau) = \frac{1}{(2\pi)^{d/2}}\int d\tilde{\mathbf{w}}\exp(\lambda\tau)\mathbf{f}(\mathbf{w}\exp(\lambda\tau))\exp\left[-\frac{(\mathbf{v}-\mathbf{w})^2}{2}\right], \quad (3.12)$$

(where f is the inverse Fourier transform of ϕ) which gives the correct asymptotics

$$\lim_{\tau\to\infty} P(\mathbf{v},\tau) = (2\pi)^{-d/2}\exp(-\mathbf{v}^2/2)\,, \tag{3.13}$$

as expected from the H-theorem.

The problems with this techniques are due to the positivity of the final solution which is not guaranteed or, given $\phi(\mathbf{x})$, not even easy to prove. A complete review of methods and results is given in Ref. 4, together with a discussion on the so-called Krook–Wu conjecture about the relevance of the scaling solutions.

3.3. *Inelastic Maxwell models*

An interesting inelastic version of the Ulam model has recently been proposed by Ben Naim and Krapivsky (BK).[13] As before, random pairs of particles are selected, but now their velocities are updated accordingly with the collision rule (2.1a), where the inelasticity is modeled through a restitution coefficient α. The Boltzmann equation of the corresponding Maxwell model (3.2) is modified as follows:

$$\frac{\partial P(\mathbf{v},\tau)}{\partial t} = \int d\mathbf{v}_2 \int_{(\mathbf{v}-\mathbf{v}_2)\cdot\hat{\mathbf{n}}>0} d\hat{\mathbf{n}}\left[\frac{1}{\alpha}\mathbf{P}(\mathbf{v}',\tau)\mathbf{P}(\mathbf{v}_2',\tau) - \mathbf{P}(\mathbf{v},\tau)\mathbf{P}(\mathbf{v}_2,\tau)\right]\,. \tag{3.14}$$

The inelasticity has several major consequences:

(1) In the absence of external energy injection the total kinetic energy of the fluid decreases, i.e. the velocity distribution becomes narrower with time, i.e. the granular temperature $\varepsilon(\tau) = \langle v^2\rangle$ decreases.
(2) While in the elastic case for $d = 1$ any initial distribution is left unchanged by the dynamics since the particles upon colliding merely exchange their state, when the collisions are inelastic the model becomes nontrivial and the equation reads, setting $\beta = 2/(1+\alpha)$:

$$\partial_t P(v,t) = \beta\int du\, P(u,t)P(\beta v + (1-\beta)u, t) - P(v,t)\,. \tag{3.15}$$

The first term on the R.H.S. represents the average gain and the second the average loss in the collision process.

Multiplying both sides of the equation by v^2 and integrating, a closed equation for the evolution of the energy can be obtained which gives:

$$\varepsilon(\tau) = \varepsilon_0\exp(-\lambda\tau)\,, \tag{3.16}$$

where ε_0 is the initial energy of the system, which can arbitrarily be chosen equal to 1 without loss of generality, and λ depends on the restitution coefficient α

$$\lambda = \frac{1-\alpha^2}{2}\,. \tag{3.17}$$

(The exponential decay of the energy can be simply proved for any dimension, with $\lambda = (1-\alpha^2)/(2d)$.) The same result can be obtained starting from the Fourier transformed equation, which reads:

$$\partial_\tau \tilde{P}(k,\tau) + \tilde{P}(k,\tau) = \tilde{P}[k/(1-\beta),\tau]\tilde{P}[k/\beta,\tau] \tag{3.18}$$

differentiating twice with respect to k and computing the result for $k = 0$. In fact, since $\tilde{P}(k,t)$ is the generating function for the moments of the distribution $P(v,t)$, then

$$\partial_k^2 \tilde{P}(k,t) \mid_{k=0} = -\langle v^2 \rangle = -\varepsilon(\tau)\,.$$

In principle the dissipative nature of the problem reintroduces the possibility of finding a scaling solution of (3.18) of the form (3.10) for the Boltzmann equation, at odds with the elastic case. This means finding a scaling solution

$$P(v,\tau) = \frac{f(v/v_0(\tau))}{v_0(\tau)}\,, \tag{3.19}$$

where $v_0 = \sqrt{\varepsilon(\tau)}$ and f is the inverse Fourier transform of ϕ. Formally, a scaling solution of this kind imposes a temporal dependence of the higher moments:

$$\langle v^{2m} \rangle = v_0(\tau)^{2m} \mu_{2m}\,, \tag{3.20a}$$

where

$$\mu_{2m} = \int dy f(y) y^{2m} \tag{3.20b}$$

does not depend on time.

Ben-Naim and Krapivsky showed that it is possible to write the equations for every moment of the velocity distribution $P(\mathbf{v},\tau)$. The second moment has a closed equation (which gives the simple exponential decay mentioned) while the others depend on the lower order ones. They computed the asymptotic decay of every moment and found that

$$\lim_{\tau\to\infty} \frac{\langle v^{2m} \rangle}{(\langle v^2 \rangle)^m} = \infty\,.$$

Considering Eqs. (3.20), this result seems to rule out the very existence of a physical scaling solution. For instance even if

$$\phi(x) = (1+x)\exp(-x) \tag{3.21}$$

is a valid scaling solution, it does not correspond to a real f, since it does not satisfy:

$$\phi(-x) = [\phi(x)]^\dagger\,.$$

In fact this is not the case if one considers the possibility of a scaling function f with diverging moments $\mu_{2m} = \infty$ for $m > 1$. In such a case $\phi(x)$ should lose analyticity for $x = 0$. For instance

$$\phi(|x|) = (1+|x|)\exp(-|x|) \tag{3.22}$$

corresponds to the positive

$$f(y) = \frac{2}{\pi[1+y^2]^2}\,,$$

whose large algebraic tails are the signature that moments higher then the second diverge. Note the nonanalytic structure of (3.22) for $x \to 0$:

$$\phi(x) = 1 - \frac{1}{2}x^2 - \frac{1}{3}|x|x^2 + o(|x|x^2)\,. \tag{3.23}$$

The singular term $|x|x^2$ is the counterpart of tail y^{-4} for large $y \gg 1$, i.e. of the divergence of μ_4.

A direct inspection shows that the corresponding velocity distribution

$$P(v, \tau) = \frac{2}{\pi v_0(\tau)[1 + (v/v_0(\tau))^2]^2} \tag{3.24}$$

is indeed a solution of the nonlinear Boltzmann equation, for every value of α.

In fact we believe that (3.24) represents the asymptotic solution for a large class of initial distributions, for the following arguments:

(1) as shown by Ben Naim and Krapivsky, the dynamics of the moments for a generic starting distribution can be computed, giving $\lim_{t\to\infty}\langle v^{2m}(t)\rangle / \langle v^2(t)\rangle^m = \infty$ for $m > 1$;
(2) secondly we performed numerical simulations of the BK model, collecting evidence of the convergence to the solution (3.24) for several starting velocity distributions, namely uniform, exponential (see Fig. 1(a)) or Gaussian.

Interestingly the asymptotic probability distribution function (pdf) (3.24) does not depend on the restitution parameter α. A similar asymptotic universality is expected for a real one-dimensional granular gas, as shown by recent extensive numerical simulations.[8] However, when the BK model is generalized to vectorial velocities, the tails of the pdf depend on α. Results of our numerical simulations for the two-dimensional case are shown in Fig. 1(b). For $\alpha = 1$ we recover the asymptotic Maxwell distribution predicted by Ulam, whereas for $\alpha = 0$ our data suggest the formation of algebraic tails.

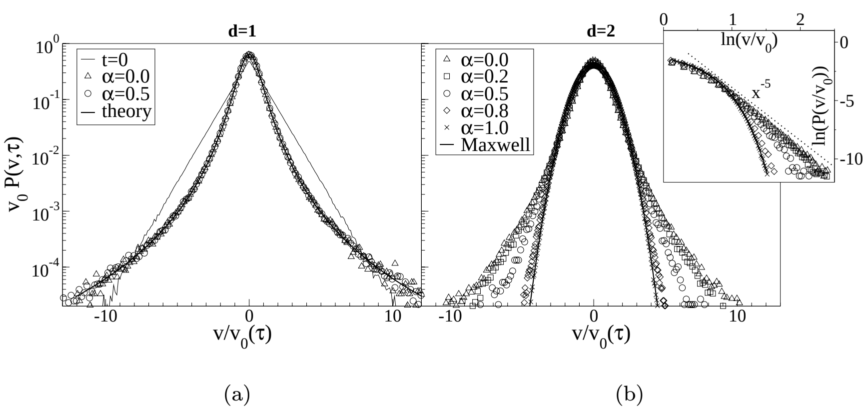

Fig. 1. Asymptotic velocity distributions $P(v, t)$ versus $v/v_0(t)$ for different values of α from the simulation of the inelastic pseudo-Maxwell (Ulam's) model in (a) 1D and (b) 2D.

3.4. *Higher dimensions*

The numerical indication shown in Fig. 1 of large algebraic tails for $d > 1$ has been recently confirmed by several analytical study.[26,27] These works compute self-consistently the exponents at every dimension considering the first singular term in the $x \to 0$ behavior for the Fourier transformed scaling function $\phi(\mathbf{x})$. First consider the isotropic solution

$$\phi(\mathbf{x}) = \psi(\mathbf{x}^2)\,.$$

If the corresponding scaling solution has algebraic tails for large y of the form

$$f(\mathbf{y}) \propto \mathbf{y}^{-2a-d}\,,$$

then its Fourier transform for small values of its argument

$$\psi(z) \simeq 1 + \frac{1}{2}z + \sum_{m<a} \frac{\mu_{2m}}{(2m)!} z^m + Az^a + o(z^a)\,. \tag{3.25}$$

In the one-dimensional case, for instance, the large y^{-4} tails correspond to $a = 3/2$, i.e. $\psi(z) \simeq 1 + z/2 + 1/3z^{3/2} + o(z^{3/2})$.

Inserting the form (3.25) in the Fourier transformed equation for the isotropic scaling solution and equating the coefficients of equal powers of z an equation for a can be obtained. We return to Refs. 11 and 27 for the detailed derivation of the final transcendental equation

$$1 - \lambda(a - d/2) = \int_0^1 \mathcal{D}\mu[\xi^{a-d/2} + \eta^{a-d/2}]\,, \tag{3.26}$$

where

$$\mathcal{D}\mu = \frac{\mu^{-1/2}(1-\mu)^{(d-2)/2}}{B(1/2,\, \frac{d-1}{2})} d\mu\,, \tag{3.27a}$$

$$\xi = 1 - [3 + \alpha(2-\alpha)]\frac{\mu}{4}\,, \tag{3.27b}$$

$$\eta = (1+\alpha)\frac{\mu}{4} \tag{3.27c}$$

and $\lambda = (1 - \alpha^2)/d$, while B is the beta function which guarantees the proper normalization $\int_0^1 \mathcal{D}\mu = 1$.

Equation (3.26) (which can be solved numerically) gives the exponent a for a generic dimension $d > 1$ and restitution coefficient α. In the elastic limit $\alpha \to 1$ the exponent $a \to \infty$, indicating that one recovers the Gaussian Boltzmann distribution tail.

3.5. *Relevance of mean-field models*

In spite of these nontrivial features Mean Field models do not bear a strong resemblance with physical reality. Obviously, their mean field character prevents the onset of any kind of inhomogeneities. On the other hand, theoretical approaches

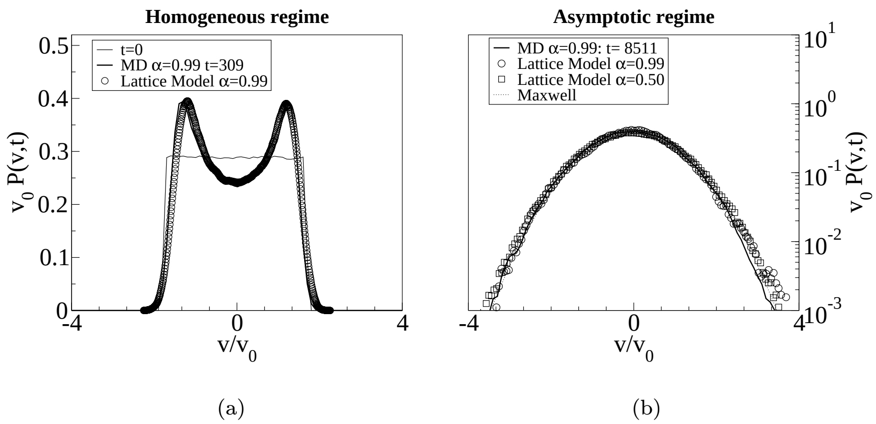

Fig. 2. Rescaled velocity distributions for the 1D MD and in the 1D lattice gas, during (a) the homogeneous and (b) the inhomogeneous phase. (a) also shows the initial distribution (both models). The distributions refer to systems having the same energy. Data refer to $N = 10^6$ (both models) particles with $\alpha = 0.99$ and $\alpha = 0.5$ (for the lattice model in the inhomogeneous regime).

based on linear stability analysis predict three distinct and consecutive dynamical regimes:[9,11] homogeneous, inhomogeneous in the velocity field, inhomogeneous in the velocity and density fields. Realistic tests of this state of affairs are provided by Molecular Dynamics or Event Driven simulations (see for example Refs. 12 and 13 in 1D and Refs. 9, 11, 14, 19 and 20 in 2D or 3D). These simulations agree well with the theory in the homogeneous regime, while in the correlated stage do not provide a clear answer, since they become exceedingly demanding; in fact, the instabilities appear only in large systems and at late times. However, even the homogeneous cooling regime of a one-dimensional granular gas seems very different from that predicted by the BK model. In Fig. 2(a), we show the velocity distribution before the onset of extensive correlations in the velocity fields for a quasielastic systems. In this case, and more generally for larger inelasticity, we observe a suppression of the tails, in contrast with the algebraic behavior of (3.24).

4. Lattice Models

In a realistic description of the dynamics of granular gases one needs to account for the spatial structure of the systems. In fact, one observes in numerical simulations of hard inelastic bodies that the local average velocity and local average density become non-uniform as the system evolves.

In such simulations, the evolution of a system of particles having initial random positions and velocities consists of three different stages:[11]

(a) a completely homogeneous stage, extensively studied since the first contribution by Haff.[21] In such a regime both the density and the velocity field are homogeneous. The energy decays, after a very brief transient of the order of a collision per particle, as

$$\varepsilon(t) = \frac{\sum_{i=1}^{N} |\mathbf{v}_i(\mathbf{t})|^2}{N} \sim t^{-2}\,, \tag{4.28}$$

which corresponds to an exponential decay

$$\varepsilon(\tau) \sim \exp(-\lambda\tau)\,, \tag{4.29}$$

if the time is measured by the number of collisions per particle τ.

(b) a second stage in which the density is still homogeneous, but the velocity field develops inhomogeneities and the energy decay exhibits a power-law behavior in the number of collisions τ, which depends on the dimensionality of the ambient space;

(c) a third stage in which the density field also exhibits strong inhomogeneities.

The three stages are clearly separated (at least for not too high inelasticity). Analytical confirmations of this scenario have been obtained by means of linear stability analysis of the macroscopic (hydrodynamics) description of the system.[9–11]. Studies of the deviations from homogeneity have been obtained by means of fluctuating hydrodynamics analysis[11] and mode-coupling theory,[14] obtaining scaling forms for the structure factors of the velocity and density fields and estimates for the asymptotic energy decay.

In the following sections, we shall deal with a natural extension of the Maxwell models, able to incorporate the correlations which characterize the more realistic descriptions of granular gases. This extension is obtained by placing immobile particles, endowed with a velocity, on the nodes of a regular lattice (with periodic boundary conditions). The evolution of the system is obtained by choosing a random nearest neighbor pair and updating their velocities according to the transformation Eq. (2.1), where now $\hat{\sigma}$ represents the unit vector pointing from site j to i. In this model the time is measured by means of the number of collisions per particle τ. We shall show that such a model captures the formation of dynamical correlations.

In the lattice model the particles are fixed to their lattice positions, so that there is no relation between their velocities and their displacements. As a consequence the proposed lattice models fail to describe stage c), because we are not including density inhomogeneities. Nevertheless they are able to probe the physically interesting regime characterized by an inhomogeneous velocity field.

The velocity field initially prepared in a state characterized by random uncorrelated velocities, remains homogeneously random (i.e. without correlations) during a first dynamical stage, in agreement with the so-called Homogeneous Cooling Regime (or Haff regime) observed in simulations of inelastic hard bodies. Afterwards, one observes the formation of spatial correlations in the velocity field, in the form of structured domains, i.e. shocks and vortices. This is analogous to the formation of magnetic domains in standard quench processes.

In fact, the free cooling process bears a strong resemblance with a quench from an initially stable disordered phase to a low temperature phase in a magnetic system.[1] In the granular case the relaxation occurs due to the inelasticity. Since many possible configurations are compatible with the linear and angular momentum conservation and compete in order to minimize the energy dissipation, the system does not relax immediately towards a motionless state, but displays a behavior similar to that observed in a coarsening process.

We have studied one-[5,6] and two-dimensional[7,6] versions of this lattice model and some results will be briefly discussed below.

4.1. *One-dimensional models*

One-dimensional models represent a favorite playground for theoretical physicists and in fact systems of inelastic hard rods on a ring have extensively been studied.[8,12,16] Here we want just to briefly show the results for the velocity distributions obtained with our lattice model. At odds with the BK (scalar) model, the one-dimensional lattice model seems to recover quantitatively the distributions measured in the inelastic hard rod system, in both the homogeneous and the inhomogeneous phase.

In Fig. 2 we show the good agreement obtained with comparing velocity probability distribution function of the lattice model and that measured in Molecular Dynamics simulations of the inelastic hard rod gas.

- in the left frame the velocity probability distribution function in the early homogeneous regime of a nearly elastic system ($\alpha = 0.99$) is shown: it displays the characteristic two-peaks form that has been predicted by Benedetto *et al.*[15] studying the quasielastic limit of the corresponding Boltzmann equation; for larger inelasticities the formation of the peaks is less evident, but a suppression of the tails is generically observed;
- for larger times the asymptotic probability distribution function turns Gaussian in both models, contrary to the expectation, based on the Burgers equation, that the tails of the velocity probability distribution function should be of the form $\exp(-v^3)$.

The tentative of comparing the lattice model against the Inelastic Hard Rod model encounters a major obstacle in the functional form of the energy decay, which has been measured to be $\sim t^{-2/3}$ in the IHR model, while is $\sim \tau^{-1/2}$ in the lattice model: in order to directly compare those results, the mapping $\tau \to t$ is needed, but this has been observed to depend upon the particular regularization of the dynamics used to avoid the *inelastic collapse* in the simulations of the IHR.[8]

Other features, such as shock fronts, observed in recent extensive simulations of hard rods,[8] have their counterparts in our one-dimensional lattice model and are discussed in detail in Ref. 5.

4.2. *Two-dimensional lattice model*

In the present section we consider a slightly more realistic situation: a system of particles sitting on a regular two-dimensional triangular lattice and endowed with a two-dimensional velocity.[7]

The cross-over from the homogeneous to the inhomogeneous regime is again manifest in the change of the energy decay law. As shown in Fig. 3, at first the average energy per particle $\varepsilon(\tau) = \sum v_i(\tau)^2/N$ decreases exponentially at a rate $\lambda = (1-\alpha^2)/4$. This behavior reflects the fact that each velocity evolves independently of the others.[21] On the other hand, for times larger than $t_c \sim \lambda^{-1}$, a second regime arises, where correlations play a major role and the average energy per particle decays as $\varepsilon(t) \sim t^{-1}$.

During the early stage the velocity probability distribution function changes, as already explained in the case of the one-dimensional lattice model. In two dimensions, during the early regime the velocity distribution deviates sensibly from a Maxwell distribution and shows more pronounced high velocity tails. These tails seem to be determined by the lack of spatial correlations up to t_c. As soon as the energy begins to decay as t^{-1} the velocity distribution changes to a Gaussian.

The inelasticity of the collisions and the presence of the Θ have the effect of reducing the quantity $(-(\mathbf{v}_i - \mathbf{v}_j)\cdot\hat{\sigma})$, i.e. inducing an alignment of the velocities. The most dramatic consequence, in two dimensions, is the spontaneous formation of vortices as shown in Fig. 4. Vortices form spontaneously and represent the boundaries between regions which selected different orientations of the velocities during the quench and are an unavoidable consequence of the conservation laws which forbid the formation of a single domain (conservation of linear and angular momentum).

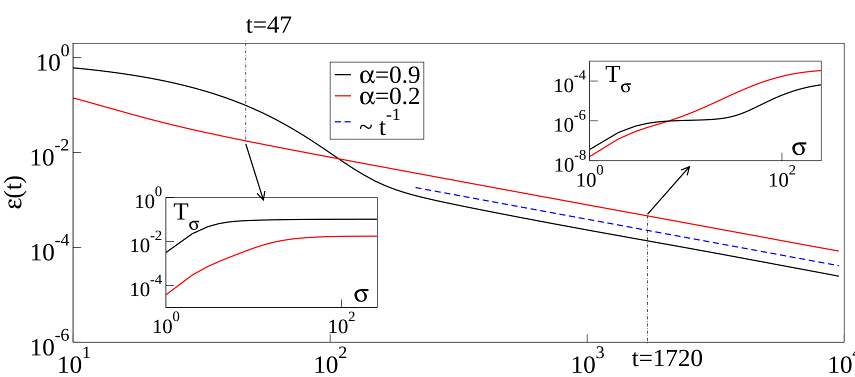

Fig. 3. Energy decay for $\alpha = 0.9$ and $\alpha = 0.2$ (1024^2 sites) in the two-dimensional lattice model. The dashed line $\sim 1/\tau$ is a guide to the eye for the asymptotic energy decay. In the insets we reported the scale-dependent temperature, T_σ, defined in the text, as function of the coarse graining size σ for $\tau = 47$ and $\tau = 1720$. The total energy per particle and T_σ remain nearly indistinguishable in the early incoherent regime, but for $\sigma < L(\tau)$ the thermal energy becomes much smaller than the kinetic energy, a clear indication of the onset of macroscopic spatial order.

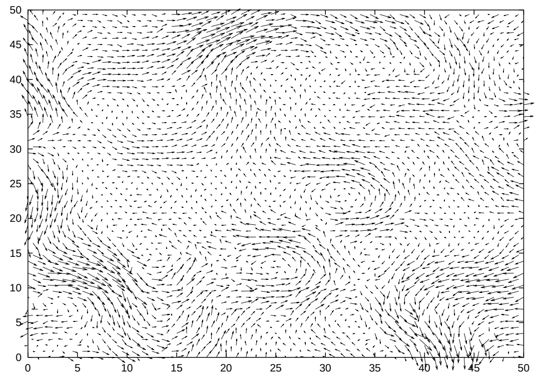

Fig. 4. A (zoomed) snapshot of the velocity field at time $t = 52$ for the lattice model in two dimensions, $d = 2$, with $\alpha = 0.7$ and size $N = 512 \times 512$. The time has been chosen at the beginning of the correlated regime. The presence of vortices is evident. All the velocities have been rescaled to arbitrary units, in order to be visible.

Such a cross-over between homogeneous and inhomogeneous phase can be directly investigated studying the statistical properties of the velocity field. The characterization of structures is achieved by means of correlation functions $G_{ij}(\mathbf{r}, \mathbf{t})$ or structure factors $S_{ij}(\mathbf{k}, \mathbf{t})$, which are their Fourier transforms:

$$G_{ij}(\mathbf{r}, \mathbf{t}) = \frac{1}{V} \int d\mathbf{r}' \langle \delta \mathbf{v}_i(\mathbf{r} + \mathbf{r}', \mathbf{t}) \delta \mathbf{v}_j(\mathbf{r}', \mathbf{t}) \rangle \,, \tag{4.30a}$$

$$S_{ij}(\mathbf{k}, \mathbf{t}) = \frac{1}{V} \langle \delta v_i(\mathbf{k}, \mathbf{t}) \delta \mathbf{v}_j(-\mathbf{k}, \mathbf{t}) \rangle = \int d\mathbf{r} \mathbf{e}^{-ik \cdot r} \mathbf{G}_{ij}(\mathbf{r}, \mathbf{t}) \,, \tag{4.30b}$$

where $V = L^d$ is the volume of the system and i, j are Cartesian components.

The function S_{ij} is an isotropic tensor and can be decomposed in two scalar isotropic functions:

$$S_{ij}(\mathbf{k}, \mathbf{t}) = \hat{\mathbf{k}}_i \hat{\mathbf{k}}_j \mathbf{S}_{\parallel}(\mathbf{k}, \mathbf{t}) + (\delta_{ij} - \hat{\mathbf{k}}_i \hat{\mathbf{k}}_j) \mathbf{S}_{\perp}(\mathbf{k}, \mathbf{t}) \,. \tag{4.31}$$

It is immediate to verify that, if the vector $\mathbf{v}$ is decomposed into $(d-1)$ components $v_\perp$ perpendicular to $\mathbf{k}$ and one component $v_\parallel$ parallel to $\mathbf{k}$, then

$$S_{\parallel}(k, t) = \frac{1}{V} \langle \delta v_{\parallel}(\mathbf{k}, \mathbf{t}) \delta \mathbf{v}_{\parallel}(-\mathbf{k}, \mathbf{t}) \rangle \,, \tag{4.32a}$$

$$S_{\perp}(k, t) = \frac{1}{V} \langle \delta v_{\perp}(\mathbf{k}, \mathbf{t}) \delta \mathbf{v}_{\perp}(-\mathbf{k}, \mathbf{t}) \rangle \,. \tag{4.32b}$$

These correlation functions (shown in Fig. 5) represent a useful statistical indicator of the spatial order of the system and are often employed to describe the ordering process in reaction–diffusion processes. There one finds the remarkable phenomenon known as dynamical scaling. In other words, there exists at late times of the evolution a single characteristic length scale $L(t)$ such that the domain structure is in a statistical sense independent of time when lengths are scaled by $L(t)$.

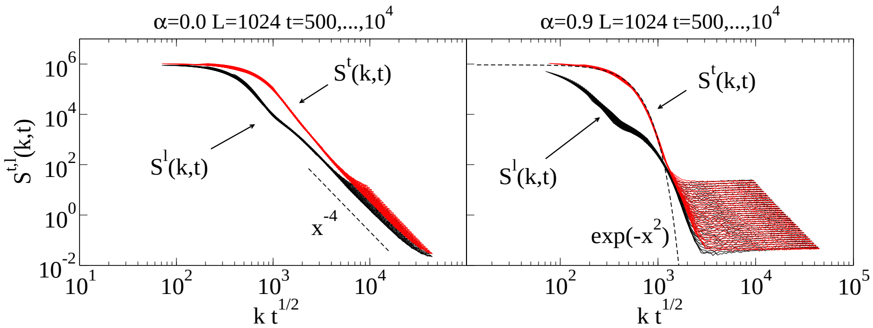

Fig. 5. Data collapse of the transverse (S^t) and longitudinal (S^l) structure functions for $\alpha = 0.$ and $\alpha = 0.9$ (system size 1024^2 sites, times ranging from $t = 500$ to $t = 10^4$). The wave number k has been multiplied by $\sqrt{t}$. Notice the presence of the plateaus for the more elastic system. For comparison we have drawn the laws x^{-4} and $\exp(-x^2)$.

The existence of a single characteristic length scale implies that the pair correlation function and the structure factor have the scaling form:

$$G_{\parallel(\perp)}(r,t) = f_{\parallel(\perp)}(r/L(t))\,, \tag{4.33a}$$

$$S_{\parallel(\perp)}(k,t) = L(t)^d g_{\parallel(\perp)}(kL(t))\,. \tag{4.33b}$$

In our case, the Fourier transform $S_{\parallel(\perp)}(k,t)$ turns out to be a function of a single scaling argument kt^z where z is the so-called growth exponent.

The scaling of the structure factors is illustrated by the good data collapse in Fig. 5, which identifies two growing lengths $L^{\parallel(\perp)}(t)$ both proportional to $t^{1/2}$.

The form of the energy decay, the distribution of the velocity field and the growth $L^{\parallel(\perp)}(t)$ seem to suggest that the evolution can be represented by some effective diffusive dynamics. In fact, in the absence of the kinematic constraint the evolution of the velocity field would be satisfactorily described by an effective diffusion equation.

The analysis of the structure functions $S^{\parallel(\perp)}(k,t)$, instead, indicates the presence of a long-wavelength region which is diffusive in character, whereas at intermediate wavelength the structure functions decay according as $k^{-\beta}$ with $\beta \sim 4$. Finally a plateau region is observed (for $\alpha > 0$) where $S^{\parallel(\perp)}(k,t)$ remain nearly constant with respect to k, but decay in time with a power law t^{-2}. The observed intermediate and small wavelength behaviors have no counterparts in the pure diffusive model, where one always observes Gaussian structure functions.

The $L^{-2}(t)k^{-4}$ intermediate region in the structure functions is understood simply as a consequence of the existence of topological defects in the velocity field. Such a phenomenon is known in the area of phase ordering processes as the generalized Porod's law.[1,22] In the cooling process in $d = 2$ is the signature of the presence of a particular kind of topological defects, namely vortices.

With the random initial conditions adopted, vortices are born at the smallest scales and subsequently grow in size by pair annihilation, conserving the total

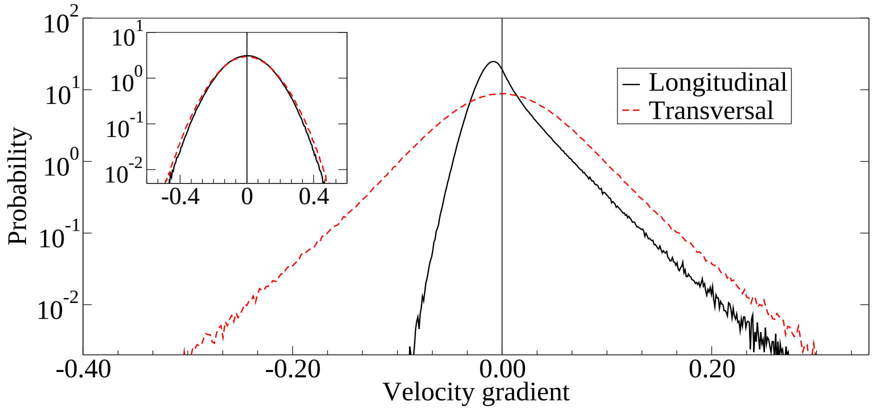

Fig. 6. Probability densities of the longitudinal and transverse velocity increments. The main figure shows the p.d.f. of the velocity gradients ($R = 1$). The inset shows the Gaussian shape measured for $R = 40$ (larger than $L(t)$ for this simulation: $\alpha = 0.2$, $t = 620$, system size 2048^2).

charge. By locating the vortex cores, we measured the vortex density $\rho_v(\tau)$, which represents an independent measure of the domain growth, and in fact it decays asymptotically (when $\tau \gg t_c$) as an inverse power of time:

$$L_v(\tau) = \rho_v^{-1/2}(\tau) \propto \tau^{1/2} \,. \tag{4.34}$$

The vortex distribution turns out to be not uniform for α not too small. Its inhomogeneity is characterized by the correlation dimension d_2, defined through the cumulated correlation function:

$$H(R) = \frac{\sum_{i<j} \Theta(R - (\mathbf{r}_i - \mathbf{r}_j))}{N_v^2} \sim R^{d_2} \,, \tag{4.35}$$

where $\mathbf{r}_i$ are the core locations. For $\alpha \to 1$ the vortices are clusterized ($d_2 < 2$) i.e. do not fill homogeneously the space, whereas at smaller α their distribution becomes homogeneous ($d_2 \to 2$).

Vortices are not the only topological defects of the velocity fields. In fact we observe shocks, similarly to recent experiments in rapid granular flows.[23] Shocks have a major influence on the statistics of the velocity field, i.e. on the probability distributions of the velocity increments. The probability density function (p.d.f.) of the longitudinal increment is shown in Fig. 6 for $R = 1$ (longitudinal velocity gradient) in the main frame, and for $R = 40 > L(t)$ in the inset. For small $R \ll L(t)$ the longitudinal increment p.d.f. is skewed with an important positive tail, whereas for $R \gg L(t)$ it becomes Gaussian. The distribution of transverse increments

$$(\mathbf{v}_{i+\mathbf{R}} - \mathbf{v}_i) \times \hat{\mathbf{R}} \,, \tag{4.36}$$

instead, is always symmetric, but non-Gaussian distributed for small R. A similar situation exists in fully developed turbulence.[24]

Though vortices and shocks explain the power law decay of the structure factors, the plateau in the tail of the structure function is related to the so-called internal noise, i.e. to the presence of short range spatial fluctuations induced by the collisions.[11] A small α determines a rapid locking of the velocities of neighboring elements to a common value, while in the case of $\alpha \to 1$, short range small amplitude disorder persists within the domains, breaking simple scaling of $S^{\|(\perp)}$ for large k and having the effect of a self-induced noise.

The internal noise observed in the study of the longitudinal and transversal structure factor can be characterized by means of an average local granular temperature T_σ:

$$T_\sigma = \langle |\mathbf{v} - \langle \mathbf{v} \rangle_\sigma|^2 \rangle_\sigma \,, \tag{4.37}$$

where $\langle \cdots \rangle_\sigma$ means an average on a region of linear size σ.

If we call $L(t)$ a characteristic correlation length of the system, since when $\sigma \gg L(t)$ the local average tends to the global (zero) momentum, then $\lim_{\sigma\to\infty} T_\sigma = E$ For $\sigma < L(t)$, instead, $T_\sigma < E$. The behavior of T_σ in the uncorrelated (Haff) regime and in the correlated (asymptotic) regime for two different values of α is presented in the inset of Fig. 3.

A very important observation is the following: for quasielastic systems T_σ exhibits a plateau for $1 \ll \sigma \ll L(t)$ that identifies the strength of the internal noise and individuates the mesoscopic scale necessary to find a hydrodynamic description. The local temperature ceases to be well-defined for smaller α: this clearly suggests the absence of scale separation between microscopic and macroscopic fluctuations in the strongly inelastic regime.[7,25]

5. Conclusions

To conclude, we have studied the kinetics of granular gases using different models and following a path of increasing complexity: the mean field inelastic Maxwell model (or Ulam model) has an exact asymptotic solution for scalar velocities and, in general, displays power-law velocity tails; however it cannot account for spatial correlations and therefore is a very poor approximation of an inelastic gas. The successive step is putting the same model onto a spatial lattice: in one dimension, with scalar velocities, this lattice version displays a very good agreement with the kinetics of an inelastic hard rod gas, in particular it reproduces the velocity distributions in the first Haff regime and in the consequent regime. The last step of this modeling procedure is to study the lattice model in two dimensions, with vectorial velocity field. In this model the expected asymptotic decay of the energy is reproduced and the dynamics of the growth of correlations in the velocity field is investigated by measuring the structure factors. The analysis of the structure factors and the study of other statistical properties (e.g. the distribution of the velocity gradients) indicate that the evolution of the model is consistent with that of a diffusive model with corrections due to the kinematic constraint.

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