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Orientational and Translational Cooling in Two Dimensional Systems of Granular Needles

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We present molecular dynamics results of a two-dimensional gas of inelastic needles. At high number densities such a system forms a macroscopically ordered nematic phase. A simple dissipation model is introduced which takes into account geometry and number density of interacting bodies. Freely cooling of the dissipative system leads to orientational clusters (bundles), local inelastic collapse and decrease of the order parameter.

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1 Introduction

Dissipative granular materials are omnipresent in our environment. First scientific records about them date back to the 19th century and are associated to names like Reynolds and Faraday. However, only recently systematic investigations have been undertaken. Practically most advanced papers on this fascinating subject have been published in the last decade (Pöschel and Luding, 2001; Luding, 1998). A very satisfactory collection of references can be found also on the webpage http://www.ica1.uni-stuttgart.de/ lui/REFS/references.html. They report a number of properties of freely cooled and driven (excited) granular gases like clustering (Goldhirsch and Zanetti, 1993; McNamara and Young, 1996; Luding, Huthmann, McNamara and Zippelius, 1998; Luding and McNamara, 1998), inelastic collapse (Goldhirsch and Zanetti, 1993), non-Gaussian profiles of the velocity distribution (Olafsen and Urbach, 1998), surface fluidisation (Clement, Duran and Rajchenbach, 1992) or convection rolls (Evesque and Rajchenbach, 1989). All these works are concerned with spherical particles. By now very little is still known about the behaviour of anisotropic granular materials that play so large a role in industrial and geological processes.

One of the first attempts to investigate properties of a system composed of anisotropic constituents is the study of the granular cooling in an ensemble of 3D hard needles (Huthmann, Aspelmeier and Zippelius, 1999). Such a system does not exhibit ordered phases because the excluded volume of the hard needles is virtually zero. The authors of (Huthmann, Aspelmeier and Zippelius, 1999) have reported on the two-step cooling: (1) a fast exponential decay to a state that is characterised by a time independent ratio of translational to rotational energy; (2) a slow algebraic decay like t^{-2} of the total kinetic energy. In dense regimes they observe large scale structures in the translational velocity field. Neither local ordering nor correlations between velocity and density fields are encountered.

Boundary conditions, as can be expected, can significantly influence the granular structure. In an experiment on the mechanically tapped cylinder filled with rods Villarruel *et al.* (2000) showed that initially unordered rods undergo compaction to a highly ordered smectic like phase with the process of order being seeded at the walls. Similar effects of confinement has been found in molecular systems of, for instance, confined ellipsoids (Chrzanowska, Teixeira, Ehrentraut and Cleaver, 2001) in which the walls also tend to promote an ordered phase.

The very short list of the recent papers on anisotropic granular materials ends the work of Aspelmeier *et al.* (1998), where the simulation results for a 1D dilute gas of inelastic rods situated on a ring and interacting via a short range repulsive potential have been presented. This model allows for fluctuations in the transfer of energy into internal vibrational modes, although it does not include orientational degrees of

freedom. The authors show the possibility of kinetic aggregation of the particles due to energy dissipation into internal vibrations and then break up through the energy feedback without inelastic collapse. Such a situation can be compared to the erythrocyte systems, although they are much more complicated to study, since the strong shape elasticity of red cells also allows for internal energy storage.

The purpose of this paper is to demonstrate the influence of dissipation on a system composed of anisotropic particles. For this purpose we have chosen two dimensional hard needles, which are known to form a nematic phase at sufficiently high number densities (Frenkel and Eppenga, 1985), where as a relevant "number density" we understand the reduced number density $\rho^* = 4\rho L^2$ with L being the half length of the needle. (For simplicity we will be using throughout the paper only the word "density".) Note that as a "hard needle" an infinitesimally thin needle-shaped particle is treated. For such objects in literature there are two terms used interchangeably: "hard needles" and "hard lines". As a matter of fact neither of them is perfect: the first does not convey the fact that the particle is infinitesimally thin and the second does not show that it has a finite length. The chosen system is the simplest example of an orientationally ordered medium. Its other big benefit lies in the fact that 2D systems can be easily visualised. This is also why 2D systems are so popular in the study of granular materials (McNamara and Young, 1996; Luding, Herrmann and Blumen, 1994; McNamara and Young, 1994; Andrade, Trevino and Medina, 1996; Baumann, Janosi and Wolf, 1995; Cafiero, Luding and Herrmann, 2000). As concerns orientational properties, to our knowledge, there has been no report about granular cooling so far.

In genuine liquid crystals cooling is understood to take place if a sample is immersed in a medium or put in contact with some other thermostat of a lower temperature. This involves for a short time temperature gradients and heat transfer in the system, but finally the equilibrium is obtained that corresponds to the new thermodynamic parameters. If the word "cooling" is used here it concerns more the equilibrated state at the last stage of cooling than the way of its approaching. By monitoring then the liquid crystal order versus diminishing temperature one standardly gets a simple scenario of the phase transitions: isotropic $\rightarrow$ nematic $\rightarrow$ smectic $\rightarrow$ solid (with exceptions for the systems not exhibiting a nematic phase at all). Since the moment the system becomes ordered, after the transition from the isotropic phase, a decrease of temperature is followed by an increase of the order parameter or by appearance of new types of the order parameters like, for example, the ones involved in the characteristics of the smectics and their rich variety (de Gennes, 1974; Vertogen and de Jeu, 1988; Chandrasekhar, 1971) (here again there are a very few exceptions of the reentrant phases).

In computer simulations the role of the thermostat should be realized differently. In molecular dynamics control of the temperature is performed by rescaling *at the same time* all the particles velocities accordingly to the condition of the constant temperature. A desired large change of the thermostat temperature can be undertaken by imposing small subsequent rescalings until the assumed temperature is obtained, at each step allowing the system to attain equilibrium. This can be done either for an increase or for a decrease of the temperature and is aimed to mimic the cooling/heating of a real experimental system. It is not infrequent then that subsequent heating of a previously cooled system does not reproduce the chain of phases (and also meta phases) that have been observed while cooling (Affouard, Kröger and Hess, 1996).

This is much different in the case of granular liquid crystals. First of all one should realize that no equilibrium situation is possible. Although in both cases, in molecular liquid crystals and in granular liquid crystals, we talk about diminishing of the energy the main difference between these systems lies in the form how the energy is removed from the system. In granular materials this is uniquely done due to the dissipation conditions that influence the collision rules. Loss in energy depends on the particles kinetic energy, the friction coefficient, the local density and the configuration that determines the local collision rate. As a consequence a granular system is inevitably driven into an inhomogeneous state in which there coexist the areas with different pressures and densities. Moreover, there is not one definition of the granular temperature. There is not even a notion of universal temperature since the equipartition theorem no longer holds.

An attempt to propose an effective temperature definition has been recently made by Makse and Kurchan (2002), which is based on the well known Einstein diffusivity to mobility ratio. This proposition holds only for ideally homogenous materials in the slow flow regime which are, in a sense, close to thermal equilibrium molecular ensembles.

In inhomogenous states in general each degree of freedom can have its own much different level of the

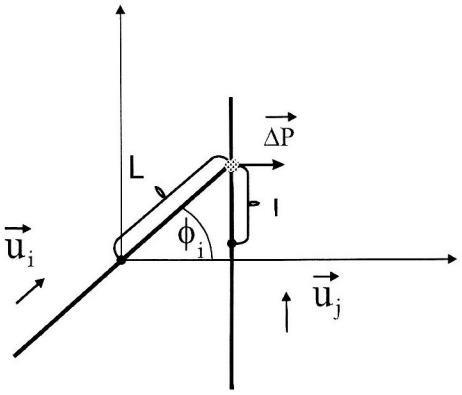


Figure 1: Geometry of the Collision

mean kinetic energy and its own measure of the granular temperature. For these granular temperatures a working formula can be used $< E^i_{kin} >= kT^i_{gran}/2$, where i numbers the degree of freedom, but one should also be aware of the fact that the appropriate velocity profiles might not be of the Maxwellian type.

In this paper we present that the order of the granular system that is macroscopically ordered can decrease upon diminishing temperature, a unique feature that is quite opposite to liquid crystals, where lower temperatures entails higher order. Also we give evidence for the presence of orientational clusters and inelastic collapse.

2 Orientational Cooling

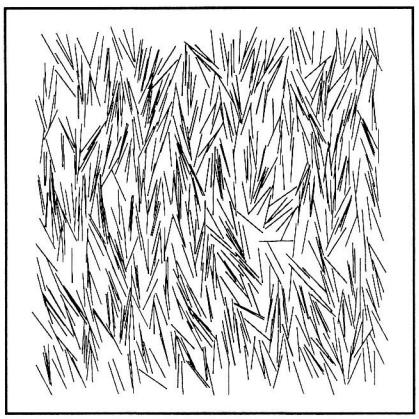
Two spherical particles can collide only once. For the collision to reoccur an intervention of a third particle or a wall is needed. This is completely different in case of anisotropic bodies. The same pair of particles can undergo collisions one after another under appropriate orientational and kinetic conditions. In peculiar circumstances the number of elastic collisions of hard needles may even reach hundreds (Mukoyama and Yoshimura, 1997). Such a chain collision is called a chattering collision. In granular materials composed of spherical particles a diverging collision rate is purely an effect of dissipation and indicates an inelastic collapse. In hard needles ensembles divergent collision frequencies can be driven both by chattering collisions and dissipation.

In our investigation the system comprising 800 hard needles of unit mass m and moment of inertia I with applied periodic boundary conditions has been equilibrated by means of the MD technique. As an initial spatial configuration we have chosen a system of perfectly ordered particles situated on a lattice. This choice has an advantage over randomly chosen positions, which in fact leads to a prolonged run with a small advance in time. The simulation box is standardly taken of unit length. The half-length of the particles L is 0.05, which corresponds to a reduced density $\rho^* = 4\rho L^2 = 8.0$, for which the system forms a nematic phase.

The MD method used is of the event driven type. Its main objective is to resolve for the instant of time in which two particles are in contact. We assume that this happens always when the end of one needle touches the other needle at any point (See Fig.1). The transfer of momentum is naturally within the plane spanned by the needles (in plane collision). This is opposite to the three dimensional case considered by Frenkel and Maguire (1981, 1983) (non dissipative) and by Huthmann *et al.* (1999) (dissipative) in which collisions are always side to side but the momentum transfer is out of plane. Assessment of the collision time has to be done for all possible couples of needles, from which the shortest time is chosen and used to update all the particles' coordinates. After this the system is exactly at the collision point and an exchange of momentum and angular momentum has to be performed due to the collisional formulas. This cycle is repeated as many times as needed.

The time of collision is found as the smallest root of the function $\Psi^{p,k}(t)$ that comes from the algebraic

a)



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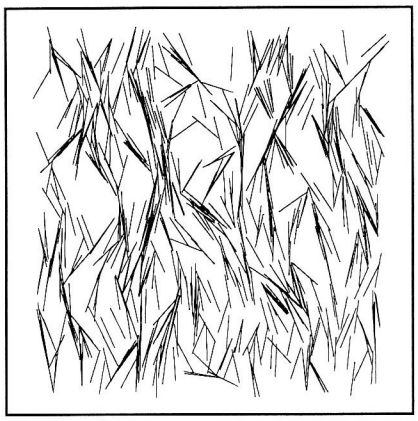

Figure 2: Typical configurations of the 2D hard needle system. a) is an equilibrium configuration exhibiting nematic phase obtained for the density ($\rho^* = 8$) at temperature $kT = 2.0$; It has the global order parameter around 0.82. b) is an configuration obtained form the configuration in (a) after 20000 collisions under dissipation condition with the restitution parameter $\epsilon = 0.4$. The order parameter of this configuration is substantially lower ($S = 0.644$) than the order of the starting configuration and the temperature is $kT = 0.3920$.

condition for the point of contact (see Fig.1)

$$\Psi^{p,k}(t) = \left(X^{ij} + V_x^{ij}t \pm L\cos(\phi_i(t))\right)\sin(\phi_j(t)) - \left(Y^{ij} + V_y^{ij}t \pm L\sin(\phi_i(t))\right)\cos(\phi_j(t)) \tag{1}$$

and the point of contact l (see Fig.1), which can attain values from the interval $(-L < l < L)$ is given by

$$l^{p,k} = \frac{Y^{ij} + V_Y^{ij}t \pm L\sin(\varphi_i + \Omega_i t)}{\sin(\varphi_j + \Omega_j t)}. \tag{2}$$

p and k have been used to distinguish between cases where the beginning or the end of the needle is involved in a collision (since we use L as always positive). In the above $+$ is associated to the index "p" and $-$ to the index "k"; $\phi_i(t)$ stands for $(\varphi_i + \Omega_i t))$, $X^{ij}(Y^{ij})$ denotes the $X(Y)$ coordinate of the relative distance between the particles' centres. Similarly, V_x^{ij} and V_y^{ij} are coordinates of the relative translational velocity. Equation $\Psi^{p,k}(t) = 0$, where $\Psi^{p,k}(t)$ is given by (1) is strongly nonlinear, so we have to resort to numerics to find its smallest root. The method we use is "climbing the rope", where we walk along the values of the function $\Psi^{p,k}(t)$ till the zero value is crossed, with the step of walk adjusted due to the behaviour of the derivatives of the function. The last pair of values having opposite signs is then used as the bracketing points for the Newton-Raphson method of root finding.

Starting from a random distribution of the linear and angular velocities adjusted to the temperature $kT = 2$ the system evolves towards the state in which these distributions have the Gaussian profiles due to the equipartition theorem. Such an equilibrated configuration has been used as the system initial state for the dissipative process. We have found that already after 125 collisions per particle we get appropriate Gaussian velocity characteristics. However, because of the changes in the order parameter S we performed equilibration for a longer time corresponding to 200 collisions/particle. Nonetheless, the system always exhibits relatively strong fluctuations in the order parameter S. This fact has already been shown by the Monte Carlo investigations (Frenkel and Eppenga, 1985).

The 2D order parameter S discussed here differs from the 3D case. It is introduced through the order parameter tensor $\mathbf{Q}$ defined as $\mathbf{Q} = \frac{1}{N}\sum_{i=1}^{N}\left(2\mathbf{a}^i\mathbf{a}^i - \mathbf{1}\right)$, where $\mathbf{a}^i$ is confined to the XY plane orientation of the particle i. $\mathbf{Q}$ is traceless and has eigenvalues of the form $\{S, -S\}$, with S being the scalar order parameter. Eigenvectors of $\mathbf{Q}$ give the direction of the most preferred orientation in the system (the director) and the vector perpendicular to it. We calculate the order parameter tensor in accordance to the above definition and after its diagonalisation we find the global strength of order S.

During collision both momenta and angular momenta of the actors are changed to new values

$$\begin{aligned} \mathbf{P}'_i &= \mathbf{P}_i + \Delta\mathbf{P} & \mathbf{P}'_j &= \mathbf{P}_j - \Delta\mathbf{P} \\ \mathbf{J}'_i &= \mathbf{J}_i + L\mathbf{u}_i \times \Delta\mathbf{P} & \mathbf{J}'_j &= \mathbf{J}_j - l\mathbf{u}_j \times \Delta\mathbf{P} \end{aligned} \tag{3}$$

Due to the geometry of a 2D collision without tangential friction, that we consider here, the exchange of $\Delta\mathbf{P}$ has orientation perpendicular to the needle j, $\mathbf{u}_\perp$. For the elastic case its value can be obtained from the equation

$$\begin{aligned} 0 \;=\; & \frac{\Delta\mathbf{P}}{m} \cdot \mathbf{P}_{ij} + \frac{L}{I}\mathbf{J}_i \cdot (\mathbf{u}_i \times \Delta\mathbf{P}) - \frac{l}{I}\mathbf{J}_j \cdot (\mathbf{u}_j \times \Delta\mathbf{P}) \\ & + \frac{L^2}{2I}(\mathbf{u}_i \times \Delta\mathbf{P})^2 + \frac{l^2}{2I}(\mathbf{u}_j \times \Delta\mathbf{P})^2 + \frac{\Delta P^2}{m} \end{aligned} \tag{4}$$

that is based on the energy balance. We will use this expression for $\Delta\mathbf{P}$ as the reference for an inelastic case. For this case dissipation is introduced through a general ansatz

$$\mathbf{u}_\perp \cdot \Delta\mathbf{P}_{inel} = \epsilon\mathbf{u}_\perp \cdot \Delta\mathbf{P}_{elas}, \tag{5}$$

where ϵ is the normal restitution parameter. The formula (5) simply says what fraction of momentum is preserved after a collision.

In Fig.2 we present a needle configuration obtained in the equilibrated state and a typical configuration obtained after dissipation. To measure how much energy has been dissipated we will use an auxiliary mean temperature kT defined by the working formula $kT = 3E/2$ which corresponds rather to the global energy of the system. Comparing the two pictures in Fig.2 one notices a visible change in the particles organisation. Under dissipation the system has developed thick bundles comprised of several needles together with spaces free of particles. The growth of bundles depends on the magnitude of the restitution parameter. For large dissipation (small restitution parameter) two particles remain after collision in their neighbourhood which leads to shorter times until next collisions and to larger collision frequency. For small dissipation the needles preserve much of their energy and can still interact with more distant particles and the growth of bundles is slower. In terms of the density a dissipative system becomes strongly inhomogeneous with very dense areas. Usually to study short and long range structures of dense systems one uses the radial distribution function (Frenkel and Smit, 1996). Here however, this function is not a good tool since at short distances it exhibits wild fluctuations that depend on the width of the histogram cell. Instead of it we propose a nearest neighbourhood density in order to detect inhomogeneities and quantify the process of the bundles creation.

Around the centre of each particle we consider an ellipsoidal box with the long axis corresponding to the particle orientation and the length equal to 2L. As short axis we take L/2. Next we calculate the number of particles whose centres are found in each box.

In Fig.3 we plot the number of nearest neighbourhood boxes N_{box} that have density ρ^*_{box} (we use the subscript *box* to indicate that this density is calculated with respect to an individual box) and which are present in our configurations. The resulting distribution function (also normalised to unity) seems to be a satisfactory tool to detect inhomogeneities. The distribution obtained for the elastic case fits very well to the Gaussian profile which is centred at a certain density higher than the global density ρ^*. For $\rho^* = 8.0$ and the ellipsoidal box whose axes have lengths $a = 2L$ and $b = L/2$ the box mean density is $\rho^*_{box} = 16.0$. This difference is caused by the box anisotropy (Chrzanowska and Ehrentraut, in preparation). The curve obtained for the system after dissipation is *non symmetrical* with a well pronounced slope towards higher densities. This slope is a direct evidence of new structures - bundles. To obtain the figures in Fig.3 we have performed averaging over 21 different configurations for the elastic case (at kT=2.0) and over 10 configurations for the inelastic case (at kT=0.53).

In Fig.4 we present the order parameter that has been calculated for each individual type of the box. (This type is given by the box density). If no box with a given density is encountered in our configurations then no order parameter is assigned. It is, then, clearly seen from Fig.4 that in the granular case new boxes with high degrees of order have formed which we refer to as orientational clusters.

Newly created voids in the system are also an opportunity for the particles (or whole bundles) to rotate

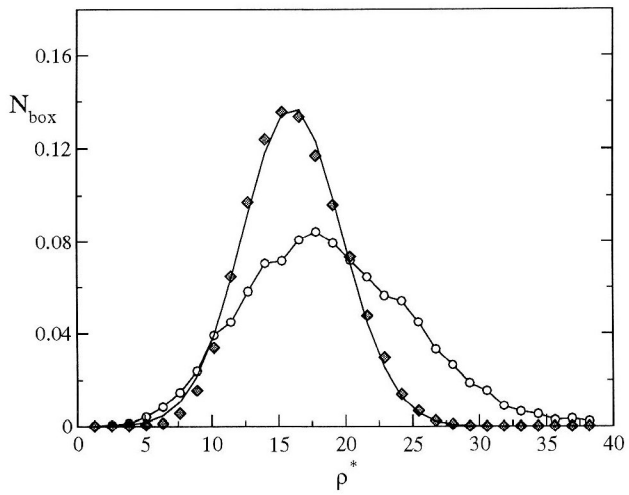

Figure 3: Nearest neighbourhood density N_{box}; diamonds correspond to the non dissipative case and the solid line is the fitted Gaussian profile; circles are obtained after dissipation; a dashed line is used to guide the eye.

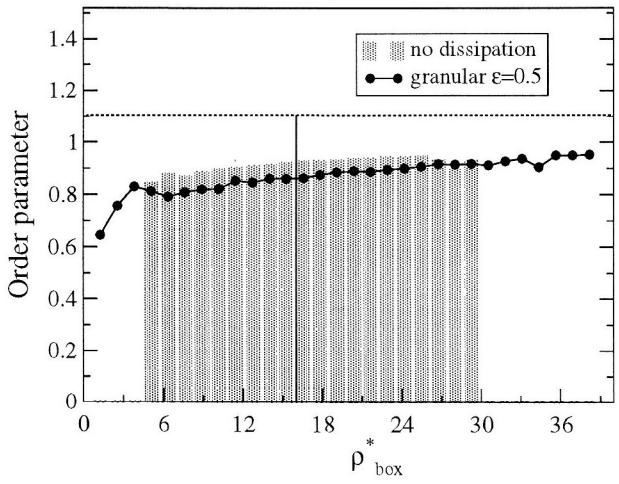

Figure 4: Order parameter of the nearest neighbourhood boxes vs. their density ρ^*_{box}. Shadowed area is the histogram type presentation of the boxes order in the equilibrium and dots are the data of the order S in the system after dissipation with $\epsilon = 0.5$. If no box with a given density is present no order parameter is assigned.

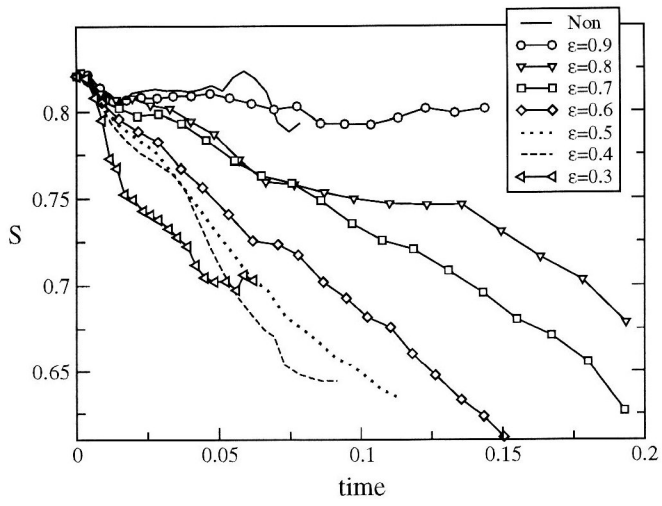

Figure 5: Order parameter S vs. time presented after 20000 dissipative collisions. The restitution parameters ϵ are given in the inset. Different time lengths are due to the different collision frequency which depends on ϵ (see Fig.7).

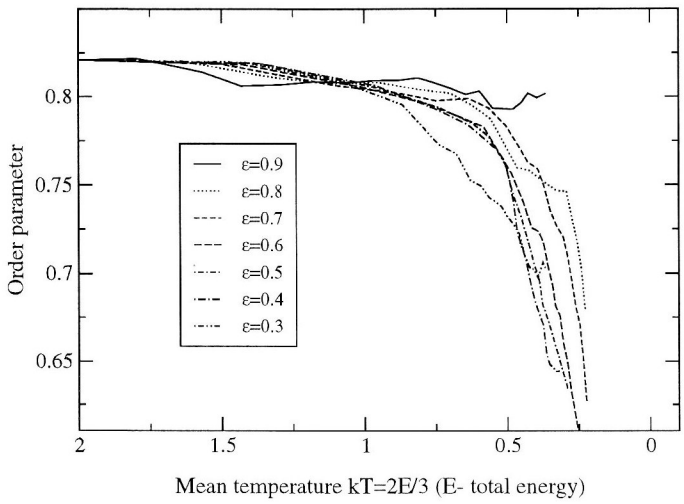

Figure 6: The change of the order parameter vs. the mean temperature (the total energy) for different restitution parameters ϵ for a nematic at the density $\rho^{ast} = 8.0$.

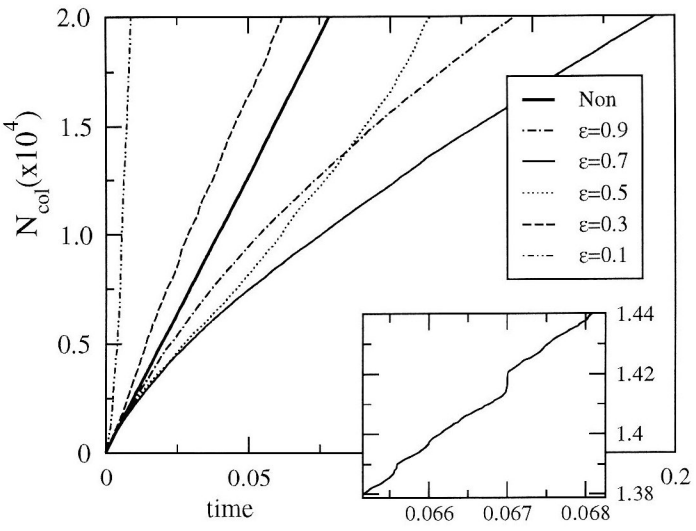

Figure 7: Number of collisions for different restitution parameters ϵ for the ordered system at the density ρ^* vs. time. The inset profile shows a magnified part of the collision number from a clustering state; vertical steps with divergent collision frequency are examples of the inelastic collapse phenomenon.

to more off-the director positions. Indeed we observe a diminishing tendency of the order parameter upon cooling of the system which we refer to as orientational cooling. In Fig.5 we present the decay of the order parameter versus the passing time for different restitution parameters. Although the behavior of S under cooling is irregular (since here, accordingly to our computer capacities, the time evolution of only *one* configuration is presented), we detect a general tendency (besides the last curve for $\epsilon = 0.3$) that for the same time intervals stronger dissipation is followed by stronger decrease of the system order.

Fig.6 shows the order parameter changes with respect to the system global kinetic energy (the sum of the translational and the rotational energy) given in terms of the introduced mean temperature. Different curves correspond to different restitution parameters (a description is given in the inset). It is characteristic that large drops in the order parameter can occur only when the system has lost about 75% of the energy. Only then the restitution strength seems to play a role. Before its influence is minute. More simulation and more detailed study based on the statistical averaging is needed to establish true functional dependencies in the regime where the restitution influences the order parameter. From Fig.6 we can expect the tendency that larger dissipation during a collision can lead to smaller order at the same value of the global energy.

The above discussed results presented in Fig.5 and Fig.6 convince us of a possibility to obtain a cooling driven transition to the isotropic phase if the initial thermodynamic conditions are appropriately chosen (to be searched for).

In the equilibrium state the particles collide with one collision frequency which depends on the system density and the dependence of the collision number upon the time is a linear function. When dissipation is present this is no longer true. In Fig.7 we show the number of collisions vs. time for different values of the restitution parameter ϵ. The behaviour of $N(t)$ is quite complex. Collisions of the dissipative system with ϵ from the interval 0.6-1.0 are less frequent than in the equilibrium state and the profiles of $N(t)$ are concave. The whole process is prevailed by the loss in the global kinetic energy. Then below 0.6 the situation changes dramatically. On average the collision rate (dN/dt) is growing upon diminishing ϵ and at a certain value between 0.3 and 0.4 the profile becomes close to the equilibrium case. This growth is caused by a creation of the cluster- bundles. At the same time we observe small steps in the curves that are almost parallel to the N_{col} axis ie. with divergent collision frequency. This is an evidence of inelastic collapses which last over a maximum of a few hundreds of collisions and are dissolved afterwards. This surprising behaviour is the result of the strong relation between the system energy and the inhomogeneities.

All kinetic characteristics and correlation functions will be reported elsewhere. No theory is available at

the moment due to the strong non homogenous character of the system.

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