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Transient clusters in granular gases

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Abstract

The most striking phenomenon in the dynamics of granular gases is the formation of clusters and other structures. We investigate a gas of dissipatively colliding particles with a velocity dependent coefficient of restitution where cluster formation occurs as a transient phenomenon. Although for small impact velocity the particles collide elastically, surprisingly the temperature converges to zero.

1. Introduction

Granular gases, i.e. gases of dissipatively colliding particles in the absence of external forces, reveal a variety of interesting phenomena, such as characteristic deviations from the Maxwell distribution [1–3], overpopulation of the high energy tail of the distribution function [4], anomalous diffusion [5, 6], and others (see [7–9] for an overview). However, the most striking phenomenon which distinguishes granular gases from molecular gases is the self-organized formation of spatio-temporal structures such as clusters [10] and vortices [11].

The loss of mechanical energy of dissipatively colliding particles i and j is characterized by the coefficient of restitution, which relates the normal component of the relative velocity before a collision, g, to that after, g':

$$\varepsilon \equiv \frac{g'}{g} = -\frac{\vec{v}'_{ij} \cdot \vec{e}_{ij}}{\vec{v}_{ij} \cdot \vec{e}_{ij}}, \qquad \vec{e}_{ij} \equiv \frac{\vec{r}_i - \vec{r}_j}{\left|\vec{r}_i - \vec{r}_j\right|} \tag{1}$$

with $\vec{v}_{ij} \equiv \vec{v}_i - \vec{v}_j$ and with $\vec{v}'_{ij}$ being the corresponding post-collision value. Frequently it is assumed that the coefficient of restitution is a material constant; however, this assumption contradicts experiments [12] and disagrees with a dimension analysis [13, 14]. Instead, ε is a function of the impact velocity g.

The coefficient of restitution can be obtained by integrating Newton's equation for the collision. The elastic component of the contact force for spheres of diameter σ is given by Hertz' law $F^{(\mathrm{el})} = B\xi^{3/2}$, with $\xi(t) \equiv \sigma - \left|\vec{r}_i - \vec{r}_j\right|$ and $B(\sigma)$ being the elastic material parameter [15]. Assuming viscoelastic material properties, the dissipative part of the contact

force reads $F^{(\mathrm{dis})} = A\sqrt{\xi}\dot{\xi}$ [16–18] with the dissipative material constant $A(\sigma)$. Integration of Newton's equation of motion yields [14, 19]

$$\varepsilon_{\mathrm{v}}(g) = 1 - D_1 g^{1/5} + D_2 g^{2/5} \mp \cdots, \tag{2}$$

where the coefficients $D_{1/2}$ depend on the elastic and dissipative particle material properties and on the radii of the particles (for details see [19]).

The temperature of homogeneous granular gases in the absence of macroscopic flows can be defined as the mean kinetic energy of the particles. Due to dissipative collisions the temperature decays persistently and, therefore, the thermal velocity $v_{\mathrm{T}}(t) \equiv \sqrt{2T(t)/m}$ decays too. For vanishing temperature the particles collide elastically, i.e., $\lim_{T\to 0} \varepsilon_{\mathrm{v}} = 1$. Since the formation of clusters in granular gases is a consequence of dissipative particle collisions the question arises whether clusters may occur and persist for gases of viscoelastic particles. The linear stability analysis of the hydrodynamic equations of such gases [20, 21] as well as molecular dynamics simulations and the numerical solution of the hydrodynamic equations [21] support the hypothesis that the cluster state is only a transient phenomenon. The analysis is, however, restricted to small inelasticity which is the precondition of equation (2). Moreover, the clusters that have been observed in gases of viscoelastic particles always grow until they reach the border of the periodic system [21]. Although we believe that the dissolution of clusters is an inherent property of the system, it is not evident how it is affected by the unphysical self-interaction of clusters via the periodic boundary. Therefore, it is desirable to study a granular gas with a simplified collision model which demonstrates the most essential property of the restitution coefficient, $\lim_{g\to 0} \varepsilon(g) = 1$, but nevertheless is not affected by unphysical influences of the boundary conditions.

2. Model

The molecular dynamics of force-free granular gases of viscoelastic particles with periodic boundary conditions is problematic, due to the emergence of system size clusters in the long time behaviour. Therefore, in this paper we assume a coefficient of restitution with an extremely simplified impact velocity dependence: the particles collide with a constant coefficient of restitution ε^* if the impact velocity exceeds a certain value g^*, and otherwise they collide elastically:

$$\varepsilon(g) = \begin{cases} \varepsilon^* & \text{for } g > g^* \\ 1 & \text{for } g \leqslant g^*, \end{cases} \tag{3}$$

where $0 < \varepsilon^* < 1$, that is, the inelasticity of particle collisions need not be small.

A granular gas which is initialized at uniform number density n stays homogeneous during the first stage of its evolution, called the *homogeneous cooling state*. In this regime the kinetic energy of the gas may be characterized by the granular temperature T, defined in terms of the second moment of the velocity distribution function $f(v)$:

$$\frac{d}{2} nT \equiv \int \frac{mv^2}{2} f(v)\, \mathrm{d}\vec{v}, \tag{4}$$

(m is the mass of particles and d is the dimension). For $\varepsilon =$ constant the decay of the temperature due to inelastic collisions is described by Haff's law $T_{\mathrm{H}}(t)$ [22], whereas for gases of viscoelastic particles it is given by $T_{\mathrm{v}}(t)$ [19]:

$$T_{\mathrm{H}}(t) = \frac{T_0}{(1 + t/\tau_{\mathrm{H}})^2}, \qquad T_{\mathrm{v}}(t) = \frac{T_0}{(1 + t/\tau_{\mathrm{v}})^{5/3}}, \tag{5}$$

where τ_{H} and τ_{v} are the relaxation times [23].

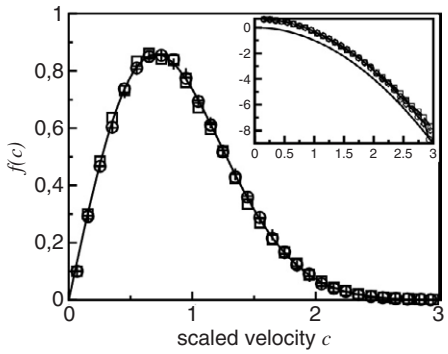

Figure 1. Scaled velocity distribution $f(c)$ at times $t_1 < t_2 < t_3$ where $v_T(t_1) \gg g^*$ (circles), $v_T(t_2) \approx g^*$ (squares) and $v_T(t_3) \ll g^*$ (plus symbols), together with a Maxwellian (full curve). Inset: the same data as $\ln(f(c)/c)$. The full curve shows a parabola for comparison (shifted for better visibility).

Equations (5) were first derived with the assumption of a Maxwell distribution; however, their functional form remains conserved also when we take into account the known deviations from the Maxwell distribution [1–3]. Before investigating the temperature decay let us first check whether the assumption of an approximative Maxwell distribution is justified for our case too.

Starting at a certain temperature which corresponds to a thermal velocity $v_T \gg g^*$, almost all collisions occur with ε^*; hence, in this range, we expect to find a velocity distribution close to a Maxwellian with the small deviations mentioned above. At late times when $v_T \ll g^*$ the majority of the collisions occurs elastically. In this range we expect, therefore, a Maxwell distribution too, just as for molecular gases. In the intermediate range $v_T \approx g^*$ a sizable part of the collisions, i.e. collisions between slow particles, occur elastically, whereas fast particles mainly undergo dissipative collisions. Therefore, it is not *a priori* clear whether the distribution function is close to the Maxwell distribution.

We have simulated a 2D granular gas of $N = 10^5$ particles of unit mass which collide according to equation (3). The parameters are: $\varepsilon^* = 0.6$, $g^* = 0.1$ and the initial temperature is $T(0) = 1$ which corresponds to an initial thermal velocity $v_T(0) = \sqrt{2} \gg g^*$. Figure 1 shows the scaled velocity distribution function $\tilde{f}(c)$ defined by

$$f(\vec{v}, t) = \frac{n}{v_T^d(t)} \tilde{f}(\vec{c}), \qquad \vec{c} \equiv \frac{\vec{v}}{v_T(t)}, \tag{6}$$

for the three cases mentioned together with the Maxwell distribution. From the results we conclude that even in the transition region $v_T \approx g^*$, the Maxwell distribution is a good approximation.

3. Temperature decay

Using the standard approach based on the Boltzmann equation (e.g. [1–3, 23]) with the assumption of a Maxwell distribution we obtain

$$\frac{dT}{dt} = -\frac{2}{d} g_2(\sigma) \sigma^{d-1} n v_T T \mu_2, \tag{7}$$

where $g_2(\sigma)$ is the contact value of the pair distribution function,

$$g_2(\sigma) = \frac{1 - 7\eta/16}{(1-\eta)^2} \qquad \text{with } \eta = \tfrac{1}{4} n \pi \sigma^2, \tag{8}$$

for a two-dimensional gas and in three dimensions

$$g_2(\sigma) = \frac{2-\eta}{2(1-\eta)^3} \qquad \text{with } \eta = \tfrac{1}{6}n\pi\sigma^3. \tag{9}$$

The second moment of the dimensionless collision integral reads [3, 23]

$$\mu_2 = \tfrac{1}{4}\int \mathrm{d}\vec{c}_1 \int \mathrm{d}\vec{c}_2 \int \mathrm{d}\vec{e}\,\Theta(-\vec{c}_{12}\cdot\vec{e})\,\tilde{f}(\vec{c}_1)\,\tilde{f}(\vec{c}_2)(1-\varepsilon^2)\,|\vec{c}_{12}\cdot\vec{e}|^3\,. \tag{10}$$

The integration is performed over the velocities $\vec{c}_1$, $\vec{c}_2$ of the colliding pair and over the unit vector $\vec{e} = \vec{e}_{12}$ as introduced in equation (1). The unit step function $\Theta(x)$ guarantees that only approaching particles collide. Approximating the velocity distribution function by the Maxwell distribution, $\tilde{f}(\vec{c}) \equiv \phi(c) = \pi^{-d/2}\exp(-c^2)$, and transforming the variables, $\vec{c}_1, \vec{c}_2 \to \vec{C}, \vec{c}_{12}$, where $\vec{C} \equiv (\vec{c}_1 + \vec{c}_2)/2$ and $\vec{c}_{12} \equiv \vec{c}_1 - \vec{c}_2$, we can write

$$\tilde{f}(\vec{c}_1)\,\tilde{f}(\vec{c}_2) = \phi(c_{12})\phi(C) \tag{11}$$

with

$$\phi(c_{12}) = \frac{1}{(2\pi)^{d/2}}\exp\left(-\frac{1}{2}c_{12}^2\right) \tag{12}$$

$$\phi(C) = \left(\frac{2}{\pi}\right)^{d/2}\exp\left(-2C^2\right). \tag{13}$$

Substituting the latter expressions into equation (10) and taking into account $\int \phi(C)\mathrm{d}\vec{C} = 1$, we obtain μ_2 for a two-dimensional gas:

$$\mu_2 = \frac{1}{4}\left(1-\varepsilon^{*2}\right)2\pi\int_{g^*/v_\mathrm{T}}^{\infty} c_{12}\frac{1}{2\pi}\exp\left(-\frac{1}{2}c_{12}^2\right)\mathrm{d}c_{12}\int_{-\varphi_0}^{\varphi_0} c_{12}^3\cos^3\varphi\,\mathrm{d}\varphi, \tag{14}$$

with $\varphi_0 \equiv g^*/(v_\mathrm{T}c_{12})$, where we take into account that the integral in equation (10) vanishes if the normal component of the impact velocity $|\vec{c}_{12}\cdot\vec{e}| = |c_{12}\cos\varphi| < g^*/v_\mathrm{T}$. Simple calculations then yield the coefficient μ_2 for general dimensions ($d = 2$, $d = 3$):

$$\mu_2 = A_d\frac{\sqrt{2\pi}}{2}(1-\varepsilon^{*2})\left(1+\frac{g_0^2T_0}{2T}\right)\exp\left(-\frac{g_0^2T_0}{2T}\right), \tag{15}$$

where $A_2 = 1$ (see also [24]) and $A_3 = 2$. In equation (15), $T_0 \equiv T(0)$ denotes the initial temperature and $g_0 \equiv g^*/v_\mathrm{T}(0)$. Introducing the variable $x = 2T/(T_0g_0^2)$ we obtain from equation (7)

$$\dot{x} = -\alpha\left(x^{3/2}+x^{1/2}\right)\mathrm{e}^{-1/x}, \tag{16}$$

$$\alpha = A_d g_0\left(1-\varepsilon^{*2}\right)g_2(\sigma)\sigma n\sqrt{\pi T_0/2m}. \tag{17}$$

If at the initial stage of the temperature evolution $v_\mathrm{T}(0) \gg g^*$, i.e. $g_0 \ll 1$, then $x \gg 1$. Equation (16) reduces then to $\dot{x} = -\alpha x^{3/2}$, yielding Haff's law (5) with

$$\tau_\mathrm{H} = \frac{\alpha}{g_0\sqrt{2}} = \frac{1}{2}\left(1-\varepsilon^{*2}\right)g_2(\sigma)\sigma n\sqrt{\frac{\pi T_0}{m}}. \tag{18}$$

For large time, i.e., for sufficiently small x, the general solution of equation (16) can be found in the form of a series

$$\frac{x^{3/2}\mathrm{e}^{1/x}}{1+x}\left[1+\frac{3+x}{2(1+x)}x+\frac{15+10x+3x^2}{4(1+x)^2}x^2+\cdots\right] = \alpha t + C, \tag{19}$$

where C is an integration constant. For large times, i.e., $x \ll 1$, it simplifies to

$$x^{3/2}\mathrm{e}^{1/x} = \alpha t. \tag{20}$$

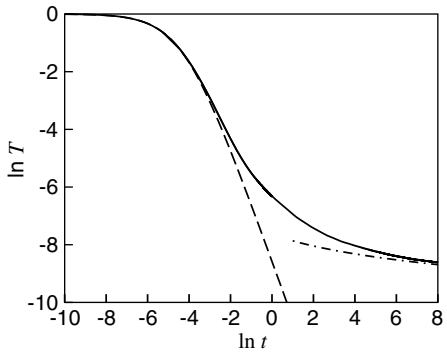

Figure 2. Granular temperature of a gas of $N = 10^5$ particles and critical velocity $g^* = 0.1$. Full curve: molecular dynamics, dashed curve: Haff's law, equation (5), dash–dotted curve: asymptotics, equation (21).

With the definition of Lambert's W function [25], $W(x)\exp[W(x)] = x$, we find the solution of equation (20):

$$\frac{1}{x} = -\frac{3}{2}W\left(-\frac{2}{3(\alpha t)^{2/3}}\right), \qquad x = \frac{2}{g_0^2}\frac{T}{T_0}. \tag{21}$$

For large t, equation (21) may be approximated by

$$\frac{1}{x} = \frac{3}{2}\left[\ln\left(\frac{3}{2}(\alpha t)^{2/3}\right) + \ln\ln\left(\frac{3}{2}(\alpha t)^{2/3}\right) + \cdots\right] \tag{22}$$

which yields the asymptotics for $t \to \infty$:

$$T(t) = \frac{g_0^2}{2}\frac{T_0}{\log \alpha t}, \tag{23}$$

with the constants g_0 and α defined above. The asymptotic temperature relaxation is much slower as compared with the power law equation (5) (see figure 2) since at late times most of the collisions occur elastically according to equation (3). Therefore, only collisions of particles whose velocities belong to the high energy tail contribute to the decay of temperature. With similar arguments, logarithmically slow cooling was also obtained for a system of electrically charged particles [26]. The above temperature dependence is the same for two- and three-dimensional gases, differing only through the pure number α.

Strictly speaking, equation (23) is only valid for infinite systems. For any finite system the cooling process terminates when the total energy of the system drops below $0.5\,(g^*/2)^2 + 0.5\,(g^*/2)^2 = (g^*)^2/4$, i.e., when the total energy of the system is insufficient to afford the relative particle velocity g^* which is necessary for a dissipative collision. This energy corresponds to the temperature $T_{\rm crit} = (g^*)^2/(4N)$, i.e. for our case ($N = 10^5$, $g^* = 0.1$) $T_{\rm crit} = 2.5 \times 10^{-8}$, or $\ln T_{\rm crit} \approx -17.5$. This value is *far* below the temperature reached in the simulation[3]. Therefore, here the limited cooling due to finite number of particles is not relevant.

[3] Evidently the temperature does indeed decay to $T < T_{\rm crit}$: assume $T = T_{\rm crit} + \delta$ ($\delta \gtrsim 0$). As long as the particles collide elastically, due to ergodicity in the course of time the system scans the full phase space volume which is compatible with conservation of energy, momentum and angular momentum. This includes such configurations where sufficient energy is concentrated in the pair of particles colliding next such that $g \gtrsim g^*$, i.e. the next collision occurs dissipatively. Consequently temperature decays until $T \lesssim T_{\rm crit}$.

4. High energy tail of the distribution function

For granular gases of particles which collide with $\varepsilon =$ constant the high energy tail of the reduced distribution function does not obey a Maxwell distribution ($\sim \exp(-c^2)$) but decays as $\exp(-ac)$ (for details see [4]). This behaviour can be understood if one notices that the number of particles of the reduced velocity $c = v/v_\mathrm{T}$ is determined by a balance of *three* processes: (i) losses due to collisions of particles at velocity c (thus changing their velocity to some c'), (ii) gains due to particles resulting at c after a collision and (iii) variations without collisions due to decaying thermal velocity v_T of a cooling gas, i.e. although the particle's velocity v stays the same, its reduced velocity $c = v/v_\mathrm{T}$ changes due to temperature decay. For gases of elastic particles process (iii) is irrelevant and the balance of the processes (i) and (ii) yields the Maxwell distribution. For dissipative gases of particles which collide with $\varepsilon =$ constant, process (ii) for the high velocity tail may be neglected as compared to (i). Process (iii) causes in this case an increase of the number of particles in the high velocity tail with $c \gg 1$. The resulting balance of (i) and (iii) yields the steady-state exponential overpopulation of the high energy tail [4].

For the coefficient of restitution according to equation (3) the temperature decay is logarithmically slow as compared with the power law for $\varepsilon =$ constant. Therefore, the loss of particles (process (i)) is not balanced any longer by process (iii) due to the extremely slow decay of temperature; hence, we do not expect overpopulation of the tail, but rather underpopulation. The depopulation of the tail will continue until the number of high velocity particles becomes so small that process (ii) cannot be neglected any longer with respect to (i). This gain process (ii) is most efficient for small velocities due to the elastic particle interaction for these velocities. One might even suspect that there is a maximal velocity above which (practically) no particles can be found.

5. Cluster formation

The spontaneous formation of clusters in a force-free cooling granular gas can be understood from simple arguments [10]: consider density fluctuations in an otherwise homogeneous granular gas. In denser regions the particles collide more frequently than in more dilute regions; therefore, dense regions cool faster than dilute regions and the local pressure decays in these colder regions. The resulting pressure gradient causes a flux of particles into the denser region, which leads to further increase of the density. Hence, small fluctuations of the density are enhanced which leads to the formation of clusters.

These arguments are certainly valid for the case $\varepsilon =$ constant, but not necessarily for a gas of viscoelastic particles with $\varepsilon = \varepsilon_\mathrm{v}(g)$: in the latter case collisions become less and less dissipative since the velocities decrease over time in the cooling gas. Hence the question arises whether clusters persist in granular gases of viscoelastic particles. The numerical investigation of these gases reveals dissolution of clusters after long time [21]. However, at a certain time the clusters grow to a size comparable with the size of the periodic system. From this instant on the simulation becomes questionable due to the unphysical effect of the cluster self-interaction via the periodic boundary conditions. To prove the dissolution of clusters by means of molecular dynamics for a gas of viscoelastic particles without encountering the above-mentioned unphysical effect, we need a system which is large enough to ensure that at no time the cluster size reaches the system size. At the moment we are able to simulate systems up to about $N = 3 \times 10^6$ particles, which seems to be far below the necessary size. Therefore, we use the simplified collision law, equation (3), which should exhibit similar features to a gas of viscoelastic particles since for both $\lim_{g\to 0} \varepsilon = 1$. Figure 3 shows snapshots of a simulation of $N = 10^5$ particles.

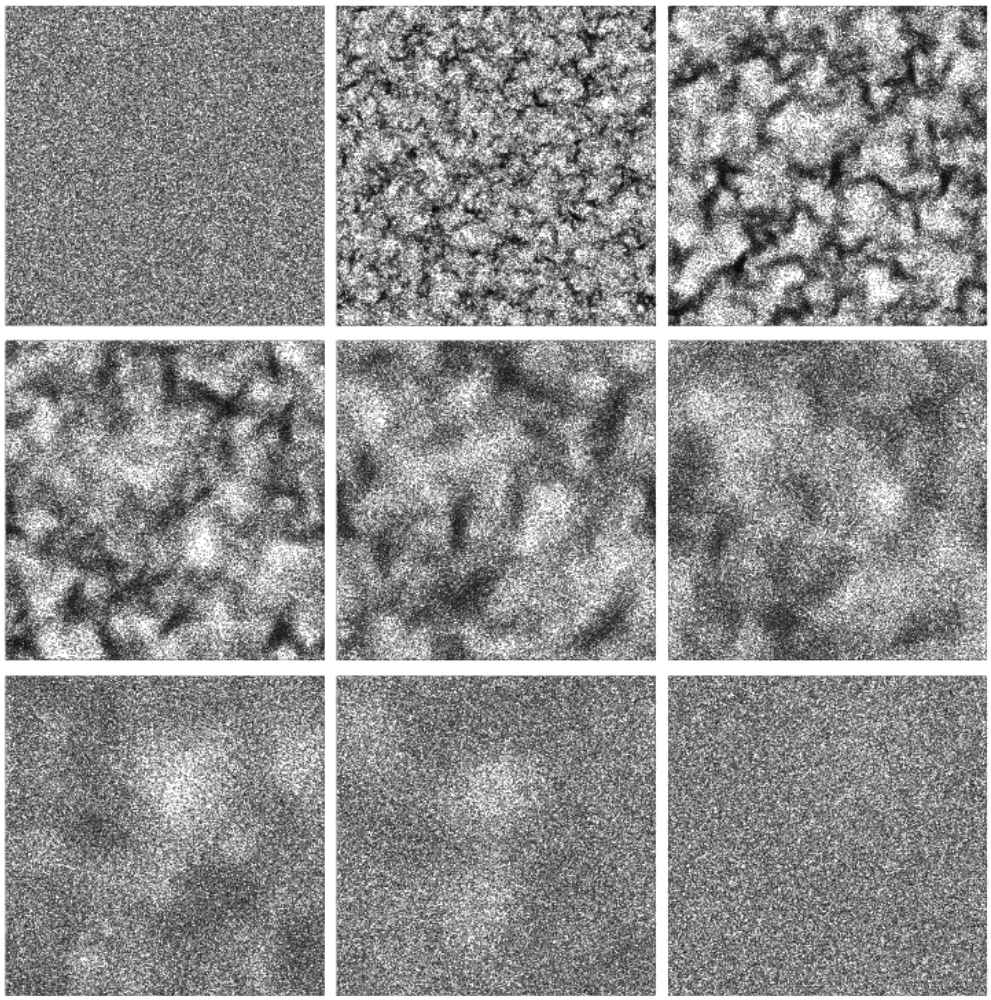

Figure 3. Snapshots of a simulation ($N = 10^5$, $\varepsilon^* = 0.6$, $g^* = 0.1$, $\eta = 0.1$) after 0, 50, 100 (first row), 150, 200, 250 (second row), 500, 1000 and 5000 (last row) collisions per particle. The corresponding fractions of dissipatively occurring collisions read (in the same order) 0.998, 6×10^{-3}, 1.1×10^{-3}, 5.1×10^{-4}, 3×10^{-4}, 2.8×10^{-4}, 8.5×10^{-5}, 2.6×10^{-5}, 3.8×10^{-6}. The initial temperature $T_0 = 1$ corresponds to the thermal velocity $v_T = \sqrt{2}$. Starting at a homogeneous distribution we observe cluster formation up to a certain cluster size. At late times the system returns to the homogeneous cooling state.

Starting from a uniform distribution density, inhomogeneities appear after a short period of homogeneous cooling, and grow up to a certain typical size. The collision frequency in dense regions is larger than in dilute regions, which leads to decreasing thermal velocity. In the course of time more and more collisions inside the clusters occur with relative velocities $g < g^*$, i.e., elastically. Therefore, the clusters dissolve. At late times the system returns to the homogeneous cooling state.

Why do we not observe system spanning clusters as in the case of $\varepsilon =$ constant? We start the simulation at a temperature for which the thermal velocity $\sqrt{2T_0/m}$ is well above g^*, i.e. the system has the properties of a granular gas with $\varepsilon =$ constant. Therefore, clusters

begin to form and grow due to the above-described pressure instability. At a certain time the typical velocity inside the clusters falls below g^*; from this moment on the clusters start to dissolve, i.e., this time determines the typical cluster size which is significantly smaller than the system size for an appropriate choice of parameters. According to these arguments we expect the dissolution of clusters in granular gases of viscoelastic particles not to be related to the periodic boundary conditions.

6. Conclusion

We have investigated a granular gas of particles which collide by means of a stepwise coefficient of restitution used to mimic collisions of viscoelastic particles. This simplified collision law reflects the main feature of viscoelastic particles that collisions tend to occur elastically for decreasing impact velocity. In such gases clustering takes place only as a transient process. Using this collision model, clusters dissolve before they grow to system size. Hence, the model allows us to investigate the total process without the drastic influence of boundary conditions. The results support the previous findings [21] that clustering occurs only as a transient process for realistic gases of viscoelastic particles.

The model investigated, equation (3), compromises between physical correctness (viscoelastic collisions with $\varepsilon(g)$ given by equation (2)) and numerical feasibility. Although the two models have the same asymptotics, $\lim_{g\to 0}\varepsilon = 1$, they differ in an important point: for $g \ll g^*$ viscoelastic particles collide *almost* elastically but not *exactly*. Therefore, our result is not a rigorous proof for the dissolution of clusters in the long time behaviour of gases of viscoelastic particles but a strong hint, supporting the linear stability analysis [20] and the previous numerical results [21] where periodic boundary conditions affected the dynamics of the gas.

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