

Inelastic granular gas: Computer simulations and kinetic theory of the cooling state

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We developed computer simulations of an inelastic granular gas which show that the energy decay proposed by Goldhirsch and Zanetti [Phys. Rev. Lett. **70**, 1619 (1993)] has a limited validity. Moreover, we give an exact solution of the Liouville equation for the moments of the two-body homogeneous cooling distribution. The latter includes velocity correlations which raises questions about the derivation of kinetic equations for inelastic gases. [S1063-651X(99)07802-2]

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I. INTRODUCTION

During the last 30 years the study of granular media has been very active, and has provided important results which have enlarged our knowledge on this research field. Some authors have developed theoretical descriptions based on hydrodynamiclike equations whose validity is restricted in density and for weakly inelastic systems (a restitution coefficient near 1). The partial success of these efforts is due to the fact that these formulations do not reveal some of the most characteristic and intriguing features of granular media such as the formation of clusters, segregation phenomena, inelastic collapse, etc. It is precisely these features, absent in a usual hydrodynamic behavior, which make a formulation of granular media an extremely difficult task. This last fact has led several researchers to start to develop a kinetic theory of inelastic gases [1,2] whose main objective is to derive macroscopic flow equations from basic principles. However, since collisions between grains are inelastic, intrinsic attractors exist in the phase space [3,4] which are associated with correlations among particles. Henceforth, a derivation of the kinetic equation for an inelastic gas should start at the level of the exact Liouville equation and proceed by an adequate reduction of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy associated with it. On the other hand, even if we suppose that an adequate kinetic equation can be obtained, another crucial difficulty remains. That is, for inelastic gases not submitted to external constraints or forces, the local Maxwellian distribution is generally not a solution. In the case of an inelastic gas, the reference state cannot be the final evolution stage since the latter corresponds to the rest state for all the particles. Recent works in this field based on kinetic theory assume the existence of the so-called homogeneous cooling state. For instance, Brey, Ruiz-Montero, and Cubero [5] started from the Liouville equation and looked for a solution corresponding to an homogeneous state by assuming that it depends only on the average kinetic energy. This led to their closed equation for the granular temperature. In the first step of our work, we developed com-

puter simulations to verify previous results reported by other authors. These simulations were performed for an inelastic gas for which the restitution coefficient α was varied between 1.0 and 0.7. Moreover, the simulations, which are based on the Boltzmann equation [direct simulation Monte Carlo (DSMC) method] exhibited deviations with respect to the Maxwellian distribution. These facts motivated us to reconsider from the most basic principles the kinetic approach to inelastic gases. That is, in our approach, instead of starting with the Boltzmann equation or any of its enhanced versions, we investigated the properties that could be extracted from the complete Liouville equation, but we tried to find a resolution with a minimal assumption, i.e., the homogeneity of the state. This led us to find an exact solution for the homogeneous regime which shows that the temperature is not the only relevant parameter describing this regime. More precisely, we find exactly all the moments for this distribution. The differences between the results in Ref. [5] and ours are the following. First, our distribution is a two-body distribution which does not factorize. Second, it depends on an infinite set of moments, and the result of Ref. [5] can be found from ours.

The work reported here is organized as follows: In Sec. II we present the computer simulations developed for an inelastic granular gas by using an enhanced version of the direct Monte Carlo simulation method. In Sec. III we propose a Liouville equation for an inelastic granular gas for which the moments of the two-body distribution function are exactly computed and where the demonstration is given in the appendix. Finally, in Sec. IV we give several conclusions concerning the results obtained.

II. DIRECT MONTE CARLO SIMULATIONS FOR AN INELASTIC GRANULAR GAS

An interesting feature of granular gases is their tendency to form dense clusters [6–8] of particles characterized by a collision rate larger than in the less dense regions. This last implies processes involving more than two particles, and we believe that a simulation based only on the Boltzmann equation without some necessary modifications will not reproduce important observations of inelastic granular gases. This situation is similar to the case of a dense hard-sphere gas

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described by the Boltzmann equation, which gives an excellent description when the density and the range of forces are small, but, as the density increases, ceases to be valid [9]. In order to overcome the difficulty of taking into account collisions involving more than two particles we proceed in a similar way as was proposed in Ref. [10], where the authors proposed a modified version of the direct simulation Monte Carlo method originally proposed by Bird [12], which includes an additional displacement in the advection process and an enhanced collision rate [11]. Here we report two-dimensional DSMC simulations of a granular gas composed of identical hard disks performing inelastic collisions between them without an energy input. The formulation of the collision rate follows the lines given in Ref. [9], and allows us to study granular gases with high and low density regions. It is important to point out that these enhancements to the DSMC method do not modify the natural evolution of the gas, and they play their role only when spatial inhomogeneities appear. This last permits us to avoid wasting CPU time in high collisional regions as it occurs when we use the Monte Carlo method for studying granular media. The analysis of our simulations was focused to study the time evolution of the granular temperature [7] and the velocity distributions.

The simulations were performed in a two dimensional simulation box of area $(0.2 \text{ m})^2$ under periodic boundary conditions. The number of particles used were 2.0×10^4 , the time step used was equal to 2.0×10^{-5} sec, and for each simulation we performed 2.0×10^5 iteration steps, which in real time represents 4 sec. Under these conditions the mean free path λ was equal to 1.78×10^{-2} m and the dimensions of the simulation box in terms of λ are of $11.245 \times \lambda$ in the x and y directions. Under these conditions the gas may be considered as dilute at the initial time. In average each particle experienced 200 collisions. The particles are characterized by a mass of 3.0×10^{-6} kg and a diameter of $d = 2.0 \times 10^{-3}$ m. In the simulations the inelasticity of the collisions is represented by the restitution coefficient α , which varied between 1.0 (elastic case) and 0.7 by steps of 0.2. Moreover, the results reported for each value of α were averaged over ten simulations. Only the seed of the random numbers generator was changed at each simulation.

A. Temperature

Several authors [5,7,8], inspired by the works of Jenkins and Richman [19], have studied the formation of spatial inhomogeneities of a granular gas by a kinetic theory approach. These works have deduced, from hydrodynamiclike assumptions, that the time evolution of the kinetic energy (KE) of an inelastic granular gas in a homogeneous state, and obeys an equation of the form $E(t) = E_0 / (1 + At)^2$, where E_0 is the initial energy and A is a function of the restitution coefficient α . Moreover, the formation of spatial instabilities were obtained by considering a Maxwellian velocity distribution in the homogeneous initial state. This last assumption seems justified for almost elastic collisions by experimental studies [13–15] on dilute disk gases connected to a reservoir of energy, which showed that the velocity distribution functions are very close to a Maxwell-Boltzmann distribution for α close to 1.0. Moreover, density profiles show the forma-

tion of dense slowly moving clusters and particles outside the clusters with high velocities which violates the equipartition of energy [8]. Another important point obtained from experimental studies is that the exchange of energy in shocks is not sufficient to equalize the distributed energy. It is important to remark that in most works the granular gas described by kinetic approaches does not include any energy source to equilibrate the energy loss due to the collisions between particles, while the experiments are connected to a reservoir of energy. In Sec. II B we show, as an exact consequence of the Liouville equation for an inelastic hard sphere gas, that the two- and one-body distributions are not necessarily Maxwellian. Moreover, the nonfactorizability of the two-body distribution raises questions about the derivation of the kinetic equations for such systems.

As mentioned above, various authors [5,7,8] found that the time evolution of the energy in a homogeneous cooling regime (HCR) is of the form

$$E(t) = \frac{E(0)}{(1 + t/\tau)^2}$$

or, equivalently,

$$E(t)^{-1/2} = \eta t + \beta. \quad (1)$$

In Fig. 1 we give the results obtained for the time evolution of the inverse of the square root of the KE, $E^{-1/2}$, for the first 900 iteration steps with $0.98 \leq \alpha \leq 0.70$. This figure shows that for $\alpha = (0.8, 0.98)$ the energy time dependence is, qualitatively, in agreement with the results given in Refs. [7,8]. But for $0.7 < \alpha < 0.8$, Eq. (1) is obeyed only for the first 300 iteration steps, which in average represent less than one collision per particle. Figure 2(a) shows the time evolution of the KE for the granular gas defined above and for the first 7×10^4 of 2×10^5 iteration steps. This time corresponds, on average, to 200 collisions per particle. The last figure illustrates the decay of the KE for different values of the restitution coefficient, and we can observe, as expected, that the cooling state is reached more rapidly as α is decreased. In Fig. 2(b) we give the time evolutions of $E(t)^{-1/2}$ for the different values of α used, and we show that these time evolutions do not obey Eq. (1) for long times. The best fitted curve we obtained for the time evolution of $1/\sqrt{E}$ is given by

$$E(t)^{-1/2} = a_2 \frac{(a_1 - a_2)}{1 + \exp\left(\frac{t - t_0}{a_3}\right)}, \quad (2)$$

This last result, which encloses those given in Fig. 1, suggests that the time evolution of the energy proposed by Eq. (1) has a limited validity. The important point to stress here is that the region where Eq. (1) is valid in our simulations corresponds to a state where, on average, the particles has experienced less than a collision. Therefore, we can reasonably assume that the system has not yet reached the homogeneous regime.

B. Velocity distributions

We analyzed the velocity distributions obtained from simulations performed for the granular gas described in Sec.

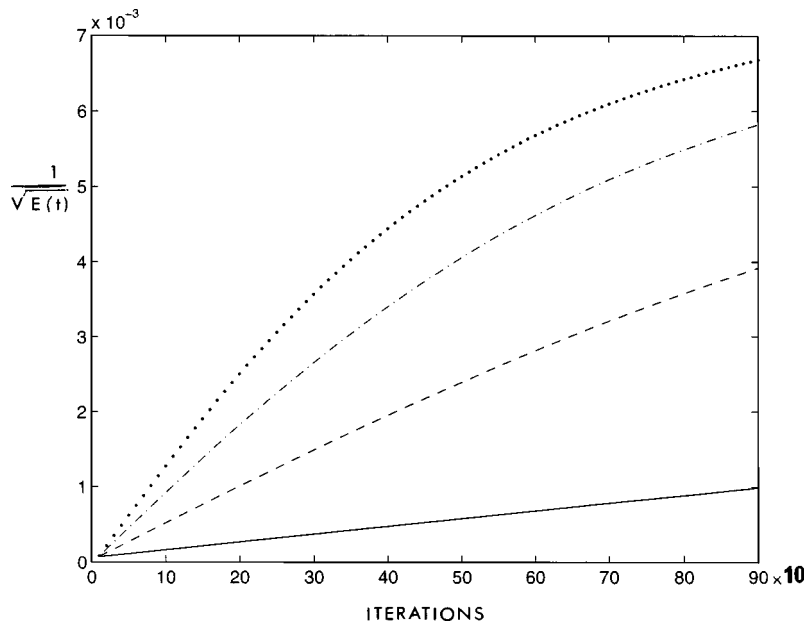


FIG. 1. Time evolution of $E^{-1/2}$ for values of the restitution coefficient varying from $\alpha=(0.7,0.98)$ for the first 900 iteration steps.

II A for $\alpha=(1.0,0.7)$. We considered the speed distribution $v=(v_x^2+v_y^2)^{1/2}$ and the v_x component of the velocity. Several simulations were performed by considering as initial conditions one of the three following initial velocity distribution functions: a Maxwellian, a Gaussian, and a constant distribution. We observed that these distributions led the granular gas to the same class of asymptotic velocity distribution. The results presented here used a constant initial velocity distribution with random initial positions and averaged over ten simulations. Figure 3(a) shows the speed distribution for an elastic granular gas which exhibits an excellent agreement with its corresponding Maxwell-Boltzmann (MB) distribution. For α in the range $(0.98,0.70)$ we obtained, instead of a Maxwellian, a distribution which can be assimilated to a Gaussian where the width of the distribution decreases as the inelasticity increases [Fig. 3(b)].

The analysis of the v_x distribution for $\alpha=1.0$ yields a Gaussian distribution [Fig. 4(a)] of the form

$$f(v_x)=y_0+\frac{A}{w\sqrt{(\pi/2)}}\exp\left(-2\left(\frac{v_x-v_c}{w}\right)^2\right). \quad (3)$$

A similar result was obtained for $\alpha=(0.98,0.70)$. In Fig. 4(b) we show that the width of the distribution decreases as the inelasticity increases. This last is in accordance with the results obtained for the speed. We believe that this decrease in the velocity range implies velocity correlations which should be included in the distribution function. A possibility to include these velocity correlations is detailed in the next sections.

III. HOMOGENEOUS STATE: EXACT RESULTS ON THE VELOCITY DISTRIBUTION

In this section we study theoretically the homogeneous regime of an inelastic hard sphere gas. Our objective is a complete specification of the velocity distribution for that state. The reason behind this analysis is twofold. The first is

related to the derivation of the kinetic equations for inelastic hard sphere gases. The second concerns the derivation of hydrodynamiclike equations for such systems. Indeed, in an inelastic gas not submitted to external forces or constraints there is no equilibrium distribution except the state of complete rest for all the particles. Thus hydrodynamic expansions like the Chapman-Enskog scheme must be reconsidered. Such an expansion must be performed around a velocity distribution valid in a locally homogeneous state. This means that the knowledge of an explicit solution for a complete homogeneous state is essential: It would provide the zero order distribution around which a gradient expansion may be performed. We show below that a promising answer to this question has been found [16]. More precisely, we find the complete set of moments for the reduced two-body distribution. This result is exact since it has been derived without any approximation from the complete Liouville equation for an inelastic hard sphere gas. The distribution function can be inferred from the infinite set of its moments under certain conditions on the parameters.

A. Liouville equation

We consider a gas of identical macroscopic spheres of finite radius interacting by inelastic and instantaneous collisions of restitution coefficient α ($0\leq\alpha\leq 1$). Each particle moves, between collisions, with constant velocity in a straight line motion. The collision takes place when the center of two particles are at a distance equal to the diameter a of a particle. The particles are smooth spheres, so that no change affects the projection of the relative velocity on the tangential plane at the contact point of the two colliding spheres. The construction of the pseudo-Liouville equation for inelastic hard spheres is quite similar to that for elastic collisions [2,10,17,18]. The only difference is the nonconservation of the phase space volume due to the inelasticity of the hard sphere collisions. This feature is taken into account in the collision term by the Jacobian of the phase-space transformation corresponding to the collision:

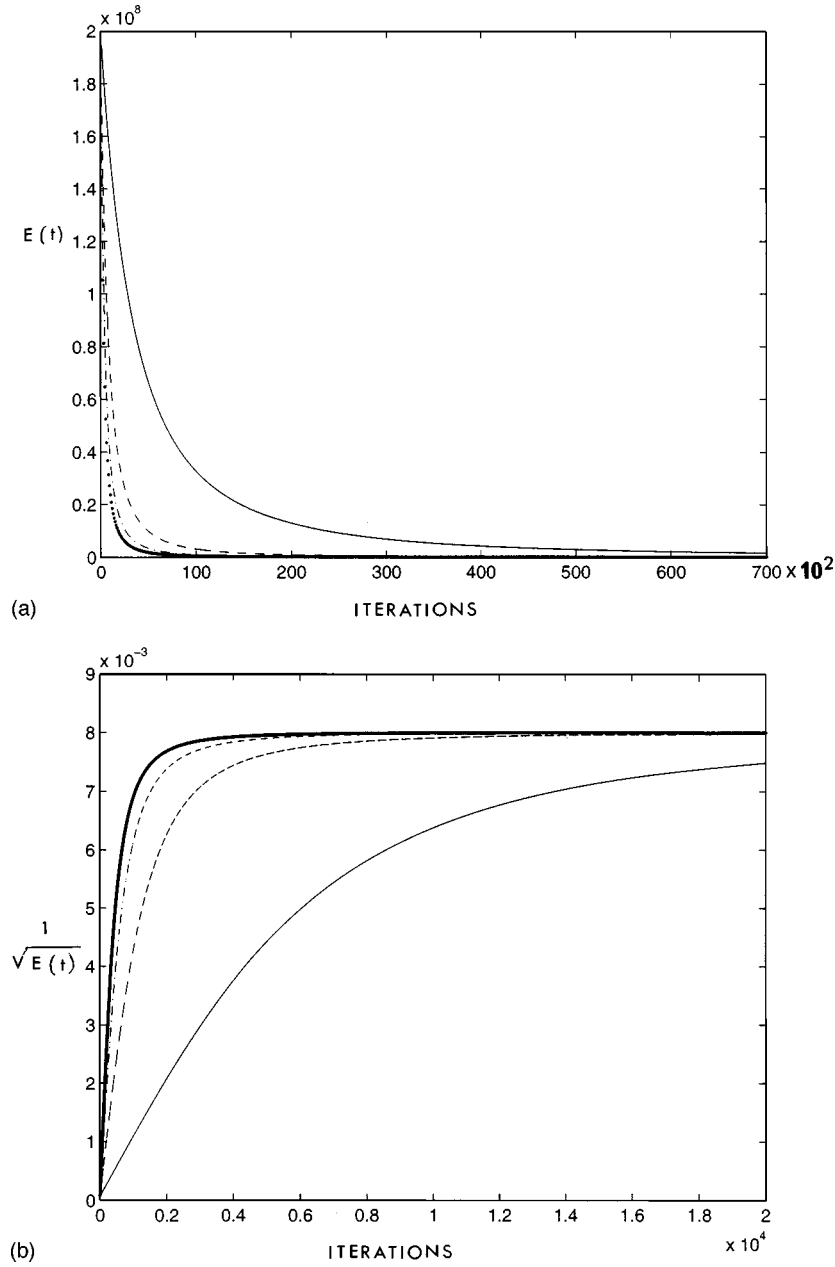


FIG. 2. (a) Time evolution of the kinetic energy (in Joules) for the first 7×10^4 iteration steps for $\alpha=0.98$ (continuous line), $\alpha=0.90$ (–), $\alpha=0.80$ (· –), and $\alpha=0.0$ (·). (b) Time evolution of $E^{-1/2}$ obtained from simulations for 2×10^4 iterations. The continuous bold line corresponds to $\alpha=0.7$, while the thin continuous line corresponds to $\alpha=0.98$.

$$\vec{v}'_i = \vec{v}_i - \left(\frac{1+\alpha}{2}\right) \vec{\epsilon}(\vec{\epsilon} \cdot \vec{v}_{ij}), \tag{4}$$

$$\vec{v}'_j = \vec{v}_j + \left(\frac{1+\alpha}{2}\right) \vec{\epsilon}(\vec{\epsilon} \cdot \vec{v}_{ij}), \tag{5}$$

where $\vec{\epsilon}$ is the unit vector along the direction from the center of particle j to the center of particle i , and the primed velocities represent the post-collision data. The relative velocity \vec{v}_{ij} is defined as

$$\vec{v}_{ij} = \vec{v}_i - \vec{v}_j.$$

Transformations (4) and (5) conserve the total momentum of the two particles, but their total kinetic energy decreases:

$$E' = E - \frac{m}{4}(1-\alpha^2)(\vec{\epsilon} \cdot \vec{v}_{ij})^2, \tag{6}$$

where m is the mass of a particle. With these remarks in mind, the Liouville equation can be written as

$$\frac{\partial \rho_N}{\partial t} + \sum_{i=1}^N \vec{v}_i \cdot \frac{\partial \rho_N}{\partial \vec{r}_i} = \frac{1}{2} \sum_{i,j=1}^N K^{(ij)} \rho_N, \tag{7}$$

where ρ_N is the N -body distribution function and the collision term for two particles i, j reads

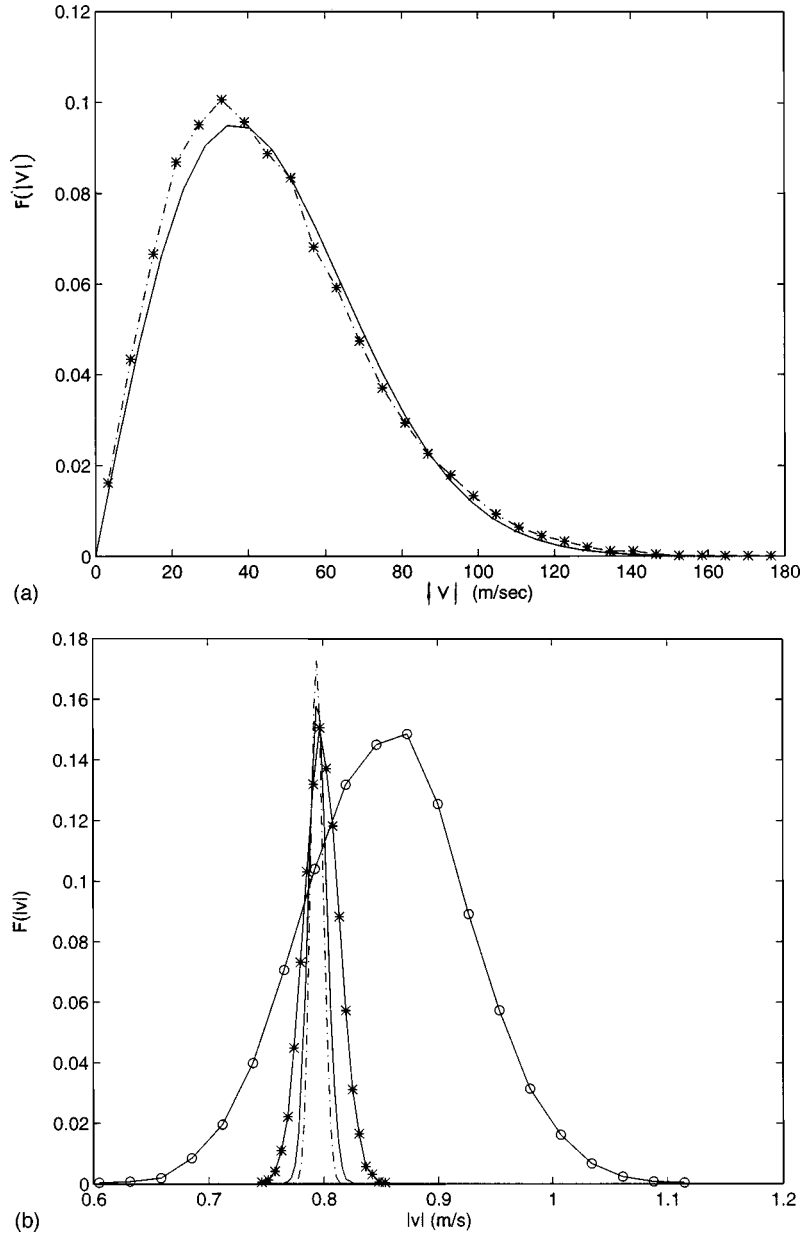


FIG. 3. (a) Comparison between the Maxwell-Boltzmann distribution of $v = (v_x^2 + v_y^2)^{1/2}$ (solid line) and the results obtained by simulations for $\alpha = 1.0$. (b) Speed distributions obtained for $\alpha = 0.98$ (O), $\alpha = 0.90$ (*), $\alpha = 0.8$ (-), and $\alpha = 0.7$ (-.).

$$\begin{aligned}
 K^{(ij)} \rho_N &= a^2 \int d^2 \epsilon (\vec{\epsilon} \cdot \vec{v}_{ij}) \Theta(\vec{\epsilon} \cdot \vec{v}_{ij}) \\
 &\times \left\{ \frac{1}{a^2} \delta(\vec{r}_{ij} - a \vec{\epsilon}) \rho_N(\{\vec{r}_k\}, \{\vec{v}_k\}_{k \neq i, j}, \vec{v}'_i, \vec{v}'_j) \right. \\
 &\left. - \delta(\vec{r}_{ij} + a \vec{\epsilon}) \rho_N(\{\vec{r}_k\}, \{\vec{v}_k\}) \right\} \quad (8)
 \end{aligned}$$

and where $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$, \vec{v}'_i and \vec{v}'_j are given by Eqs. (4) and (5). Here we do not give the proof of this result since a similar equation has been recently obtained independently by Brey, Dufty, and Santos [2].

B. Liouville equation for the HCR

For a spatially homogeneous state such as the HCR the distribution ρ_N depends only on the relative positions \vec{r}_{ij} . Hence, the free flow term of Eq. (7) is replaced by

$$\frac{1}{2} \sum_{i, j=1}^N \vec{v}_{ij} \cdot \frac{\partial \rho_N}{\partial \vec{r}_{ij}}.$$

By integrating over the positions and velocities of $N-1$ particles, Eq. (7) leads to an equation for the one-body distribution f_1 which reads

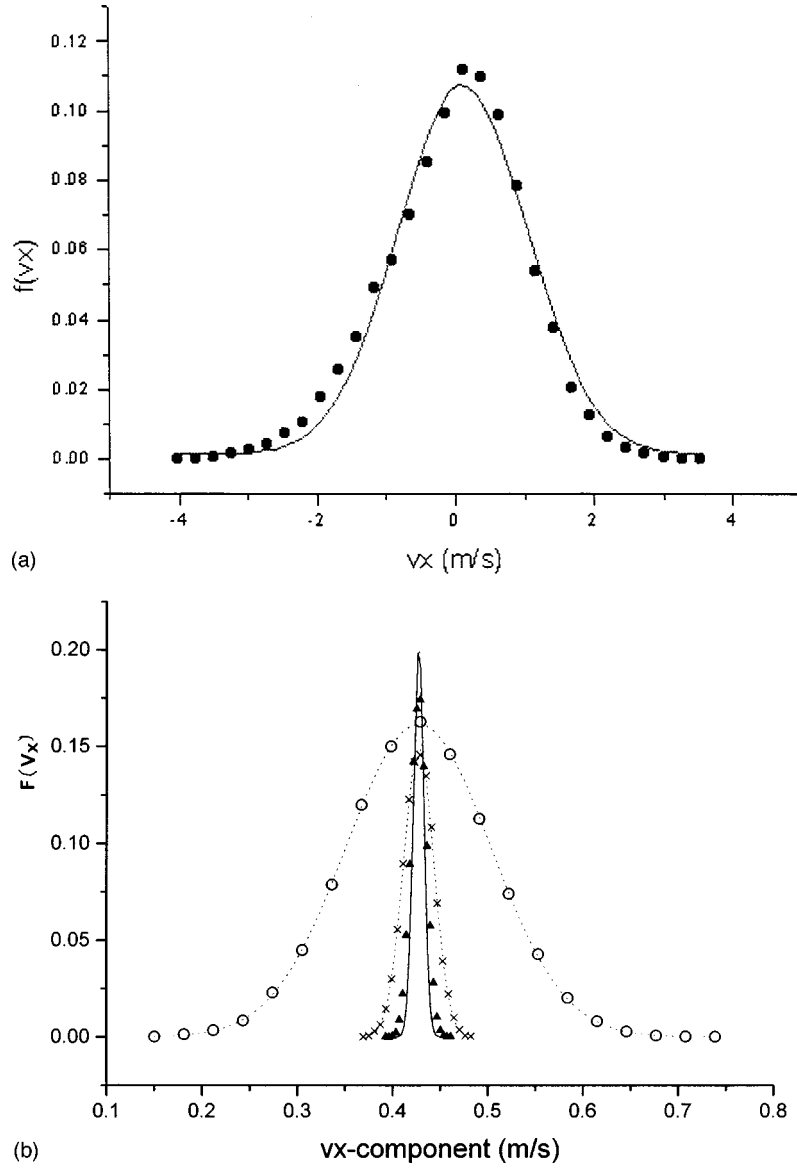


FIG. 4. v_x distributions and fitted curves (dashed line) for $\alpha=0.98$ (\circ), $\alpha=0.90$ (*), $\alpha=0.8$ (triangle), and $\alpha=0.7$ (solid line).

$$\begin{aligned} \frac{\partial f_1(\vec{v}_1, t)}{\partial t} = & a^2 \int d^3 \vec{v}_2 \int d^2 \vec{\epsilon} (\vec{\epsilon} \cdot \vec{v}_{12}) \Theta(\vec{\epsilon} \cdot \vec{v}_{12}) \\ & \times \left(\frac{1}{\alpha^2} f_2(\vec{r}_1, \vec{r}_1 - a \vec{\epsilon}, \vec{v}'_1, \vec{v}'_2) \right. \\ & \left. - f_2(\vec{r}_1, \vec{r}_1 + a \vec{\epsilon}, \vec{v}_1, \vec{v}_2) \right). \end{aligned} \quad (9)$$

In the collision term of this reduced equation appears the two-body distribution f_2 which, in turn, obeys an equation whose collision term contains f_3 . In this way, an infinite BBGKY hierarchy of equations is generated for the reduced distribution functions of growing order. For dilute gases of elastic hard spheres, this hierarchy is truncated by the molecular chaos assumption which, in a few words, amounts to factorizing f_2 into $f_1 f_1$. This factorization implies the smallness of the velocity correlations. However, for inelastic hard sphere gases, numerical simulations show the existence of

attractors in phase space [3,4]. Such attractors imply non-trivial velocity correlations. Henceforth, we believe that the above truncation hypothesis should be carefully revised.

C. An exact result for the HCR two-body distribution

First, let us show that although the kinetic energy is not conserved in the collision of two particles, there remains a part of that energy which is invariant. To show this, we introduce the center of mass velocity of the two particles,

$$\vec{u}_{12} = \frac{\vec{v}_1 + \vec{v}_2}{2}, \quad (10)$$

along the relative velocity \vec{v}_{12} already defined above. The latter may be projected along the unit vector $\vec{\epsilon}$ which lies on the direction from the center of particle 2 to the center of particle 1:

$$\vec{v}_{12} = \vec{\gamma} + \vec{\epsilon} g, \quad (11)$$

with

$$\vec{\gamma} = (I - \vec{\epsilon} \times \vec{\epsilon}) \cdot \vec{v}_{12} \quad (12)$$

and

$$g = \vec{\epsilon} \cdot \vec{v}_{12}. \quad (13)$$

The definitions of \vec{u}_{12} and \vec{v}_{12} , allow us to write

$$\vec{v}_1 = \vec{u}_{12} + \frac{\vec{v}_{12}}{2}, \quad (14)$$

$$\vec{v}_2 = \vec{u}_{12} - \frac{\vec{v}_{12}}{2}. \quad (15)$$

Thus we can write

$$\vec{v}_1 = \vec{u}_{12} + \frac{\vec{\gamma} + \vec{\epsilon}g}{2}, \quad (16)$$

$$\vec{v}_2 = \vec{u}_{12} - \frac{\vec{\gamma} + \vec{\epsilon}g}{2}. \quad (17)$$

When Eqs. (16) and (17) are inserted into $E = (m/2)(v_1^2 + v_2^2)$, one obtains

$$E = m \left(u_{12}^2 + \frac{\gamma^2}{4} + \frac{g^2}{4} \right), \quad (18)$$

where we have used the fact that $\vec{\gamma}$ is orthogonal to $\vec{\epsilon}g$. However,

$$E_0 = m(u_{12}^2 + \gamma^2/4), \quad (19)$$

is invariant in the inelastic collision. Indeed, \vec{u}_{12} is the center of mass velocity which is proportional to the total momentum of the two particles. The latter and the kinetic energy of the center of mass are invariants, as can be seen from Eqs. (4) and (5). For $\vec{\gamma}$, its value after collision is

$$\vec{\gamma}' = (I - \vec{\epsilon}' \times \vec{\epsilon}') \cdot \vec{v}'_{12}. \quad (20)$$

More explicitly, we have

$$\vec{\gamma}' = (I - \vec{\epsilon}' \times \vec{\epsilon}') \cdot [\vec{v}_{12} - (1 + \alpha)\vec{\epsilon}(\vec{\epsilon} \cdot \vec{v}_{12})], \quad (21)$$

and, by using

$$(I - \vec{\epsilon}' \times \vec{\epsilon}') \cdot \vec{\epsilon} = 0, \quad (22)$$

we obtain

$$\vec{\gamma}' = \vec{\gamma}. \quad (23)$$

A glance at Eq. (18) shows that the kinetic energy may be decomposed as $E = E_0 + E_1$, with

$$E_1 = \frac{m}{4} g^2. \quad (24)$$

The variation of E_1 after collision is given by

$$E'_1 = \frac{m}{4} g'^2 \quad (25)$$

or, equivalently,

$$E'_1 = \frac{m}{4} (\vec{\epsilon}' \cdot \vec{v}'_{12})^2, \quad (26)$$

with

$$(\vec{\epsilon}' \cdot \vec{v}'_{12}) = \vec{\epsilon}' \cdot (\vec{v}_{12} - (1 + \alpha)\vec{\epsilon}(\vec{\epsilon} \cdot \vec{v}_{12})). \quad (27)$$

Using the fact that $\vec{\epsilon}$ is a unit vector, one obtains

$$g' = -\alpha g, \quad (28)$$

and finally we obtain

$$E'_1 - E_1 = -\frac{m}{4} (1 - \alpha^2) g^2. \quad (29)$$

The above decomposition of E suggests that the time evolution of the HCR is essentially due to the variation of the successive moments of the quantity g [see Eq. (13)]. In fact, as we show next, these moments obey an exact infinite hierarchy of equations independently of the moments of the other phase-space variables of the system. This is readily proved by computing the time evolution of the successive moments of $|g|$ (see the Appendix for the detailed demonstration):

$$x_k = \langle |g|^k \rangle. \quad (30)$$

Using the Liouville equation (7), for the HCR and integrating over all space variables, one readily obtains an expression depending only on the two-body distribution. This is due to the fact that g is a two-body phase-space quantity. Next a change of variables to the center of mass and to the relative positions and velocities leads, after some simple but tedious algebra, to the hierarchy

$$\frac{\partial x_k}{\partial t} = 2\pi n a^2 (\alpha^k - 1) x_{k+1} \quad (31)$$

for any integer value of k . These last equations are an exact consequence of the Liouville equation. To our knowledge, these equations constitute a new result. This difference-differential equation can be exactly solved by calculating the Taylor series of x_k in time. The recursion relation between successive time derivatives generated by this equation enables us to derive the exact general term of the above Taylor series. The derivation is straightforward, and one obtains the solution

$$x_k(t) = \sum_{l=0}^{\infty} \frac{[2\pi(\alpha-1)na^2t]^l [k+l-1]!}{l! [k-1]!} x_{k+l}(0), \quad (32)$$

where

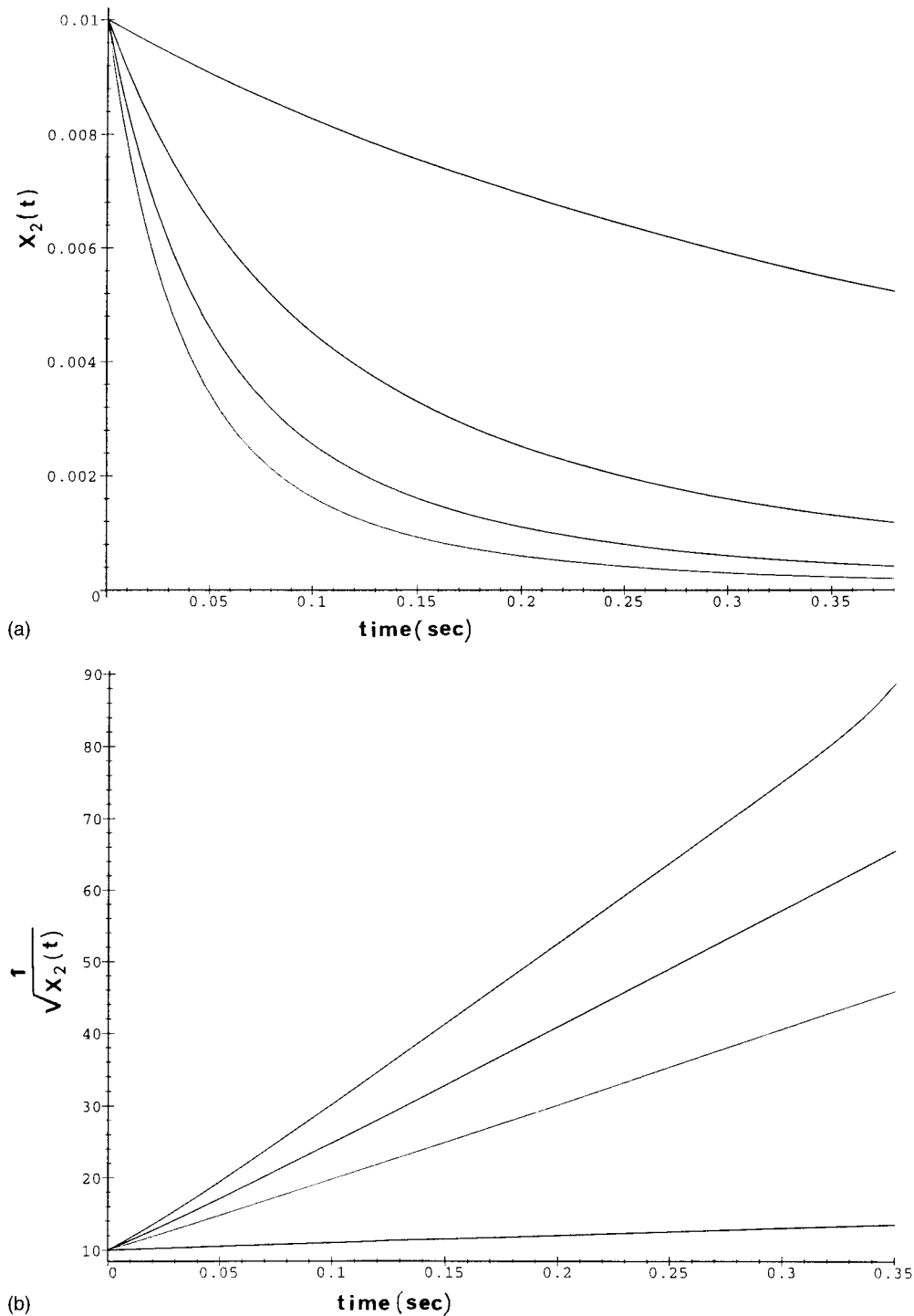


FIG. 5. (a) Time dependence for $x_2(t)$ and for $\sqrt{x_2(t)}$ in arbitrary units of time for $\alpha=0.98, 0.90, 0.80, 0.70$, and 0.60 . In (a) the closest curve to the x axis corresponds to $\alpha=0.6$, and the upper curve was obtained for $\alpha=0.98$. In (b) the nearest curve to the x axis corresponds to $\alpha=0.98$, and the upper curve corresponds to $\alpha=0.6$.

$$[k]! = \prod_{l=1}^k \left(\frac{\alpha^l - 1}{\alpha - 1} \right) \quad (33)$$

is the q factorial of k [19] for $q = \alpha$. The above solution is valid for any $k \geq 1$. Clearly, the above series have generally a finite radius of convergence since $\alpha < 1$.

Let us analyze more closely the series giving the moment $x_2(t)$. Generally, for a large set of initial conditions, the series has a finite radius of convergence. However, this con-

vergence is very slow. This is perhaps due to singularities in the complex plane of the time which cannot be detected directly from the Taylor series. Hence an excessively large number of terms is needed to obtain the correct long time behavior of $x_2(t)$. In Fig. 5 we give the curves for $x_2(t)$ and $1/\sqrt{x_2(t)}$ obtained with our series. These curves should be compared with our simulation results (see Fig. 1) and the theoretical results of Ref. [2]. It can be seen that our curves agree with those of Ref. [2] for a short time. However, in

order to compare the behavior for larger times, some convergence acceleration algorithm, such as Shanks transformation or Padé summation, should be applied to our series. Furthermore, analytical methods may be envisaged to find the asymptotic behavior of the function defined by our series, such as the Borel integral summation. This analysis needs some time to be developed, and will be presented in a further publication. Nevertheless, an important point that can be clarified already at this level of our work is the following: it can be shown, without ambiguity, that our series [Eq. (32)] gives, for values of α near 1, the equation proposed in Ref. [2] [see Eq. (43), given in Sec. IV]. This can be demonstrated in the following way. Equations (32) and (33) give, for $k=2$,

$$x_2(t) = \sum_{l=0}^{\infty} [2\pi(\alpha-1)na^2t]^l \frac{[1+l]!}{l![1]!} x_{2+l}(0). \quad (34)$$

For α near 1, the α factorial behaves like the factorial

$$\lim_{\alpha \rightarrow 1} [n]! = n! \quad (35)$$

since

$$[n]! \equiv \prod_{m=1}^n \left(\frac{\alpha^m - 1}{\alpha - 1} \right)$$

and

$$\lim_{\alpha \rightarrow 1} \left(\frac{\alpha^m - 1}{\alpha - 1} \right) = m.$$

Thus Eq. (34) may, for $\alpha \approx 1$, be rewritten as

$$x_2(t) = \sum_{l=0}^{\infty} [2\pi(\alpha-1)na^2t]^l (1+l) x_{2+l}(0). \quad (36)$$

Let us consider initial moment of the form

$$x_{2+l}(0) = \sigma_0^{2+l}, \quad (37)$$

with σ_0 a positive real number. Hence Eq. (36) becomes

$$x_2(t) = \sigma_0^2 \sum_{l=0}^{\infty} [2\pi(\alpha-1)na^2\sigma_0 t]^l (1+l), \quad (38)$$

which can be readily summed to yield

$$x_2(t) = \frac{\sigma_0^2}{(1 + 2\pi|\alpha-1|na^2\sigma_0 t)^2}. \quad (39)$$

This expression is comparable to the result of Ref. [2] for $T(t)$ [Eq. (43) given below], provided

$$\tau = \frac{1}{2\pi|\alpha-1|na^2\sigma_0}. \quad (40)$$

Thus, as a by product, we have obtained an analytic form for the characteristic time of the dissipative decay of energy. It is

already satisfying to remark that it depends on the initial state σ_0 but, it is important to notice, as expected, that it diverges for $\alpha=1$.

IV. CONCLUSIONS

The simulations presented here extend over a large range of inelasticity strength α . For most values of this last parameter we observed that the time evolution of the average kinetic equation is not that proposed by Eq. (43). Our theoretical results confirm this result (see Fig. 5). However, more systematic and quantitative verifications of these statements should be carried out.

Having in hand the exact set of moments of $|g|$ for the two-body HCR distribution function, we are now in a position to build the distribution function and to study its asymptotic behavior. Since these last calculations are still in progress, we conclude with the following remarks. First, the decomposition of E into an invariant part E_0 and a variable part E_1 indicates that a complete f_2 function, built as a product of an arbitrary function of E_0 and a function of g with its moments given by Eq. (32), is a solution of the Liouville equation. Such a two-body distribution is clearly not factorizable into two f_1 functions. Henceforth, velocity correlations are not negligible. Second, the f_2 distribution, with moments given by Eq. (32), is very unlikely to be a Gaussian for low values of α . Third, the evolution equation for the granular temperature,

$$T = \frac{2}{3nk_B} \langle E \rangle, \quad (41)$$

which is quoted by most of the authors (see Refs. [3,7,8]) has a limited validity. The corresponding evolution equation reads

$$\frac{\partial T(t)}{\partial t} = -\frac{2}{3nk_B} (1-\alpha^2) WT^{3/2}, \quad (42)$$

where W is independent of the temperature and is an integral over a rescaled two-body distribution. The parameter n represents the density and k_B is the Boltzmann constant. Equation (42) can be solved in terms of the initial conditions

$$T(t) = T(0) \left(1 + \frac{t}{\tau} \right)^{-2}, \quad (43)$$

where τ is a characteristic time constant depending on α and W . Moreover, Eq. (42) may be obtained from Eqs. (31) for $k=2$ by assuming a factorization of x_3 into x_2x_1 . Thus, the time dependence of $T(t)$ given by Eq. (43) is an approximation whose validity domain should be explored by comparing it with the exact time dependence given by Eq. (32). As far as this is concerned, the simulations reported above exhibit in some cases strong deviations with respect to Eq. (32). We think our results call into question the classical assumptions of molecular chaos and of the generality of the Gaussian shape for the asymptotic distribution when we study an inelastic granular gas. Finally, we hope our results will help to clarify these fundamental problems.

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APPENDIX: DERIVATION OF THE RECURSION EQUATION FOR THE MOMENTS $\langle |g|^{2k} \rangle$

Let us consider the moments $\langle |g_{12}|^{2k} \rangle$ where

$$g_{12} = \frac{(\vec{r}_1 - \vec{r}_2) \cdot (\vec{v}_1 - \vec{v}_2)}{|\vec{r}_1 - \vec{r}_2|}.$$

We compute them for any positive integer k with the exact distribution

$$\rho_N(\vec{r}_1, \dots, \vec{r}_N, \vec{v}_1, \dots, \vec{v}_N; t),$$

which is a solution of the Liouville equation [Eq. (10)]. That is,

$$\langle |g_{12}|^{2k} \rangle = \int d^3 r_1 \cdots d^3 v_N |g_{12}|^{2k} \rho_N(t), \quad (\text{A1})$$

which obeys the following equation for a spatially homogeneous state:

$$\begin{aligned} \frac{\partial}{\partial t} \langle |g_{12}|^{2k} \rangle = & - \int d^3 r_1 \cdots d^3 v_N |g_{12}|^{2k} \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N (\vec{v}_i - \vec{v}_j) \cdot \left(\frac{\partial}{\partial \vec{r}_i} - \frac{\partial}{\partial \vec{r}_j} \right) \rho_N(t) \\ & + \frac{a^2}{2} \int d^3 r_1 \cdots d^3 v_N |g_{12}|^{2k} \int d^2 \epsilon \sum_{i=1}^N \sum_{j=1}^N \vec{\epsilon} \cdot \vec{v}_{i,j} \Theta(\vec{\epsilon} \cdot \vec{v}_{i,j}) \\ & \times \left\{ \frac{1}{a^2} \delta(\vec{r}_{i,j} - a \vec{\epsilon}) \rho_n(\vec{r}_1, \dots, \vec{r}_N, \vec{v}_1, \dots, \vec{v}_i', \vec{v}_j', \dots, \vec{v}_N; t) \right. \\ & \left. - \delta(\vec{r}_{i,j} + a \vec{\epsilon}) \rho_n(\vec{r}_1, \dots, \vec{r}_N, \vec{v}_1, \dots, \vec{v}_N; t) \right\}. \end{aligned} \quad (\text{A2})$$

The first term on the right-hand side of the above equation corresponds to the free flow of the two particles 1 and 2, and gives a vanishing contribution to $(\partial/\partial t) \langle |g_{12}|^{2k} \rangle$. This last is easily shown as follows; let us denote the free flow term by Φ . Then it reads

$$\Phi = - \int d^3 r_1 d^3 r_2 d^3 v_1 d^3 v_2 |\hat{r}_{12} \cdot \vec{v}_{12}|^k \vec{v}_{12} \cdot \vec{\nabla}_{12} f_2,$$

and an integration by parts gives

$$\Phi = \int d^3 r_1 d^3 r_2 d^3 v_1 d^3 v_2 f_2 \vec{v}_{12} \cdot \vec{\nabla}_{12} |\hat{r}_{12} \cdot \vec{r}_{12}|^k,$$

where \hat{r}_{12} denotes the unit vector along \vec{r}_{12} . The gradient yields

$$\Phi = k \int d^3 r_1 d^3 r_2 d^3 v_1 d^3 v_2 |\hat{r}_{12} \cdot \vec{v}_{12}|^{k-1} f_2 \vec{v}_{12} \cdot \vec{\nabla}_{12} |\hat{r}_{12} \cdot \vec{v}_{12}|$$

where an easy calculation for the gradient leads to:

$$\begin{aligned} \vec{v}_{12} \cdot \vec{\nabla}_{12} |\hat{r}_{12} \cdot \vec{v}_{12}| &= \frac{1}{|\vec{r}_{12}|} \{ |v_{12}|^2 \operatorname{sgn}(\hat{r}_{12} \cdot \vec{v}_{12}) \\ & - (\hat{r}_{12} \cdot \vec{v}_{12}) |\hat{r}_{12} \cdot \vec{v}_{12}| \}. \end{aligned}$$

Hence, the free flow term can be written as

$$\begin{aligned} \Phi &= k \int d^3 r_1 d^3 r_2 d^3 v_1 d^3 v_2 f_2(\vec{r}_1, \vec{r}_2, \vec{v}_1, \vec{v}_2) \\ & \times \frac{1}{|\vec{r}_{12}|} |g_{12}|^{k-1} \{ (g_{12}^2 + \gamma_{12}^2) \operatorname{sgn}(g_{12}) - g_{12} |g_{12}| \} = 0, \end{aligned}$$

in which we used the fact that

$$|v_{12}|^2 = g_{12}^2 + \gamma_{12}^2.$$

It can be easily seen that the integrand is odd in the variable g_{12} if f_2 is supposed even in that variable, which is a natural assumption for a homogeneous state. Thus the free flow term vanishes because the integration over \vec{v}_1 and \vec{v}_2 includes an integral over g_{12} from $-\infty$ to $+\infty$. The second term on the right-hand side of Eq. (A2) provides the contribution of collisions to the time evolution of $\langle |g_{12}|^{2k} \rangle$. Three types of contributions appear in that term. The first corresponds to $i=1, j=2$ or $i=2, j=1$. The second appears for $i=1$ and $j \neq 1$ and 2 and permutation of i and j . Finally, the third case corresponds to i and $j \neq 1$ and 2. Let us start with the first contribution, $i=1, j=2$ (or the converse). Thus we can write

$$K_{12} = \frac{a^2}{2} \int d^3 r_1 \cdots d^3 r_N d^3 v_1 \cdots d^3 v_N |g_{12}|^k \int d^2 \epsilon \vec{\epsilon} \cdot \vec{v}_{12} \Theta(\vec{\epsilon} \cdot \vec{v}_{12}) \times \left\{ \frac{1}{\alpha^2} \delta(\vec{r}_{12} - a\vec{\epsilon}) \rho(\{\vec{r}\}, \vec{v}'_1, \vec{v}'_2, \vec{v}_3, \dots, \vec{v}_n; t) - \delta(\vec{r}_{12} + a\vec{\epsilon}) \rho_N(\{\vec{r}\}, \{\vec{v}\}; t) \right\}. \quad (\text{A3})$$

The integration of the last equation over the variables $\vec{r}_3, \dots, \vec{r}_N$, and $\vec{v}_3, \dots, \vec{v}_N$, which act directly on ρ_N , gives

$$\frac{\vec{r}_1 + \vec{r}_2}{2} = \vec{R}_{12},$$

$$K_{12} = \frac{a^2}{2} \int d^3 r_1 d^3 r_2 d^3 v_1 d^3 v_2 |g_{12}|^k \int d^2 \epsilon \vec{\epsilon} \cdot \vec{v}_{12} \Theta(\vec{\epsilon} \cdot \vec{v}_{12}) \times \left\{ \frac{1}{\alpha^2} \delta(\vec{r}_{12} - a\vec{\epsilon}) f_2(\vec{v}_1, \vec{r}_2, \vec{v}'_1, \vec{v}'_2; t) - \delta(\vec{r}_{12} + a\vec{\epsilon}) f_2(\vec{r}_1, \vec{r}_2, \vec{v}_1, \vec{v}_2; t) \right\}.$$

with a Jacobian equal to 1, and

$$\vec{v}_1 - \vec{v}_2 = \vec{v}_{12},$$

$$\frac{\vec{v}_1 + \vec{v}_2}{2} = \vec{u}_{12},$$

Now, by performing the transformations

$$\vec{r}_1 - \vec{r}_2 = \vec{r}_{12},$$

followed by the decomposition of \vec{v}_{12} into its projections g_{12} on $\vec{\epsilon}$ and γ_{12} on the plan orthogonal to $\vec{\epsilon}$, one obtains, after integrating over the variables \vec{R}_{12} and \vec{u}_{12} ,

$$K_{12} = \frac{a^2}{2} \int d^2 \hat{r}_{12} \int_{-\infty}^{\infty} dg_{12} \int d^2 \gamma_{12} |g_{12}|^{k+1} \left\{ \frac{1}{\alpha^2} \Theta(-g_{12}) \phi_2(\hat{r}_{12}, g'_{12}; t) - \Theta(g_{12}) \phi_2(\hat{r}_{12}, g_{12}; t) \right\}, \quad (\text{A4})$$

where ϕ_2 is the two-body distribution reduced over \vec{R}_{12} and \vec{u}_{12} . Now, since we know from the binary collision law that

$$g_{12} = -\alpha g'_{12},$$

we can insert this relation into Eq. (A4) and obtain, after a simplification of powers of α and a grouping of terms,

$$K_{12} = \frac{a^2}{2} (\alpha^k - 1) \int d^2 \hat{r} \int_0^{\infty} dg_{12} |g_{12}|^{k+1} \phi(\hat{r}_{12}, g_{12}; t),$$

which finally gives

$$K_{12} = 2\pi n a^2 (\alpha^k - 1) \langle |g_{12}|^{k+1} \rangle. \quad (\text{A5})$$

For the second type of contribution ($i=1$ and 2 and $j \neq 1$ and 2 , or the converse) on the right-hand side of Eq. (A2), we proceed as follows. For example, let us assume $i=1$ and $j=3$. Then the term to analyze is

$$K_{123} = \frac{a^2}{2} \int d^3 r_1 \cdots d^3 r_N d^3 v_1 \cdots d^3 v_N |g_{12}|^k \int d^2 \epsilon \vec{\epsilon} \cdot \vec{v}_{13} \Theta(\vec{\epsilon} \cdot \vec{v}_{13}) \times \left\{ \frac{1}{\alpha^2} \delta(\vec{r}_{13} - a\vec{\epsilon}) \rho_N(\vec{r}_1, \dots, \vec{r}_N, \vec{v}_1, \dots, \vec{v}'_1, \vec{v}_2, \vec{v}'_3, \dots, \vec{v}_N; t) - \delta(\vec{r}_{13} + a\vec{\epsilon}) \rho_N(\{\vec{r}\}, \{\vec{v}\}; t) \right\}. \quad (\text{A6})$$

Proceeding along the same lines as in the previous case ($i = 1, j = 2$), we can replace the variables $\vec{r}_1, \vec{r}_2,$ and \vec{r}_3 by the center of mass positions $R_{123}, \vec{v}_1, \vec{v}_2,$ and \vec{v}_3 by the center of mass velocity \vec{u}_{123} , and their corresponding relative velocities \vec{v}_{12} and \vec{v}_{13} and relative positions \vec{r}_{12} and \vec{r}_{13} . Afterward we perform the integrals over all the other variables with the exception of $\vec{r}_{12}, \hat{r}_{13}, g_{12},$ and g_{13} . This leads to

$$K_{123} = \frac{a^2}{2} \int d^3 r_{12} d^2 \hat{r}_{13} d g_{12} d g_{13} |g_{12}|^k g_{13} \times \left\{ \frac{1}{\alpha^2} \Theta(-g_{13}) f_3(\vec{r}_{12}, \hat{r}_{13}, g'_{12}, g'_{13}; t) - \Theta(g_{13}) f_3(\vec{r}_{12}, \hat{r}_{13}, g_{12}, g_{13}; t) \right\} \quad (\text{A7})$$

Here again we have decomposed the velocities \vec{v}_{12} and \vec{v}_{13} into g_{12} and $\vec{\gamma}_{12}$, and g_{13} and $\vec{\gamma}_{13}$, respectively, and we also integrated over $\vec{\gamma}_{12}$ and $\vec{\gamma}_{13}$. By the collision rules we have that

$$g_{13} = -\alpha g'_{13}. \quad (\text{A8})$$

Now, by using Eqs. (4) and (5) for particles 1 and 3 with Eq. (A8), we obtain that

$$g_{12} = g'_{12} - \left(\frac{1+\alpha}{2} \right) \hat{r}_{12} \cdot \hat{r}_{13} g'_{13}. \quad (\text{A9})$$

Moreover, by inserting Eqs. (A8) and (A9) into Eq. (A7), we obtain a factor in the integrand of Eq. (A7) of the form

$$\left| g'_{12} - \left(\frac{1+\alpha}{2} \right) \hat{r}_{12} \cdot \hat{r}_{13} g'_{13} \right|^k g'_{13}, \quad (\text{A10})$$

which can be rewritten as follows:

$$\left| g'_{12} - \left(\frac{1+\alpha}{2} \right) \hat{r}_{12} \cdot \hat{r}_{13} \hat{r}_{13} \cdot \vec{v}'_{13} \right|^k \hat{r}_{13} \cdot \vec{v}'_{13}.$$

The absolute value factor is clearly even in \hat{r}_{13} . Hence the whole expression is odd in that variable. This leads us to claim that the integrand appearing in Eq. (A7) is odd in \hat{r}_{13} provided that f_3 be even in g_{13} . Henceforth, the integral over \hat{r}_{13} involved in Eq. (A7) vanishes. For the third type of contribution (i and j different from 1 and 2) it is straightforward to show that it vanishes. Indeed, the integrations over all the variables except those attached to particles 1 and 2 may first be performed. Using the velocities after and before collisions, it can be seen directly that all these terms are identically zero by the same reasoning as that leading to the conservation of the norm of the distribution. Thus, we have established the differential difference [Eq. (31)] for the moments $\langle |g_{12}|^k \rangle$.

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