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Statistical mechanics of granular gases in compartmentalized systems

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We study the behavior of an assembly of *N* granular particles contained in two compartments within a simple kinetic approach. The particles belonging to each compartment collide inelastically with each other and are driven by a stochastic heat bath. In addition, the fastest particles can change compartment at a rate that depends on their kinetic energy. Via a Boltzmann velocity distribution approach, we first study the dynamics of the model in terms of a coupled set of equations for the populations in the containers and their granular temperatures and find a crossover from a symmetric high-temperature phase to an asymmetric low-temperature phase. Finally, in order to include statistical fluctuations, we solve the model within the direct simulation Monte Carlo approach. Comparisons with previous studies are presented.

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I. INTRODUCTION

In recent years considerable progress has been achieved in the understanding of granular gases, i.e., assemblies of moving inelastic solid grains mutually colliding and losing a little energy in each collision [1,2]. They exhibit a fascinating and rich phenomenology that comprehends clustering [3–5], spontaneous vortex formation [6], and breakdown of kinetic energy equipartition in granular mixtures [7,8]. More fundamentally granular gases represent one of the prototypical nonequilibrium systems.

Major progress has been achieved by considering the simplest situations, i.e., spatially homogeneous and time-independent systems. In spite of that, inhomogeneities do not always represent a nuisance or an undesired complication, but, on the contrary, they can be a source of new insight. Within such a perspective, external fields have been introduced on purpose in order to probe the inhomogeneous behavior of granular gases. The seminal work of Schlichting and Nordmeier [9] has stimulated a vivid interest in the behavior of the so called compartmentalized systems. A box, whose base moves periodically up and down, is separated by a vertical barrier into two compartments that communicate through an orifice. For strong shaking the two halves are equally populated, as it would occur in the case of a standard molecular fluid, whereas for weaker driving the symmetry is spontaneously broken. The resulting scenario resembles that of an equilibrium thermodynamical phase transition, with the population difference between the two compartments playing the role of the order parameter and the driving intensity that of temperature. Our understanding of the problem has increased since then due to a series of studies. These comprise new experiments [12,13], phenomenological flux models [10,14], hydrodynamic equations, and molecular dynamics simulation [11,22].

The scope of the present contribution is to show that by choosing a simplified yet significant model of compartmentalized granular gas it is possible not only to derive a set of equations describing the evolution of the macro state of the system, but also to obtain information about its microscopic fluctuations. The present approach represents a bridge between the phenomenological level of Refs. [12–14] and the statistical mechanical level [15].

The present paper is organized as follows: in the first section we define the model and introduce the statistical description of the system, based on a Boltzmann equation for the distribution functions, modified to take into account the stochastic driving. At this stage we follow the strategy of integrating out microscopic fluctuations going from a microscopic description based on the Boltzmann equation to a macroscopic level, where only the occupation numbers and the granular temperatures of the two compartments, i.e., the first two moments of the distribution function are taken into account. This is equivalent to neglecting inhomogeneities of the system at scales smaller than the linear size of the compartments. To obtain qualitative insight, we first try a Gaussian solution. In other words, we assume that the velocity probability density function (PDF's) are Gaussians, whose normalizations and variances (related to the occupation numbers of the compartments and to their granular temperatures, respectively), can be determined by means of a set of self-consistent differential equations. The analysis shows the existence of a transition from a symmetric phase, where the compartments are equally populated and are at the same granular temperature, to an asymmetric phase, where the two compartments have different properties. Various predictions are made: we locate the bifurcation point, obtain relations between the asymptotic values of the temperatures and densities in the compartments, estimate the characteristic times to observe the symmetry breaking, etc. In the second section, we relax the Gaussian hypothesis about the nature of the velocity fluctuations and let the populations in the two compartments fluctuate as well. This is done by solving numerically the full Boltzmann equation by means of the direct simulation Monte Carlo (DSMC) [16]. We notice deviations with respect to the treatment in Sec. I, in particular near the critical point. Finally, in the last section we present our conclusions.

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II. THE MODEL

Let us consider a system, composed of two compartments A and B of the same volume, $V_A = V/2$, and containing N_A and N_B particles, respectively. Particle pairs belonging to the same compartment may collide inelastically losing a fraction of their kinetic energy, but conserving their total momentum. The postcollisional velocities $(\mathbf{v}_1^*, \mathbf{v}_2^*)$ are determined by the transformation

$$\mathbf{v}_1^* = \mathbf{v}_1 - \frac{1}{2}(1+\alpha)(\mathbf{v}_{12}\cdot\hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}, \tag{1}$$

where $\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2$ and α is the restitution coefficient.

In addition, we assume that all the grains are subject to the action of an external stochastic driving force and their motion between two successive collisions is described by the following Ornstein-Uhlenbeck process:

$$\frac{d\mathbf{v}_i}{dt} = -\frac{1}{\tau_b}\mathbf{v}_i + \hat{\boldsymbol{\xi}}_i, \tag{2}$$

where $-\tau_b^{-1}\mathbf{v}_i$ is a friction term and $\boldsymbol{\xi}_i$ a Gaussian random acceleration, of zero average and variance given by

$$\langle \xi_{i\alpha}(t)\xi_{j\beta}(t')\rangle = 2\frac{T_b m}{\tau_b}\delta_{ij}\delta_{\alpha\beta}\delta(t-t'), \tag{3}$$

where T_b is a measure of the intensity of the driving. Notice that in the elastic case ($\alpha=1$), the average kinetic energy per particle moving in a d-dimensional space is $K = dT_b/2$, which is just the ideal gas value. The simultaneous presence of frictional dissipation and random "kicks" renders the kinetic energy of the system stationary even in the absence of collisional dissipation.

To complete the model, we allow the particles contained in $A(B)$ to move into $B(A)$ with a probability per unit time, τ_s^{-1}, provided their kinetic energy exceeds a given threshold, say $T_s = \frac{1}{2}mu_s^2$. Such a mechanism schematizes the jump process by which particles may pass from one compartment to the other by overcoming a vertical barrier of height h only if $\frac{1}{2}mv^2 > mgh$.

We shall make the key assumption, dictated by mathematical convenience, of ignoring the spatial gradients that characterize experimental situations. To be specific we stipulate which within the spatial domain, that represents a compartment, the system is homogeneous. The effect of the dividing vertical wall is schematized by a selection rule of probabilistic nature, which allows only the more energetic particles to cross the barrier.

To make analytic progress we shall transform the stochastic evolution equations for the velocities of the particles into a system of deterministic equations for the distribution functions. In order to achieve this description, we shall treat the collisions at the level of the Boltzmann molecular chaos approximation. This approximation, widely employed even in the case of granular systems, is equivalent to neglecting correlations among the colliding particles.

In order to study the statistical evolution of the system, we assume that the single particle phase-space distribution function $f(\mathbf{r},\mathbf{v},t)$ satisfies the following properties:

$$N_{A(B)}(t) = \int_{V_{A(B)}} d\mathbf{r}\int d\mathbf{v} f(\mathbf{r},\mathbf{v},t), \tag{4}$$

where $N_{A(B)}(t)$ is the average number of particles in compartment $A(B)$ at instant t. The average kinetic energy per particle, the granular temperature $T_{A(B)}$, is defined as

$$T_{A(B)}(t) = \frac{1}{N_{A(B)}(t)d}\int_{V_{A(B)}} d\mathbf{r}\int d\mathbf{v} m\mathbf{v}^2 f(\mathbf{r},\mathbf{v},t). \tag{5}$$

In the following we shall make the assumption that to describe the essential properties of the system, we do not need the detailed information contained in $f(\mathbf{r},\mathbf{v},t)$, but these can be captured by the following coarse grained distributions obtained by eliminating the $\mathbf{r}$ dependence of the original distributions:

$$f_{A(B)}(\mathbf{v},t) = \frac{1}{V_{A(B)}}\int_{V_{A(B)}} d\mathbf{r} f(\mathbf{r},\mathbf{v},t). \tag{6}$$

The change of $f_{A(B)}(\mathbf{v},t)$ is given by

$$\partial_t f_A(\mathbf{v}_1,t) = I(f_A,f_A) + \frac{T_b}{\tau_b}\left(\frac{\partial}{\partial \mathbf{v}_1}\right)^2 f_A(\mathbf{v}_1,t) + \frac{1}{\tau_b}\frac{\partial}{\partial \mathbf{v}_1} f_A(\mathbf{v}_1,t) - \frac{1}{\tau_s}\theta(|\mathbf{v}_1| - u_s)[f_A(\mathbf{v}_1,t) - f_B(\mathbf{v}_1,t)], \tag{7}$$

where $\theta(x)$ is the Heaviside function. The first term represents the change of the distribution due to collisions, the second and the third terms are due to the interaction with the heat bath and the last describes the population change due to the particles migrating from one compartment to the other [16].

In order to obtain an explicit expression for the collision integral $I(f,f)$ in the case of inelastic hard spheres, we shall follow closely the derivation of Ernst and Van Noije [17] and set

$$I(f_A,f_A) = \sigma^{d-1}\int d\mathbf{v}_2 \int' d\hat{\boldsymbol{\sigma}}(\mathbf{v}_{12}\cdot\hat{\boldsymbol{\sigma}}) \times \left\{\frac{1}{\alpha^2} f_A(\mathbf{v}_1^{**},t) f_A(\mathbf{v}_2^{**},t) - f_A(\mathbf{v}_1,t) f_A(\mathbf{v}_2,t)\right\}. \tag{8}$$

The prime on the $\hat{\boldsymbol{\sigma}}$ integration enforces the condition $\mathbf{v}_{12}\cdot\hat{\boldsymbol{\sigma}} > 0$, where $\hat{\boldsymbol{\sigma}}$ is a unit vector along the line of centers of the colliding spheres at contact, whereas $\mathbf{v}_i^{**}$ represent the precollisional velocities, which can be computed by inversion of Eq. (2).

By integrating over the spatial coordinate and over the velocity it is straightforward to obtain the equation for the rate of change of the occupation numbers N_A and N_B. It reads

$$\frac{dN_A(t)}{dt}=-\frac{V_A}{\tau_s}\int d\mathbf{v}_1[f_A(\mathbf{v}_1,t)-f_B(\mathbf{v}_1,t)]\theta(|\mathbf{v}_1|-u_s). \tag{9}$$

We see that when the typical time τ_s diverges, there is no particle exchange between the two compartments, thus N_A, N_B are constant, and the temperatures reach a constant value, which depends on the heat bath properties, the physical properties of the particles, and on their number.

In order to obtain the energy equation, instead, we multiply both sides by $m\mathbf{v}_1^2$ and integrate over coordinate and velocity space:

$$\frac{d[N_A(t)T_A(t)]}{dt}=\frac{2}{\tau_b}N_A[T_b-T_A(t)] + \frac{2}{d}\frac{N_A}{V_A}\sigma^{d-1}v_A\mu_2 N_A(t)T_A(t) \tag{10}$$

$$-\frac{V_A}{\tau_s d}\int d\mathbf{v}_1 m\mathbf{v}_1^2[f_A(\mathbf{v}_1,t)-f_B(\mathbf{v}_1,t)] \times\theta(|\mathbf{v}_1|-u_s), \tag{11}$$

where we have introduced, following Ref. [17], the nondimensional quantity μ_2,

$$\mu_2=-\frac{1}{v_A^3}\frac{V^2}{N^2}\int d\mathbf{v}_1\mathbf{v}_1^2 I(f_A,f_A) =-\frac{1}{v_A^3}\frac{V^2}{N^2}\int d\mathbf{v}_1\mathbf{v}_1^2\int d\mathbf{v}_2\int' d\hat{\boldsymbol{\sigma}}(\mathbf{v}_{12}\cdot\hat{\boldsymbol{\sigma}}) \times\left\{\frac{1}{\alpha^2}f_A(\mathbf{v}_1^{**},t)f_A(\mathbf{v}_2^{**},t)-f_A(\mathbf{v}_1,t)f_A(\mathbf{v}_2,t)\right\} \tag{12}$$

with $v_{A(B)}^2=2T_{A(B)}/m$. In the following we shall set $m=1$. A more compact notation is achieved if one introduces the collision frequency $\omega_A(t)$ and the nondimensional spontaneous cooling rate γ,

$$\omega_A=\frac{\Omega_d}{\sqrt{2\pi}}\frac{N_A}{V_A}\sigma^{d-1}v_A, \tag{13}$$

$$\gamma=\frac{\sqrt{2\pi}}{d\Omega_d}\mu_2 \tag{14}$$

with $\Omega_d=2\pi^{d/2}/\Gamma(d/2)$. The surface area of a d-dimensional unit sphere. In the remainder of the paper we shall measure the temperature in units of T_s, time in units of τ_b, and length in units of σ.

To proceed further analytically we choose $d=2$ and assume an approximate Gaussian form [18] of the distribution function:

$$f_{A(B)}(\mathbf{v},t)=\frac{N_{A(B)}}{V_{A(B)}}\frac{1}{\pi 2T_{A(B)}}\exp\left(-\frac{\mathbf{v}^2}{2T_{A(B)}}\right). \tag{15}$$

In this case one can evaluate explicitly the collision term [17]

$$\mu_2=(1-\alpha^2)\frac{\pi^{d/2-1}}{\sqrt{2}\Gamma(d/2)}, \tag{16}$$

$$\gamma\omega_A=\sigma(1-\alpha^2)\frac{N_A}{2V_A}\sqrt{\frac{T_A}{m}}. \tag{17}$$

We find

$$\frac{dN_A(t)}{dt}=\frac{1}{\tau_s}[N_B e^{-T_s/T_B}-N_A e^{-T_s/T_A}], \tag{18}$$

where the temperature T_s is given by $T_s=\frac{1}{2}mu_s^2$. Notice that the right hand side of the equation above represents the difference between the incoming flux and the outgoing flux of compartment *A*. A similar expression has been chosen by Droz and Lipowski [14] on phenomenological grounds. The model we study allows us to obtain self-consistently the temperatures T_A and T_B, a feature that was not present in most of the studies dedicated to compartmentalized systems [19]. In fact, we can write

$$\frac{d[N_A(t)T_A(t)]}{dt}=-\frac{2}{\tau_s}[N_A(T_A+T_S)e^{-T_s/T_A} - N_B(T_B+T_S)e^{-T_s/T_B}]-2\gamma\omega_A N_A T_A + \frac{2}{\tau_b}N_A(T_b-T_A), \tag{19}$$

$$\frac{d[N_B(t)T_B(t)]}{dt}=-\frac{2}{\tau_s}[N_B(T_B+T_S)e^{-T_s/T_B} - N_A(T_A+T_S)e^{-T_s/T_A}]-2\gamma\omega_B N_B T_B + \frac{2}{\tau_b}N_B(T_b-T_B). \tag{20}$$

Notice that the Arrhenius type of behavior of the transition rate $\tau_s e^{T_s/T_A}$ results from the combination of two assumptions: (a) the fact that only particles whose energy exceeds the threshold T_s can overcome the barrier; (b) the Gaussian ansatz for the velocity distribution functions. The latter ingredient, although very convenient for numerical work, could result too crude in some physically relevant situations, because the dynamics represent a severe probe of the extreme value statistics of the system. It is well known that the velocity distribution of driven and undriven granular assemblies might be characterized by fat velocity tails [16].

III. MEAN FIELD ANALYSIS

It is convenient to rewrite the coupled equations as

$$\frac{dN_A(t)}{dt}=\frac{1}{\tau_s}[N_B e^{-T_s/T_B}-N_A e^{-T_s/T_A}], \tag{21a}$$

$$N_A\frac{dT_A(t)}{dt}=-\frac{1}{\tau_s}[2(N_AT_Ae^{-T_s/T_A}-N_BT_Be^{-T_s/T_B})+(N_Ae^{-T_s/T_A}-N_Be^{-T_s/T_B})(2T_s-T_A)]-2\gamma\omega_AN_AT_A+\frac{2}{\tau_b}N_A(T_b-T_A), \tag{21b}$$

$$N_B\frac{dT_B(t)}{dt}=-\frac{1}{\tau_s}[2(N_BT_Be^{-T_s/T_B}-N_AT_Ae^{-T_s/T_A})+(N_Be^{-T_s/T_B}-N_Ae^{-T_s/T_A})(2T_s-T_B)]-2\gamma\omega_BN_BT_B+\frac{2}{\tau_b}N_B(T_b-T_B). \tag{21c}$$

Let us observe that in the temperature equations there appear two types of fluxes: the first due to the unbalance of kinetic energies, and the second due to the population difference. We identify the first with a heat conduction process and the second with a particle diffusion process.

One sees by inspection that the choice $N_A=N_B=N^*=N/2$ and $T_A=T_B=T^*$ represents a symmetric solution for all values of the control parameters. The granular temperature of the symmetric state, T^*, is given by the nonlinear equation

$$T^*\left[1+\tau_b\sigma(1-\alpha^2)\frac{N^*}{2V_A}\sqrt{\frac{T^*}{m}}\right]=T_b. \tag{22}$$

In order to ascertain the stability of such a symmetric solution we assume $T_A=T^*+\delta T_A$, $T_B=T^*+\delta T_B$, and $N_A=N^*+\delta N_A(\delta N_B=-\delta N_A)$ and expand the equations to linear order about the fixed point T^*,N^* with the result

$$\delta\dot{N}_A=-\frac{1}{\tau_s}e^{-T_s/T^*}\left[2\,\delta N_A+\frac{N^*T_s}{(T^*)^2}(\delta T_A-\delta T_B)\right], \tag{23}$$

$$\delta\dot{T}_A=-\frac{1}{\tau_s}e^{-T_s/T^*}\left[2+\frac{T_s}{T^*}+\left(\frac{T_s}{T^*}\right)^2\right](\delta T_A-\delta T_B)-\left(3\gamma\omega^*+\frac{2}{\tau_b}\right)\delta T_A-\frac{2}{N^*}\left[\frac{1}{\tau_s}e^{-T_s/T^*}(T^*+2T_s)+\gamma\omega^*T^*\right]\delta N_A, \tag{24}$$

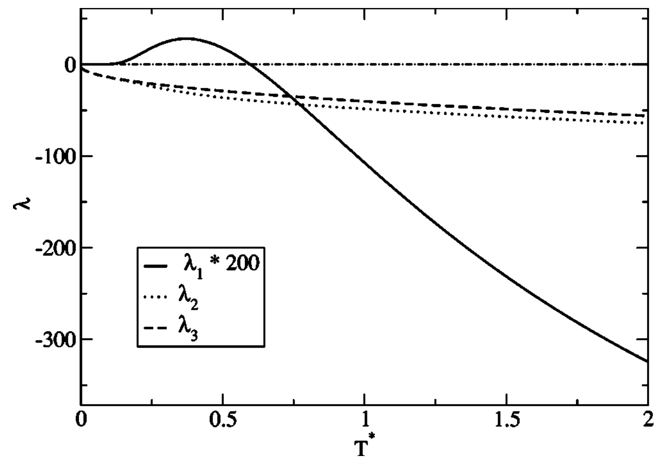

FIG. 1. Variation of the eigenvalues of the dynamical matrix with respect to the granular temperature. Notice that below the critical temperature the less negative eigenvalue displays a maximum. This is determined by the competition between the inhibiting factor due to the wall and the collisional dissipation which favors a symmetry breaking.

$$\delta\dot{T}_B=\frac{1}{\tau_s}e^{-T_s/T^*}\left[2+\frac{T_s}{T^*}+\left(\frac{T_s}{T^*}\right)^2\right](\delta T_A-\delta T_B)-\left(3\gamma\omega^*+\frac{2}{\tau_b}\right)\delta T_B+\frac{2}{N^*}\left[\frac{1}{\tau_s}e^{-T_s/T^*}(T^*+2T_s)+\gamma\omega^*T^*\right]\delta N_A. \tag{25}$$

The eigenvalues of the associated 3×3 matrix of coefficients give the three relaxation modes. By adding and subtracting the last two equations the linear system factorizes into a decoupled equation for the average value of the two temperatures $[(\delta T_A+\delta T_B)/2]$ with eigenvalue $\lambda_3=-(3\gamma\omega^*+2/\tau_b)$ and a system of rank 2 involving the temperature difference and the occupation number. The more negative of the remaining eigenvalues (we call it λ_2) is of the same order as λ_3, while the second, say λ_1, is smaller in absolute value and vanishes at the "special" temperature T_{cr}. This is obtained by solving the transcendental equation

$$\tau_s\gamma\omega^*\left(\frac{T_s}{T_{cr}}-\frac{3}{2}\right)-\frac{\tau_s}{\tau_b}=2e^{-T_s/T_{cr}}. \tag{26}$$

Figure 1 shows that above the temperature T_{cr}, λ_1 is negative, thus making the symmetric solution stable, whereas for temperatures below it λ_1 is positive. In such a case the symmetric fixed point is unstable and the solution flows away, to an asymmetric fixed point. Hereafter, we shall use the word "critical temperature" or "critical line" instead of "special" [20].

Let us also notice that when the typical collision time is much shorter than the characteristic times τ_c and τ_b the temperature $T_{cr}\to 2T_s/3$, which represents an upper bound for such a quantity.

At this stage a few comments are in order. The transition results from the competition between two effects: the diffusion due to the "thermal" agitation of the particles, i.e., the tendency to fill all the available space, and the dissipation of energy during collisions which favors clusterization.

When the external drive is sufficiently weak there appears a second fixed point. This is found by imposing the detailed balance

$$\frac{N_B}{N_A}=\frac{e^{-T_s/T_A}}{e^{-T_s/T_B}} \tag{27}$$

and the energy balance

$$-\frac{2}{\tau_s}(N_A T_A e^{-T_s/T_A}-N_B T_B e^{-T_s/T_B})-2\gamma\omega_A N_A T_A + \frac{2}{\tau_b}N_A(T_b-T_A)=0, \tag{28}$$

$$\frac{2}{\tau_s}(N_A T_A e^{-T_s/T_A}-N_B T_B e^{-T_s/T_B})-2\gamma\omega_B N_B T_B + \frac{2}{\tau_b}N_B(T_b-T_B)=0. \tag{29}$$

A good approximation to the highest eigenvalue in such a case reads

$$\lambda_1=\frac{2}{3}e^{-T_s/T^*}[\omega^*\gamma(T_s/T_*-3/2)-1/\tau_b-2e^{-T_s/T^*}].$$

One observes two regions where the solutions are apparently metastable. The first is the low-temperature region, where a detailed inspection shows that the symmetric state, in reality, is very weakly unstable. From Fig. 1 we see that at low temperatures ($T^*\to 0$) the positive eigenvalue λ_1 vanishes exponentially as e^{-T_s/T^*}, thus indicating that the symmetric solution might appear stable if the observation time is finite. In fact, the interwell diffusion for $T_b\to 0$ is almost completely suppressed by the Arrhenius factor.

The second region where the system displays genuine (meta)stability occurs just above T_{cr}. A branch with $N_A\neq N_B$ and $T_A\neq T_B$ is observed by integrating numerically the system (21) by means of an Euler scheme. These asymmetric stationary states are obtained by preparing the system in a subcritical configuration ($T^{ast}<T_{cr}$), and successively increasing the temperature above T_{cr}. The width of the region is about 10% of T_{cr}. The observed hysteresis agrees qualitatively with the results relative to the model of Ref. [14].

The numerical solutions of the coupled equations are displayed in Figs. 2 and 3. We observe that a perturbation about the symmetric solution is readsorbed for $T^{ast}>T_{cr}$, whereas for temperatures below T_{cr} the perturbation grows initially at an exponential rate, before saturating about a finite value. Let us notice that at low temperatures, due to the presence of the Arrhenius factor, the saturation process occurs extremely slowly, a phenomenon that is not related to the slowing down that occurs only in the vicinity of T_{cr}.

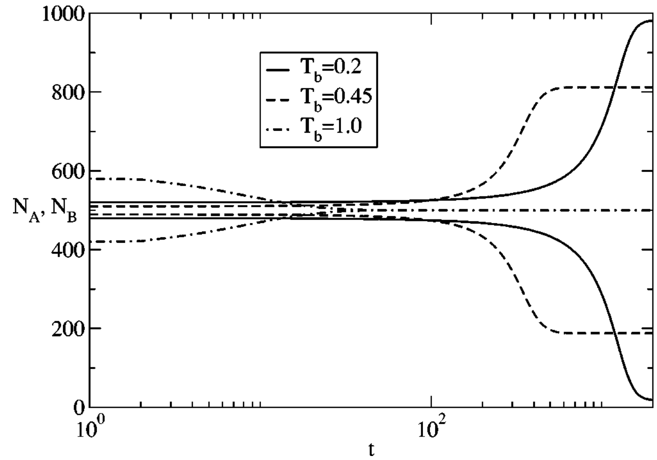

FIG. 2. Evolution of the populations in the two compartments versus time, for three different choices of the heat bath temperature, $T_b=0.2,0.3,1$. The remaining parameters are: $N=1000$, $T_s=1$, $V=100$, $\sigma=1$, $\tau_b=1$, $\tau_s=0.5$, $\alpha=0.7$.

In Fig. 4 we display the line of critical points T_{cr} as a function of the inelasticity $(1-\alpha)$ for two different values of the total number of particles. Above the line the solutions are symmetric ($N_A=N_B$), below are asymmetric. Let us observe that for $\alpha=1$ one finds $T_{cr}=0$, because there is no clustering instability in systems of elastic particles. The smaller the value of α, the higher the value of the critical temperature. We also notice that the slope of the critical line is nonnegative. When the total number of particles decreases, also the critical temperature decreases, because of the lower collision rate.

Figure 5 illustrates the behavior of the order parameter $\epsilon=|N_A-N_B|/N$ versus the heat bath temperature for two different values of the total number of particles.

Let us notice that when particles are added to the system the critical point shifts up-wards. This explains why the steady number of particles in the less populated compartment decreases when more particles are added [11].

Finally, we comment that, within our perspective, the approach of Lohse *et al.* [12] and of Lipowski and Droz [14] is equivalent to an adiabatic approximation for the temperature

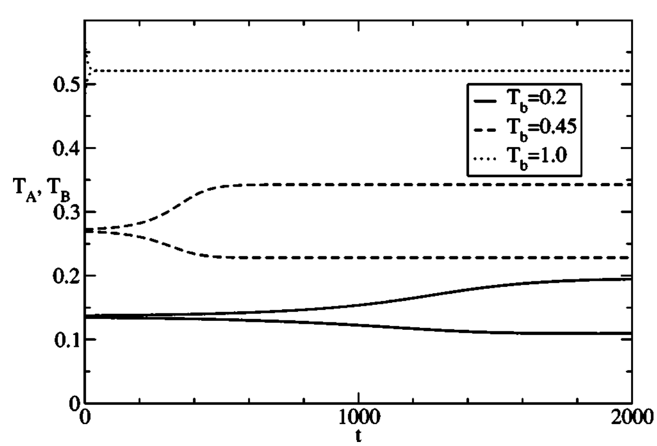

FIG. 3. Granular temperatures in the two compartments corresponding to the evolution of 2.

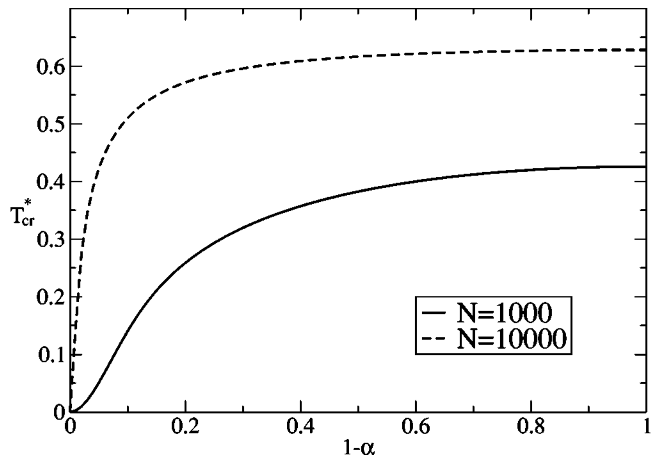

FIG. 4. Critical line for two different choices of the total number of particles 1000 (below) and 10 000 (above) according to the mean field theory. Vertical axis temperature, horizontal $(1-\alpha)$. The line represents the granular critical temperature as the inelasticity $(1-\alpha)$ varies from 0 to 1. Below the critical line the symmetric solution is unstable; above it is stable. The remaining parameters are the same as in Fig. 2.

variables. In their cases, the two granular temperatures are assumed to be slaved by the occupation number variables. In other words, one postulates that the temperatures depend on the instantaneous values of the occupation numbers. We implemented this idea within our approach, but we found a large discrepancy with the previous approximation. In reality, the temperature and the occupation variable vary on the same time scale and no slaving principle seems to occur.

IV. MONTE CARLO SIMULATIONS

In deriving the evolution equations of the preceding section, we have implicitly stipulated that the values of the occupation number and of the kinetic energy per particle in each box have narrow distributions around their mean values

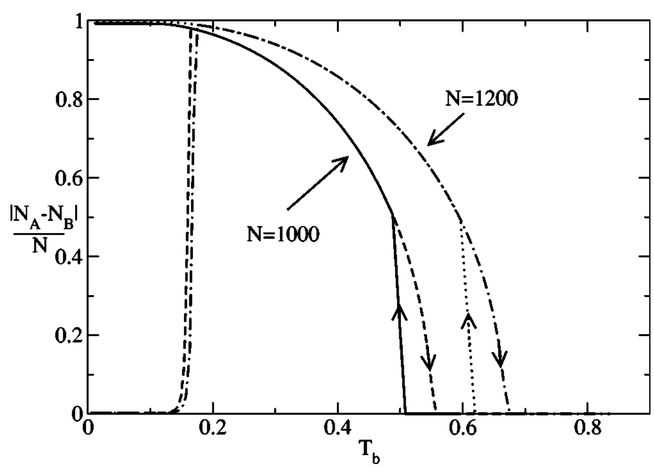

FIG. 5. Asymmetry parameter vs T_b plotted for two different choices of the total number of particles: 1000 and 1200. The remaining parameters are the same as in Fig. 2. Notice the difference between the two curves and the presence of the hysteresis.

and that these quantities are sufficient to characterize the state of the system. Do statistical fluctuations play any role or even modify the picture presented above? In the present section, which is not intended to be exhaustive, we solve the model of Sec. I by means of the DSMC method. The motivation is twofold: we want to validate the picture and the approximations introduced above and unveil some phenomena that are not accounted for by a mean field description.

We simulated two ensembles of N_A and N_B particles, respectively, subject to a Gaussian forcing, viscous friction, and inelastic collisions. In addition, the particles of high energy can change compartment with probability per unit time τ_s^{-1}.

The scheme consists of the following ingredients.

Time is discretized, i.e., $t=ndt$.

Update all the velocities to simulate the random forcing and the viscous damping,

$$v_i^\alpha(t+dt)=v_i^\alpha(t)e^{-dt/\tau_b}+\sqrt{T_b(1-e^{-2dt/\tau_b})}W(t), \tag{30}$$

where $W(t)$ is a normally distributed deviate with zero mean and unit variance.

At every time step and for both compartments, a collision step is performed, i.e., an adequate number of randomly chosen pairs of velocities are updated with the collision rule (1): the pairs are chosen with a probability proportional to their relative velocity and normalized in order to have a mean collision frequency as calculated in Eq. (13).

Place in the other compartment with probability dt/τ_s particles with kinetic energy greater than T_s.

Change the time counter n and restart.

To summarize, at every step each particle experiences a Gaussian kick and receives energy from the bath, but dissipates a fraction of its kinetic energy by collision and by damping. With respect to previous DSMC simulations of granular gases particles can migrate to another compartment, whenever their energy exceeds a fixed threshold. No packing effects are included.

The parameters chosen in the simulation are $T_s=1$, $V=100$, $\sigma=1$, $\tau_b=1$, $\tau_s=0.5$, $\alpha=0.7$, whereas the total number of particles N and T_b have been varied.

First, we analyze the evolution of the order parameter $|N_A-N_B|/N$, when the system is prepared in a symmetric configuration. The order parameter displays a behavior similar to that obtained by means of the mean field theory. In addition, it displays fluctuations around its asymptotic value. In Fig. 6, an average over 200 realizations of the evolution of the order parameter $|N_A-N_B|/N$ is shown. The numerical simulations are in agreement with the results of the mean field theory. For $T_b>0.45$ the system remains substantially homogeneous. For $T_b<0.45$ the homogeneous state becomes unstable and the stable configuration that is reached is strongly asymmetric.

Interestingly, we observe a much slower growth (see inset) near the critical temperature, $T_{cr}\sim 0.45$. The same kind of phenomenon appears at low temperatures $(T<T_s)$, because the transitions from one compartment to the other represent very rare events.

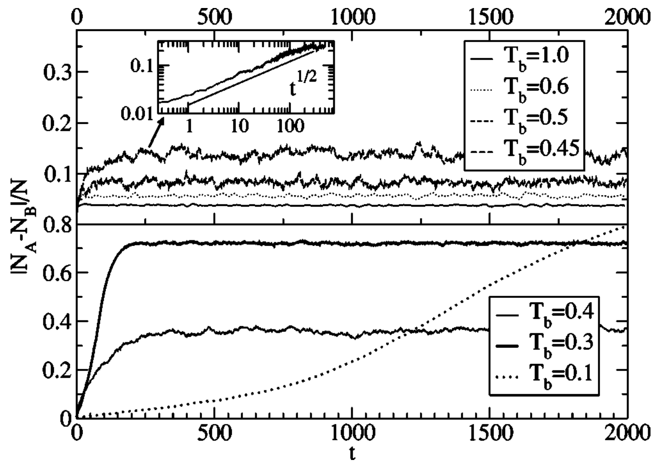

FIG. 6. Evolution of the order parameter versus time. $N=1000$, but T_b is varying, while the other parameters are: $T_s=1$, $V=100$, $\sigma=1$, $\tau_b=1$, $\tau_s=0.5$, $\alpha=0.7$.

In Fig. 7 the temperature evolutions $T_A(t)$ and $T_B(t)$ (after averaging over 200 realizations and relabeling the compartments in such a way that A is always the most populated) are displayed. The plateau values of T_A and T_B verify (with small deviations, not larger than 10%) Eq. (27).

The velocity fluctuation can be appreciated by considering the velocity PDF's of the two compartments, Fig. 8. Appreciable deviations from a Gaussian have not been detected in all cases considered (neither above, neither below, nor in the proximity of the critical temperature).

The order parameter, instead, shows less trivial fluctuations. A typical trajectory is shown in Fig. 9. The associated distribution is shown in Fig. 10. We observe that at high temperature the population distribution $P(N_A)$ is well approximated by a Gaussian distribution, but displays two symmetric peaks about the central value $N_A=500$ when the system approaches the critical temperature. Finally, at low temperature we find two very narrow peaks, well separated and centered around $N_A=950$ and $N_B=50$.

Let us consider more closely the behavior of the order parameter near the critical point. According to the mean field description of Sec. II, at T_{cr} the less negative eigenvalue of the matrix of evolution vanishes. The picture looks somehow different when microscopic fluctuations are accounted for. One observes a remarkable behavior in the order parameter evolution; namely, in the earlier regime it grows in a power law fashion as $(N_A-N_B)^2\sim t$, and not exponentially. To explain this phenomenology we remark that the evolution of the order parameter near T_{cr} can be assimilated to that of a particle undergoing a random walk. We assume that the early evolution of $\Delta N(t)=N_A(t)-N/2$ can be effectively described by the following equation:

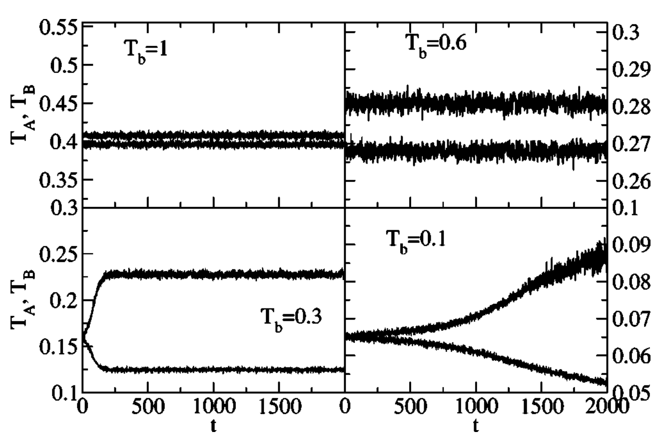

FIG. 7. Temperature evolution for various values of the heat bath temperature. The other parameters are the same as in Fig. 6.

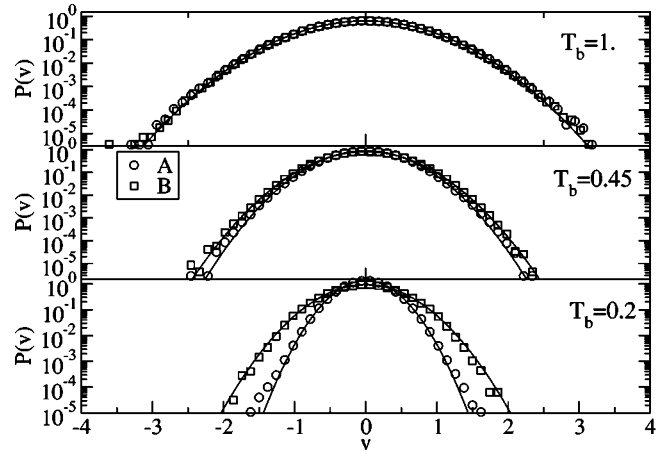

FIG. 8. Velocity distribution functions in each compartment for two different values of T_b and $N=1000$. The other parameters are the same as in Fig. 6. The lines represent Maxwellian velocity distributions, whose variances have been determined from fits of the numerical data.

$$\frac{\partial \Delta N(t)}{\partial t}=\gamma(T_b)\Delta N(t)+A(T_b)\,\eta \tag{31}$$

with γ lesser than zero above the critical temperature and greater than zero under the critical temperature and η a white Gaussian noise. In this case

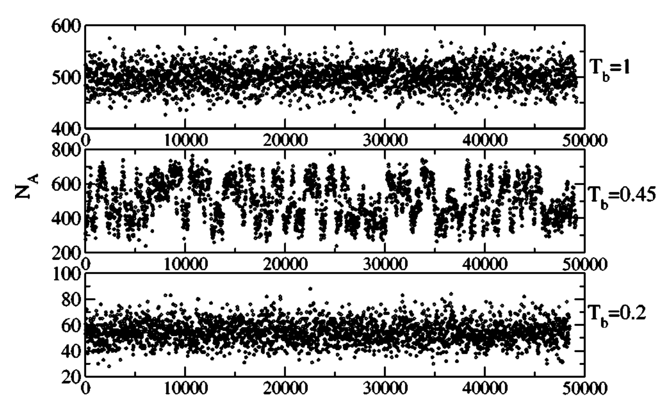

FIG. 9. Fluctuations of the occupation number $N_A(t)$ vs time, when the system is in its statistically stationary state for three different choices of T_b. The other parameters are the same as in Fig. 6.

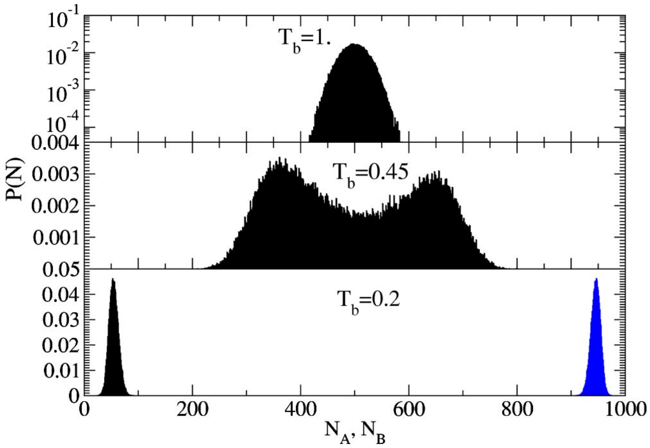

FIG. 10. Probability distribution functions of the occupation numbers in a single well (top and middle panel, respectively) and in the two wells (bottom panel), referred to a system of $N=1000$ particles. The other parameters are the same as in Fig. 6.

$$C(\tau,t)=\langle\Delta N(t+\tau)\Delta N(t)\rangle$$
$$=\left[\langle\Delta N(0)\Delta N(0)\rangle+\frac{A^2}{2\gamma}\right]e^{\gamma(2t+\tau)}-\frac{A^2}{2\gamma}e^{\gamma\tau}, \tag{32}$$

which means that if $\gamma<0$ (asymptotically in a time greater than $1/|\gamma|$) the equal time correlation function becomes

$$\langle\Delta N(t)\Delta N(t)\rangle\rightarrow-\frac{A^2}{2\gamma} \tag{33}$$

or equivalently $A=\sqrt{-2\gamma\langle\Delta N^2\rangle}$, where $\Delta N^2=\lim_{t\rightarrow\infty}C(0,t)$. On the other hand, when $\gamma=0$ (i.e., in correspondence of the critical point), the equal time correlation function displays a diffusive behavior:

$$\langle\Delta N(t)\Delta N(t)\rangle\rightarrow A^2 t \tag{34}$$

that means that the diffusion coefficient for the variable ΔN is given by $D=A^2/2$.

Eventually in the late regime the growth saturates due to the onset of nonlinear effects.

In order to verify the plausibility of Eq. (31) we determine A and γ by extracting them from numerical measures of $\lim_{t\rightarrow\infty}C(\tau,t)$ and imposing the asymptotic behavior $-(A^2/2\gamma)e^{\gamma\tau}$. In Fig. 11 we display the values of the constants obtained from simulations above the critical temperature. We also added to the plot the value of the diffusion coefficient $D=A^2/2$, as measured at the critical temperature.

Interestingly, when the characteristic time τ_s decreases (namely, $\tau_s=0.1$) an interesting phenomenon appears: the temperature of the less populated compartment exhibits an initial regime, during which it increases, due to the decrement of the number of collisions the particles experience, followed by a second regime where the temperature instead *decreases* and eventually reaches a temperature lower than the temperature of the more populated container (Fig. 12). This kind of anomaly is due to the fact that the fastest and more energetic particles are removed causing a large negative fluctuation of the associated average kinetic energy. The positive energy flux provided by the heat bath is not sufficient to compensate the energy loss due to the removal of the fast particles. This phenomenon is not observed in the mean field model, because it results from the large non-Gaussian fluctuations of the velocity PDF. We checked the fourth cumulant and observed that whereas the cumulant relative to the populated compartment corresponds to a Gaussian, the cumulant of the small population strongly fluctuates. Experimentally it might be hard to observe such a phenomenon, which is probably an artifact of the model, because the limit of small τ_s is not very realistic.

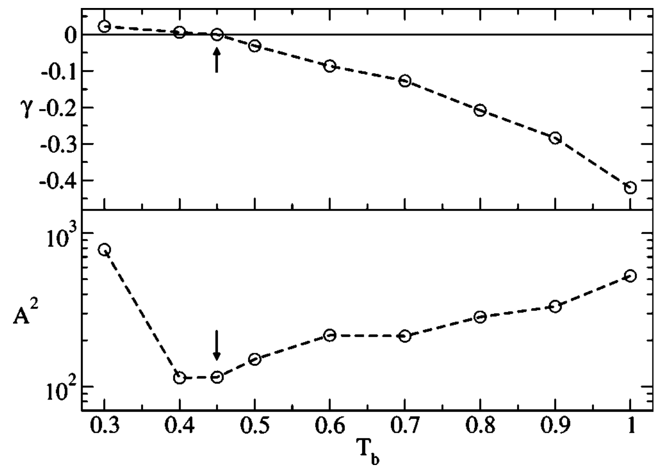

FIG. 11. Study of A^2 and γ versus T_b.

Finally, our schematization of the compartmentalized granular gas recalls the Gibbs ensemble method of equilibrium statistical mechanics, whereby it is possible to study first order phase coexistence without interfaces [21].

V. CONCLUSIONS

To summarize, we introduced a model for a compartmentalized granular gas which allows to bridge between the

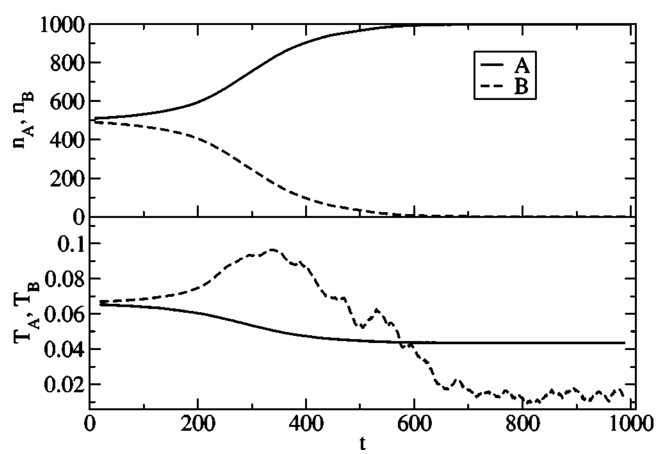

FIG. 12. Populations and granular temperatures of the two compartments when τ_s is small. Notice that the temperature of the less populated compartment initially rises, and successively decreases below the temperature of the other compartment.

microscopic level to the hydrodynamic level. In the first part of the paper we have derived a Fokker-Planck-Boltzmann description starting from the stochastic evolution of the particles' coordinates. Next, by employing a Gaussian ansatz for the velocity distribution function, we have obtained a closed set of equations for the slowly varying fields, namely, the granular temperatures and occupation numbers of each compartment. Let us comment that with respect to existing flux models, our approach treats analytically the granular temperature on equal footing as the occupation variables. The solution of the resulting equations shows the existence of two different regimes: at strong shakings the populations in the two compartments are symmetric and for weak shakings the two populations are asymmetric together with their granular temperatures. A critical point separates these two behaviors. The dynamics has been characterized in the various regimes. In the last part of the paper we have solved the full model by means of DSMC. The presence of stochastic fluctuations leads to properties not observed in a mean field description. These are the presence of critical fluctuations, of anomalies in the dynamics of the populations, and in population fluctuations.

ACKNOWLEDGMENTS

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[18] In order to improve the present approximation, one could express the probability distribution function as a Gaussian multiplied by a linear combination of orthogonal polynomials, called Sonine polynomials. After expressing the coefficients multiplying the polynomials in terms of the moments of the distribution function, one obtains the non-Gaussian corrections to the velocity distribution. The method allows to include the effect of fluctuations around the Gaussian. However, for the sake of simplicity we shall not pursue further this route.

[19] The self-consistent equations obtained above can be extended to a network of compartments in a straightforward fashion. The study of such a system will be the subject of future work.

[20] This does not mean that the transition from the symmetric behavior to the asymmetric behavior of the solutions is continuous. On the contrary, as we shall show below, we observe hysteresis, which is consistent with a discontinuous transition. Such a situation is different from the picture presented in Ref. [12], based on a flux model, that the transition is continuous when the compartments are two and discontinuous when they are more than two.

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