

# Collision properties of one-dimensional granular particles with internal degrees of freedom

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(Received 18 June 1996)

Starting from a microscopic model of interacting elastic rods, we derive an effective dissipative dynamics for the translational motion, where the internal degrees of freedom, i.e., the vibrations of the rods, are represented by a thermalized bath. Focusing on two-particle collisions, we calculate the coefficient of restitution  $\epsilon$  as a function of the relative length of the colliding rods, the center of mass velocity, and the degree of excitation of the internal vibrations. In general,  $\epsilon$  is a stochastic quantity; its distribution is interpreted as the transition probability for the Markovian jump process, which describes the loss of translational energy in successive two-particle collisions. [S1063-651X(96)12111-5]

PACS number(s): 05.20.-y, 05.40.+j, 46.30.My

## I. INTRODUCTION

Inelastic collisions of particles with internal degrees of freedom are abundant in nature. Examples are molecules with vibrational and rotational states or elastic bodies, which allow for elastic and plastic deformations. In all these processes energy of translation is lost to internal degrees of freedom. For oscillations, like elastic waves or molecular vibrations, one would expect that the transfer of energy is at least partially reversible, whereas the energy is irreversibly lost for the translational motion, if defects are generated. There is a wide range of particle sizes involved: a few atoms in a molecule, clusters of about  $10^6$  molecules in a soot or dust particle, up to truly macroscopic grains, like sand or gravel.

In recent years inelastic collisions have found renewed interest in the context of granular materials. Numerical and theoretical approaches to the dynamics of granular materials are usually based on phenomenological equations of motion for the center of mass velocities of the grains. This phenomenological ansatz has revealed surprisingly rich behavior of granular material with many fascinating features, such as surface fluidization, granular condensation, size aggregation, arching—to mention just a few. Despite a lot of activity in this field, very little effort has been put into a systematic derivation of the phenomenological equations from a microscopic theory. Instead a variety of phenomenological models is used, each with its particular strength and its limitations. For example, molecular-dynamics simulations [1] have the difficulty that *ad hoc* assumptions about microscopic interaction laws have to be made. An inadequate choice of the interaction parameters can lead [2] to spurious effects in the simulations. Other simulation techniques adopt the concept of the coefficient of restitution that determines the energy loss during collisions of granular particles. Event-driven (ED) simulations [3–6] have shown that model systems with a *fixed* coefficient of restitution evolve into clustered states where a hydrodynamic description ceases to be correct: Fundamental assumptions of hydrodynamics concerning the validity of molecular chaos and local equilibrium are violated [7]. The frequency of collisions diverges, so that the algorithm breaks down.

In this paper we aim at a *microscopic derivation* of the effective dissipative dynamics of the center-of-mass veloci-

ties of granular particles. A summary of our results has previously been published in Ref. [8]. We emphasize that our approach focuses on granular materials in the “grain inertia” regime [9], where the dynamics is dominated by inelastic collisions. Typical examples are fluidized surfaces, rapid granular flow, and the condensation of a granular gas. (We mainly refer to the latter in the following.) At this stage we have not incorporated frictional forces. Phenomena such as size aggregation and arching, for which static and dynamic friction become relevant (“quasistatic” regime), are therefore beyond the scope of the present analysis.

We start from a one-dimensional model of elastic rods. Colliding rods interact via a short-range repulsive potential. Upon collision, kinetic energy of translation is lost to the internal vibrations. Equipartition among the vibrational modes is found to be fast as compared to the relaxation of translational motion. Hence for a discussion of the cooling properties of the granular gas we model the internal oscillators by a bath temperature  $T_B$  and study in detail how energy is transferred from the translational to the internal degrees of freedom. We focus on the coefficient of restitution for inelastic two-particle collisions, expressed in terms of the parameters of the microscopic model. The principal results are as follows.

(1) In the deterministic limit ( $T_B=0$ ) we find  $\epsilon = \min(\gamma, 1/\gamma)$  with  $\gamma$  the ratio of lengths of the two colliding rods. This result is in agreement with the phenomenological wave theory. We calculate corrections due to the finite range of the potential. For a potential of small but finite range the coefficient of restitution is found to depend on the initial relative velocity, with  $\epsilon \rightarrow 1$  as the velocity goes to zero.

(2) In the general case, when  $T_B \neq 0$ , the coefficient of restitution is a stochastic quantity, whose distribution we calculate numerically. Its variance depends on the ratio of  $T_B$  to the energy of translation and on the length ratio  $\gamma$  (with the fluctuations going to zero for  $\gamma \rightarrow 1$ ).

We use a Hamiltonian approach to describe the loss of energy of translation by excitation of internal degrees of freedom. Implicit in such a Hamiltonian model is, of course, overall energy conservation. The final state after many collisions is trivial: It is characterized by equipartition among all degrees of freedom, so that the velocity of translation is typi-

cally of  $O(1/N_{mod})$ , where  $N_{mod}$  denotes the number of internal degrees of freedom per particle. We focus here on the *cooling* properties, i.e., the relaxation of a typical initial velocity of translation of  $O(1)$  to its final value of  $O(1/N_{mod})$ . One could possibly extend our approach to include dissipation of internal vibrations due to nonlinear interactions or by transfer to still other degrees of freedom. This would give rise to a decay of the internal excitations, which in the simplest case we may assume to be characterized by a single time scale  $\tau_{diss}$ . As long as the duration of collisions is small compared to  $\tau_{diss}$ , the stochastic differential equation to be derived in Sec. IV should be valid. If furthermore the frequency of collisions  $\nu_{coll}$  becomes very large or even diverges (inelastic collapse) one ultimately enters a regime such that  $1/\tau_{diss} \ll \nu_{coll}$ . Then we would expect the relaxation of internal vibrations to be irrelevant.

Our approach is conceptually related to work on a generalized Langevin equation for a heavy particle, coupled to a bath of oscillators [10–12]. Energy dissipation is modeled by the excitation of oscillators in both cases. There are important differences, however. To derive a Langevin equation one usually assumes a *bilinear* coupling between particle coordinate and bath variables. Furthermore, the frequency spectrum of the oscillators and the distribution of coupling constants can be adjusted [11,12], such that a linear damping force emerges. In our model the frequency spectrum is determined by the geometry of the particles. The coupling between center-of-mass coordinates and internal modes is dictated by physical interactions: The interparticle potential depends on the end-to-end distance between the rods and couples translational to internal coordinates. Hence there is no freedom in the choice of properties of the bath. The resulting stochastic equation for the translational coordinate is highly nonlinear and has complex correlations of the fluctuating force.

## II. MODEL

We consider a one-dimensional system of  $N$  elastic rods of homogeneous density  $\rho$ . Each rod is characterized by its length  $l_i$ , its center of mass coordinate  $R_i(t)$ , and its internal coordinates  $s_i \in [-l_i/2, l_i/2]$ , such that in the *undeformed* state the position  $r_i(s_i, t)$  of a mass element is given by

$$r_i(s_i, t) = R_i(t) + s_i. \quad (1)$$

The deformation of the rod is described by the displacement field  $u_i(s_i, t)$ , such that in the *deformed* state the position of a mass element is

$$r_i(s_i, t) = R_i(t) + s_i + u_i(s_i, t). \quad (2)$$

We require that there be no uniform displacement,  $\int_{-l_i/2}^{l_i/2} u_i(s, t) ds = 0$ , which is instead accounted for by a translation of the center of mass. The elastic energy of a deformed rod is treated in harmonic approximation

$$H_{bath}(\{u_i(s)\}) = \frac{1}{2} \sum_i \int_{-l_i/2}^{l_i/2} ds \left\{ \rho \dot{u}_i^2 + E \left( \frac{du_i}{ds} \right)^2 \right\}. \quad (3)$$

Here the elastic modulus is denoted by  $E$ , it determines the sound velocity according to  $c^2 = E/\rho$ . The displacement field

$u_i(s_i, t)$  is expanded in normal modes with wave number  $k_{i,\nu} = \pi \nu / l_i$  ( $\nu = 1, 2, \dots$ ) and frequency  $\omega_{i,\nu} = c k_{i,\nu}$ :

$$u_i(s_i, t) = \sqrt{2} \sum_{\nu=0}^{\infty} \{ (-1)^{\nu+1} q_i^{(2\nu+1)}(t) \sin(k_{i, 2\nu+1} s_i) + (-1)^\nu q_i^{(2\nu)}(t) \cos(k_{i, 2\nu} s_i) \}. \quad (4)$$

The amplitudes in this expansion are denoted by  $q_i^{(\nu)}(t)$  and the requirement of no uniform displacement implies  $q_i^{(0)}(t) = 0$ .

In one space dimension rods experience longitudinal collisions only. We model these by a short-range repulsive potential  $V(\hat{r}_{ij})$  depending on the momentary end-to-end distance between the colliding rods  $i$  and  $i+1$ ,

$$\hat{r}_{i+1,i}(t) = R_{i+1,i}(t) + u_{i+1} \left( -\frac{l_{i+1}}{2}, t \right) - u_i \left( \frac{l_i}{2}, t \right), \quad (5)$$

with

$$R_{i+1,i} = R_{i+1} - R_i - \frac{l_{i+1} + l_i}{2}. \quad (6)$$

One possibility is an exponential potential,  $V(r) = B e^{-\alpha r}$ , which includes the hard-core limit for  $\alpha \rightarrow \infty$ . The interaction only depends on the displacement fields at the ends of the rods and hence simplifies, if the expansion (4) is used. The total Hamiltonian of our model is then given by

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_{bath} \{ p_i^{(\nu)}, q_i^{(\nu)} \} + \mathcal{H}_{tr} \{ P_i \} + \mathcal{H}_{int} \{ R_i, q_i^{(\nu)} \} \\ &= \sum_{i=1}^N \sum_{\nu=1}^{\infty} \left\{ \frac{p_i^{(\nu)2}}{2m_i} + m_i \omega_{i,\nu}^2 \frac{q_i^{(\nu)2}}{2} \right\} + \sum_{i=1}^N \frac{P_i^2}{2m_i} \\ &\quad + \sum_{i=1}^{N-1} B \exp \left\{ -\alpha \left( R_{i+1,i} \right. \right. \\ &\quad \left. \left. + \sqrt{2} \sum_{\nu} [q_{i+1}^{(\nu)} - (-1)^\nu q_i^{(\nu)}] \right) \right\}. \end{aligned} \quad (7)$$

Here  $P_i$  and  $p_i^{(\nu)}$  denote the conjugate momenta for the center of mass and the amplitude of vibration, respectively. The constant  $B$  is arbitrary. It can be absorbed by rescaling time  $t' = t\sqrt{B}$  and frequencies  $\omega' = \omega/\sqrt{B}$ .

## III. NUMERICAL RESULTS

In this paper we analyze in detail the predictions of our model for two-particle interactions. We determine the asymptotic states for an inelastic collision: the change in relative velocity as a function of the degree of vibrational excitation. In a planned subsequent paper we shall extend the analysis to the entire many-body problem assuming that two-particle collisions are the dominant interactions (which is a reasonable approximation for a wide range of particle densities).

We now consider two rods with reduced mass  $\mu$ , that are placed on a circular ring of circumference  $L$ . The ring has to be sufficiently large,  $L \gg 2/\alpha$ , so that the rods are effectively decoupled for the maximal relative distance  $L/2$ . We focus

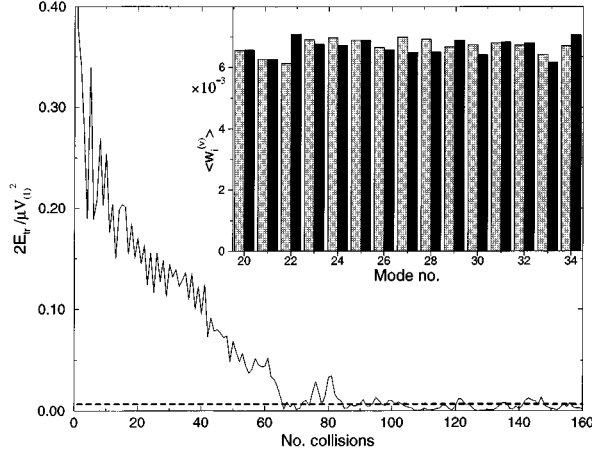


FIG. 1. Time evolution of the relative kinetic energy for a two-particle system with length ratio  $\gamma=l_1/l_2=0.6173$ ,  $\alpha V_{(1)}l/c=4000$ , and  $N_{modes}=75$ . The dashed line is the equilibrium value resulting from equipartition of energy. The inset displays a cutout from the corresponding spectrum of modal energies: After a transient time of 500 collisions the relative energies  $w_i^{(\nu)}$  have been averaged over another 4000 collisions. Gray and black bars correspond to particles 1 and 2, respectively.

on the cooling process, i.e., the transfer of translational energy to the internal vibrations. Hence we perform the following experiment repeatedly: The system is started with a cold oscillator bath,  $q_i^{(\nu)}(t=0)=p_i^{(\nu)}(t=0)=0$ . The two rods are placed maximally far apart,  $R_{2,1}=L/2$  and given relative velocity  $\dot{R}_{2,1}=-V_{(1)}$ . Subsequently Hamilton's equations of motion are solved with a Bulirsch Stoer [13] algorithm. The system undergoes a neverending cascade of inelastic collisions, thereby transferring the energy from the translational to the vibrational modes. Of particular interest is the hardcore limit  $\alpha \rightarrow \infty$ . In the following, time is counted as the number of collisions that have occurred, and hence is not simply related to real time.

A typical realization of the decay of the translational energy  $E_{tr}$  is shown in Fig. 1. It is seen to relax to a stationary state, which is characterized by equipartition among all  $(2N_{mod}+1)$  modes. In the stationary state we observe fluctuations of  $E_{tr}$  around the mean

$$E_{tr}^{stat} = \langle E_{tr} \rangle = \frac{\mu V_{(1)}^2}{2(2N_{mod}+1)}, \quad (8)$$

which goes to zero as  $N_{mod} \rightarrow \infty$ . The energy of the whole system,  $E_{tot} = E_{tr} + E_{bath}$  is conserved [14], so that we observe a microcanonical equilibrium state and the fluctuations in  $E_{tr}$  can be interpreted as canonical fluctuations of a subsystem, coupled to the bath of oscillators. Hence the fluctuations in  $E_{tr}$  are determined by the Boltzmann distribution

$$p^{stat}(E_{tr}) = \frac{1}{E_{tr}^{stat}} \exp\left(-\frac{E_{tr}}{E_{tr}^{stat}}\right). \quad (9)$$

The relaxation time of  $E_{tr}$  is essentially independent of  $N_{mod}$ , but does depend on  $\gamma=l_1/l_2$ , the ratio of the two lengths. For  $\gamma=0.6173$  it takes about 60 collisions for  $E_{tr}$  to relax to its stationary value.

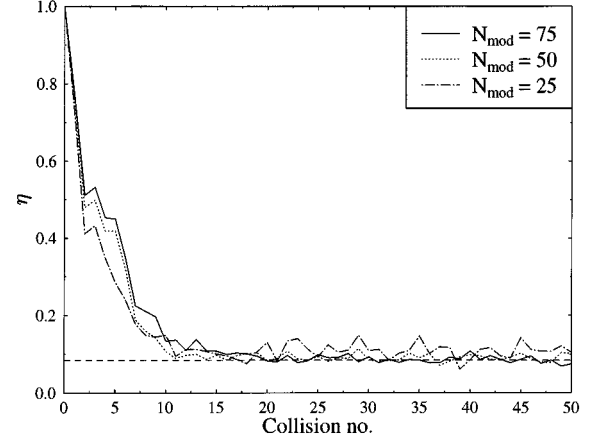


FIG. 2. Time dependence of the spectral entropy  $\eta$  for different numbers of modes. As in Fig. 1,  $\gamma=0.6173$  and  $\alpha V_{(1)}l/c=4000$ . The dashed line corresponds to the equilibrium value Eq. (11) for  $N_{mod}=75$ .

The distribution of  $E_{bath}$  over the vibrational modes is shown in the inset of Fig. 1. Equipartition implies that the relative modal energies  $w_i^{(\nu)} = E_i^{(\nu)}/E_{bath}$  are, on the average, equal to  $1/2N_{mod}$ . It is well fulfilled, provided  $\gamma$  is sufficiently irrational. An essential point is to understand the time scale, which is relevant for the equipartition of the internal modes. A measure for the degree of equipartition, which has been achieved after a time  $t$ , is the generalized entropy of information [15,16]

$$h = - \sum_{i=1}^2 \sum_{\nu=1}^{N_{mod}} w_i^{(\nu)} \ln w_i^{(\nu)}. \quad (10)$$

By definition,  $h=0$  at  $t=0$ , whereas  $h$  reaches its maximum  $h_{max} = \ln 2N_{mod}$  iff  $w_i^{(\nu)} = 1/2N_{mod}$  for all  $i$  and  $\nu$ . To compare systems of different size, it is more convenient to introduce the normalized spectral entropy:  $\eta = 1 - h/h_{max}$ . If all  $[w_i^{(\nu)}]$  are random variables, identically distributed according to Boltzmann statistics, then  $\eta$  is expected to fluctuate around a mean [17,18]

$$\langle \eta \rangle = \frac{0.423}{\ln(2N_{mod})}. \quad (11)$$

In Fig. 2 we show the decay of  $\eta$  for several  $N_{mod}$ . It takes only approximately five collisions to establish modal equipartition and this time scale does not depend significantly on the number of modes.

Based on these results, we distinguish between three time regimes:

(1) On the shortest time scales equipartition is achieved among the vibrational states.

(2) For intermediate time scales the translational energy decays to its stationary value in the presence of a bath of thermalized oscillators.

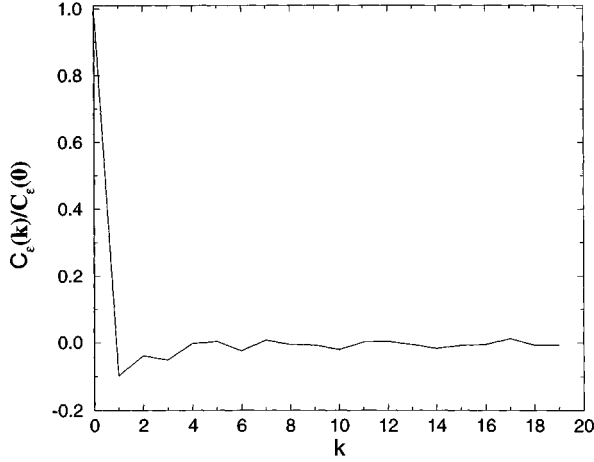


FIG. 3. The correlation function of the coefficient of restitution  $C_\epsilon(k)$  in the stationary state for the same system as in Fig. 1. The data were obtained by averaging over 4000 collisions. Apparently, successive collision events are only weakly correlated.

(3) For the longest time scales a stationary state is reached. This state is characterized by complete equipartition and hence a very small value  $O(1/N_{mod})$  of the translational velocity.

It is the *intermediate* time regime that we are interested in. For this time window we can hope to achieve a simplified description in terms of the center-of-mass coordinate only, modeling the internal oscillators as a thermalized bath. Such a coarse grained model is particularly useful if the stochastic forces of the bath are correlated over time scales much shorter than the typical time scale for translational motion. In that case, a Markov approximation for the stochastic dynamics of the particle is justified. The typical time scale for translational motion is the duration of a collision  $\tau_{coll}$ , which will be shown to be given by  $\tau_{coll} \sim 2l_i/c$ . If the states of the bath before and after collision were correlated, one would expect to see correlations among consecutive collisions on the coarse grained level. To analyze these correlations we consider the statistics of the coefficient of restitution  $\epsilon_{(j)}$ , defined for the  $j$ th collision as

$$\epsilon_{(j)} = \frac{V_{(j+1)}}{V_{(j)}}. \quad (12)$$

Here  $V_{(j)}$  is the absolute value of the center-of-mass velocity before the  $j$ th collision. The correlation function of  $\epsilon$  in the stationary state

$$C_\epsilon(k) = \frac{1}{N_{max} - k - j_0} \sum_{j=j_0}^{N_{max}} (\epsilon_{(j)} - \langle \epsilon \rangle)(\epsilon_{(j+k)} - \langle \epsilon \rangle) \quad (13)$$

has been determined as an average over many collisions. A typical realization is plotted in Fig. 3. One observes a rapid decrease of  $C_\epsilon(k)$ ; even for  $k=1$  correlations are very small. Apparently the nonlinear coupling in Eq. (7) is very effective to destroy any correlations in the internal modes. We shall come back to discuss the statistics of  $\epsilon$  in more detail, once we have shown that  $\epsilon$  is a deterministic quantity for a cold

bath of oscillators (Sec. V) and that its fluctuations are determined by the strength of the internal vibrations (Sec. VI).

#### IV. EFFECTIVE STOCHASTIC EQUATION

For a single collision of two particles one can integrate out the vibrational degrees of freedom and thereby derive an exact equation of motion for the relative velocity. For that purpose it is more convenient to consider a linear arrangement, so that the two particles move apart after collision. Our starting points are the equations of motion

$$\mu \ddot{R}_{2,1} = \alpha B \exp \left\{ -\alpha \left( R_{2,1} + \sqrt{2} \sum_{\nu} (q_1^{(\nu)} + q_2^{(\nu)}) \right) \right\}, \quad (14)$$

$$\ddot{q}_i^{(\nu)} = -\omega_{i,\nu}^2 q_i^{(\nu)} + \frac{\sqrt{2}\mu}{m_i} \ddot{R}_{2,1},$$

where we have made use of a trivial canonical transformation  $(q_i^{(\nu)}, p_i^{(\nu)}) \leftrightarrow ((-1)^{\nu+1} q_i^{(\nu)}, (-1)^{\nu+1} p_i^{(\nu)})$ . The equations have to be supplemented with initial conditions. We choose  $R_{2,1}(0) = R_0 \gg 1/\alpha$  and  $\dot{R}_{2,1}(0) = -V$  and leave  $q_i^{(\nu)}(0)$  and  $p_i^{(\nu)}(0)$  unspecified for the moment.

There are two important length scales in our model: The lengths of the rods, which we take to be different ( $l_1 \leq l_2$ ) but comparable, and the range of the potential  $1/\alpha$ . For the first it is convenient to introduce an effective length scale  $l = 2l_1 l_2 / (l_1 + l_2)$  and the ratio  $\gamma = l_1 / l_2$ . We are interested in the hard-core limit  $\alpha \rightarrow \infty$ , so that  $\alpha l \gg 1$ . The effective length of the rods  $l$  sets the time scale  $\tau_0 = l/c$  for the duration of an inelastic collision (see Sec. V). In the following we shall work with dimensionless time  $\tau = t/\tau_0$ . In these units it takes a time  $\Gamma_1 = (2l_1/c)(c/l) = 1 + \gamma$  [ $\Gamma_2 = (2l_2/c) \times (c/l) = 1 + 1/\gamma$ ] for a signal to travel back and forth on rod 1 (2). Another time scale is  $\tau_1 = 1/(\alpha V)$ , which is the collision time for the corresponding elastic collision. The latter has to go to zero in the hard-core limit, so that we shall always assume  $\kappa = \tau_0/\tau_1 = \alpha V l/c \gg 1$ .

The equation of motion for the oscillators can be integrated with help of the elastic Green function (see Appendix A). The resulting equation for the velocity increase

$$W(\tau) = \alpha \frac{l}{c} [\dot{R}_{2,1}(\tau) - \dot{R}_{2,1}(0)] \quad (15)$$

is given by

$$\frac{d}{d\tau} W(\tau) = \exp \left\{ \kappa \tau - \alpha R_0 - W(\tau) - \sum_{i=1}^2 \sum_{n=1}^{\infty} W(\tau - n\Gamma_i) + Q(\tau) \right\}. \quad (16)$$

The exponential dependence of the acceleration is, of course, due to the exponential potential, which we have chosen to represent a hard-core potential. The memory terms  $W(\tau - n\Gamma_i)$  are present because the elastic vibrations do not decay in the Hamiltonian model that we are using. Hence an applied force [ $\mu \ddot{R}_{2,1}$  in Eq. (14)] is felt forever. The function

$$Q(\tau) = \sqrt{2}\alpha \sum_{\nu} \sum_{i=1}^2 \left( q_i^{(\nu)}(0) \cos(2\pi\tau\nu/\Gamma_i) + \frac{p_i^{(\nu)}(0)}{m_i\omega_{i,\nu}} \sin(2\pi\tau\nu/\Gamma_i) \right) \quad (17)$$

accounts for the contribution to the displacements that stems from the initial excitation of the oscillator system. Note that  $(d/d\tau)W(\tau=0) \sim 0$ , i.e., the particles do not interact at  $\tau=0$ , because initially they are far apart,  $\alpha R_0 \gg 1$ .

In Sec. III we have seen that the oscillators quickly relax to a thermalized state with equipartition among the oscillators. This result suggests that for the subsequent cooling process we can model the internal degrees of freedom by a bath of temperature  $T_B = E_{bath}/(2N_{mod})$ . Then  $\{q_i^{(\nu)}(0)\}$  and  $\{p_i^{(\nu)}(0)\}$  are independent, canonically-distributed random variables with

$$\langle q_i^{(\nu)}(0) \rangle = \langle p_i^{(\nu)}(0) \rangle = 0 \quad (18)$$

$$\langle (q_i^{(\nu)}(0))^2 \rangle = \langle [p_i^{(\nu)}(0)/(m_i\omega_{i,\nu})]^2 \rangle = T_B/(m_i\omega_{i,\nu}^2).$$

Under these assumptions  $Q(\tau)$  is a Gaussian random variable with zero mean and covariance

$$\begin{aligned} C_Q(\tau) &= \langle Q(\tau')Q(\tau'+\tau) \rangle \\ &= \sigma^2 \left\{ \sum_{i=1}^2 \frac{1}{2\Gamma_i} \left( \tau - \frac{\Gamma_i}{2} - \Gamma_i \sum_{n=1}^{\infty} \theta(\tau - n\Gamma_i) \right)^2 - \frac{\Gamma_1\Gamma_2}{24} \right\}, \quad (19) \\ \sigma^2 &= \frac{\alpha^2 l^2}{\mu c^2} T_B = \kappa^2 \frac{T_B}{2E_{tr}}. \end{aligned}$$

Here  $E_{tr} = (\mu/2)V^2$  is the initial translational energy. This rather complex variance is due to the fact that  $Q(\tau)$  is the superposition of two random processes: The first (representing thermalized vibrations of rod 1) is periodic with  $\Gamma_1$  and the second (representing thermalized vibrations of rod 2) is periodic with  $\Gamma_2$ .  $C_Q(\tau)$  is a periodic function for rational  $\gamma$  and a quasiperiodic function for irrational  $\gamma$ . A typical correlation is shown in Fig. 4. It consists of pieces of parabola, joined such that the function is continuous.

The coefficient of restitution is defined as

$$\epsilon = \lim_{t \rightarrow \infty} |\dot{R}_{2,1}(t)/\dot{R}_{2,1}(0)| = \lim_{\tau \rightarrow \infty} W(\tau)/\kappa - 1. \quad (20)$$

$W(\tau)$  is expected to be of  $O(\kappa)$  and inspection of the covariance  $C_Q(\tau)$  shows that the noise  $Q(\tau)$  is of the same order of magnitude.

## V. DETERMINISTIC LIMIT

Some insight into the equation of motion can be gained from the deterministic limit  $T_B=0$ . This implies that no vibrations are excited before collision and corresponds to the initial condition in the numerical solution of Sec. III. (The deterministic limit may also be relevant for a non-

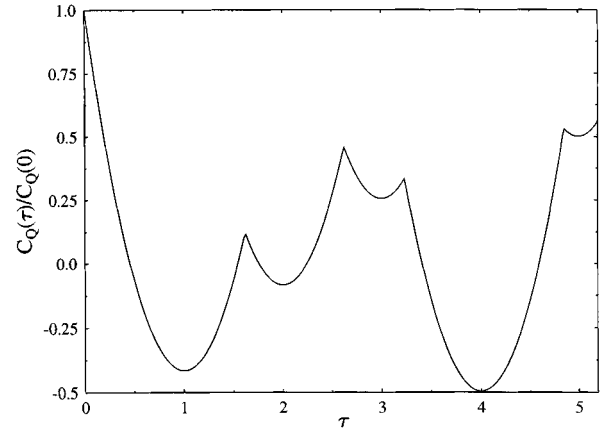


FIG. 4. The correlation function  $C_Q(\tau)$  of the noise process  $Q(\tau)$  with length ratio  $\gamma=0.6173$ . For rational  $\gamma$  the function is periodic, for irrational  $\gamma$  it is quasiperiodic.

Hamiltonian model with heavily damped vibrations, such that between collisions the vibrational energy relaxes to zero.)

The deterministic equation can be solved analytically in the limit of a hard-core interaction ( $\kappa \rightarrow \infty$ ). The solution is nontrivial due to the memory terms: To construct the solution at time  $\tau$  requires knowledge of  $W(\tau)$  at all previous times. Starting at  $\tau=0$ , with  $W(\tau)=0$  for  $\tau \leq 0$ , one solves for  $W(\tau)$  in a small time interval, such that the memory terms vanish. This solution is then fed into the memory terms of the next time interval, etc. The details of the solution are given in Appendix B. We neglect contributions, which are exponentially small in  $\kappa$  and find

$$W(\tau) = \ln \left( 1 + \frac{\exp[\kappa(\tau - \tau_{free})]}{\kappa + \exp[\kappa(\tau - 2 - \tau_{free})]} \right) \quad \text{for } \gamma=1 \quad (21)$$

and

$$W(\tau) = \ln \left( 1 + e^{\kappa\Gamma_1} \ln \left[ \frac{1 + \frac{1}{\kappa} \exp[\kappa(\tau - \Gamma_1 - \tau_{free})]}{1 + \frac{1}{\kappa} \exp[\kappa(\tau - \Gamma_2 - \tau_{free})]} \right] \right) \quad \text{for } 0.5 \leq \gamma < 1. \quad (22)$$

Here  $\tau_{free} = R_0/(V\tau_0)$  is the typical time the particles need to collide, starting with initial separation  $R_0$  and initial velocity  $-V$ .

The coefficient of restitution follows from Eqs. (21,22)

$$\epsilon = \begin{cases} 1 & \text{for } \gamma=1 \\ \gamma + \frac{\ln[\kappa(\Gamma_2 - \Gamma_1)]}{\kappa} & \text{for } 0.5 \leq \gamma < 1. \end{cases} \quad (23)$$

In the hard-core limit  $\epsilon$  is given by  $\gamma = l_1/l_2$ , the ratio of the lengths of the two rods. For rods of equal length there is no translational energy dissipation at all. Our approximate solution for large  $\kappa$  is actually remarkably good down to  $\kappa \approx 5$ . The approximate analytical solution is compared to  $\epsilon$ , as

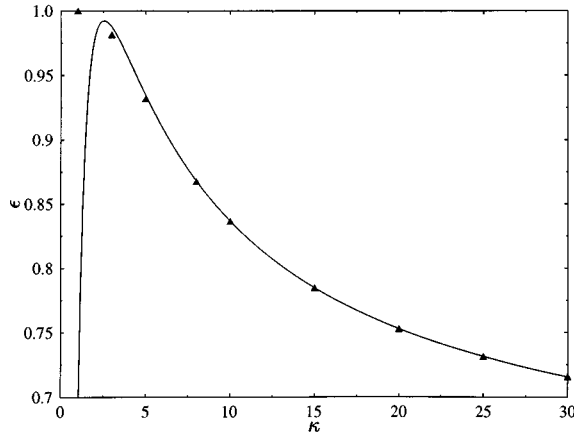


FIG. 5. The coefficient of restitution as a function of the parameter  $\kappa = \alpha V l / c$  in the deterministic limit. For  $\gamma = 0.6$ , we compare the approximate solution, Eq. (23), with the results (triangles) of a numerical integration of Eq. (16).

obtained from a numerical integration of the equation of motion, in Fig. 5. Deviations can be seen for  $\kappa \rightarrow 0$ , where the correct  $\epsilon$  approaches 1 and the approximate solution for large  $\kappa$  obviously fails.

It is only the parameter  $\kappa$  that controls the solution and hence the coefficient of restitution. For a perfect hard-core one has to require  $\alpha l \rightarrow \infty$  and hence  $\kappa \rightarrow \infty$ . If, on the other hand the range of the potential  $1/\alpha$  and the length scale of the rods are chosen such that  $\alpha l$  is large but fixed, then variations in  $\kappa$  are due to variations in  $V$ . Hence for fixed ‘‘microscopic’’ parameters  $(\alpha, l, c)$ , we interpret  $\epsilon(\kappa)$  as a velocity-dependent coefficient of restitution. Presumably this velocity dependence is not universal, in the sense that it depends on the interparticle potential.

The time evolution of  $W(\tau)$  is shown in Fig. 6 for two values of  $\kappa$ . In the hard-core limit the relative velocity is given by

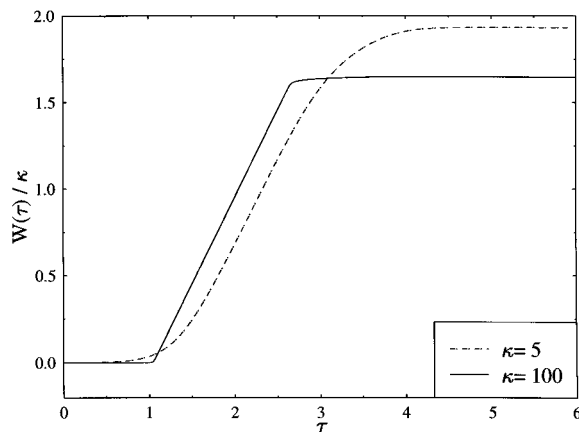


FIG. 6. The velocity increase  $W(\tau)$  in the deterministic limit. The plot displays the approximate solution Eq. (22) for  $\gamma = 0.6$ ,  $\tau_{free} = 1$ , and two different values of  $\kappa$ . In the limit  $\kappa \rightarrow \infty$ ,  $W(\tau)$  is piecewise linear [cf. Eq. (24)].

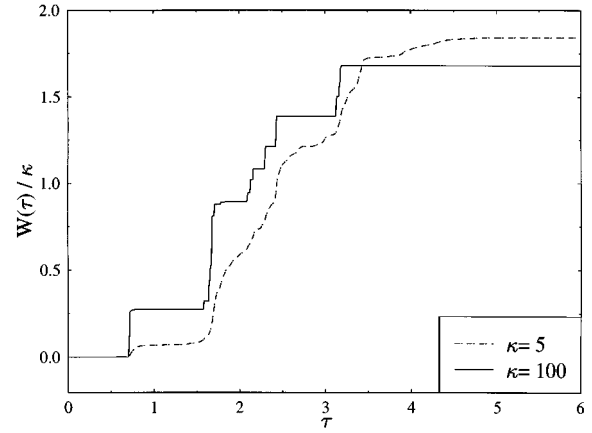


FIG. 7. Two typical stochastic trajectories of  $W(\tau)$  for  $T_B/E_{ir} = 1$  and two different values of  $\kappa$ . As in Fig. 6,  $\gamma = 0.6$  and  $\tau_{free} = 1$ .

$$V_{2,1}(\tau) = \begin{cases} -V, & \tau \leq \tau_0 \\ -V + (\tau - \tau_0)V & \text{for } \tau_0 < \tau < \tau_0 + \Gamma_1 \\ \gamma V, & \tau_0 + \Gamma_1 \leq \tau. \end{cases} \quad (24)$$

The time of interaction is equal to  $\Gamma_1$ , the time that an elastic wave needs to travel back and forth on the shorter rod. The fraction of kinetic energy that has been transferred to internal vibrations is  $(1 - \gamma^2)E_{ir}$ . It is distributed over the oscillator modes according to

$$\frac{E_i^{(v)}}{E_{ir}} = \frac{1}{\nu^2} \frac{2\Gamma_i}{\pi^2} \sin^2\left(\nu\pi \frac{\Gamma_1}{\Gamma_i}\right). \quad (25)$$

Hence all the energy lost for the translational motion is transferred to the longer rod, whereas  $E_1^{(v)} = 0$ . One can easily check that  $\sum_\nu E_2^{(v)} = (1 - \gamma^2)E_{ir}$ , as required by energy conservation.

These results are in complete agreement with the wave theory of impact [19], which analyzes the collision problem in terms of stress waves propagating through the rods. To our knowledge, a derivation in the framework of classical mechanics (with correction terms for finite  $\kappa$ ) has not been given before.

## VI. STOCHASTIC COEFFICIENT OF RESTITUTION

For  $T_B \neq 0$  we have integrated Eq. (16) numerically for various realizations of the noise process. The first step is to generate random initial conditions  $q_i^{(v)}(0)$  and  $p_i^{(v)}(0)$  with a standard procedure. The Fourier series in Eq. (17) have to be truncated after a finite number of terms ( $\nu_{max} \sim 250$  turns out to be a reasonable compromise for computation time and accuracy). The initial separation of the centers of mass has to be chosen sufficiently large compared to the noise,  $\alpha R_0 \gg \sqrt{\langle Q^2(0) \rangle}$ , so that initially the two particles move freely. Subsequently the differential equation is integrated with a Bulirsch Stoer routine.

Two typical trajectories  $W(\tau)$  are shown in Fig. 7. In the hard-core limit ( $\kappa = 100$ ) we observe a random sequence of rapid changes of  $W(\tau)$  due to the ongoing oscillations of the

ends of the rods, while for a softer potential ( $\kappa=5$ ) these changes are smoothed. The first contact of the particles may happen earlier (later) than  $\tau_{free}$ , because the ends vibrate towards (away from) each other.

Analytically, some insight into the properties of Eq. (16) can be gained in the limit  $\kappa \rightarrow \infty$ . In this case the equation can be solved [20] formally by means of a saddle-point approximation, yielding

$$\lim_{\kappa \rightarrow \infty} \frac{W(\tau)}{\kappa} = \max\{0, f(\tau)\},$$

$$f(\tau) = \max_{\tau' \in [0, \tau]} \left\{ \tau' - \tau_{free} - \sum_{i=1}^2 \sum_{n=1}^{\infty} \frac{W(\tau' - n\Gamma_i)}{\kappa} + \frac{Q(\tau')}{\kappa} \right\}. \quad (26)$$

Due to the memory terms this solution still requires a piecewise construction of  $W(\tau)$ , analogous to that performed in Appendix B for the deterministic limit. Again, it is the memory terms that end the collision process, since the remaining terms in the brackets are — on the average — increasing with time. For  $\gamma \neq 1$  the duration of the collision  $\tau_{coll}$  and the asymptotic value  $W(\tau \rightarrow \infty)$  are random variables, whose distribution we have not been able to calculate analytically.

For  $\gamma=1$ ,  $Q(\tau)$  is periodic with period  $\Gamma=2$  and the situation is totally different: For *every* realization of  $Q$  we find from Eqs. (20) and (26) that  $\epsilon=1$  and  $\tau_{coll}=\Gamma$ , which is precisely the deterministic result. In other words, the asymptotic dynamics of two colliding rods of *equal* length does not depend on whether initially internal vibrations are excited or not.

To calculate the statistics of the coefficient of restitution in the case  $\gamma \neq 1$ , we have determined the asymptotics of  $W(\tau)$  numerically and averaged over several thousand realizations of the noise. Generally, the distribution of  $\epsilon$  depends on  $T_B/E_{tr}$ ,  $\gamma$ , and  $\kappa$ . It turns out that the hard-core limit [Eq. (26)] is well represented by values of  $\kappa > 50$ , in the sense that the statistics become independent of  $\kappa$  in this range of parameters. All numerical results were obtained for this regime.

In Fig. 8 we plot the average and the standard deviation of  $\epsilon$  as a function of  $T_B/E_{tr}$  for two values of  $\gamma$ . The fluctuations of  $\epsilon$  increase with  $T_B/E_{tr}$  as expected. The variance is larger, the larger the difference in lengths of the two rods, i.e., the more inelastic the collisions are in the deterministic limit. In general the distribution of  $\epsilon$  is non-Gaussian, so that it is not sufficient to consider the two lowest moments. Instead, the full information about the statistics of  $\epsilon$  is contained in the density  $p_{E_{tr}/T_B}^\gamma(\epsilon^2)$  (which is also the relevant quantity for energy transfer, cf. below), shown in Fig. 9 together with the distribution function  $D_{E_{tr}/T_B}^\gamma(\epsilon^2) = \int_0^{\epsilon^2} p(x) dx$ . As mentioned before, the distribution broadens for increasing  $T_B$ . In the deterministic limit the distribution converges to a step-function  $D_\infty^\gamma(\epsilon^2) = \Theta(\epsilon^2 - \gamma^2)$ , corresponding to a  $\delta$  function for the density  $p_\infty^\gamma(\epsilon^2) = \delta(\epsilon^2 - \gamma^2)$ .

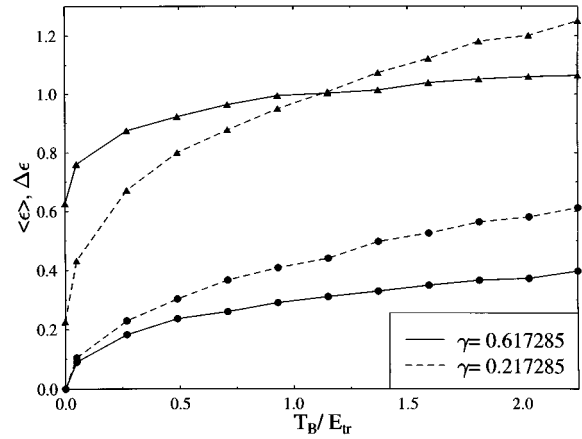


FIG. 8. The mean value  $\langle \epsilon \rangle$  (triangles) and the standard deviation  $\Delta \epsilon$  (circles) as functions of  $T_B/E_{tr}$  in the hard-core limit ( $\kappa=250$ ). We consider two different length ratios  $\gamma$ . For each data point 2500 realizations of the stochastic differential equation (16) have been integrated.

## VII. MESOSCOPIC DYNAMICS: INTERPRETATION OF $p(\epsilon^2)$ AS A TRANSITION PROBABILITY

In this section we interpret the results of the preceding sections as a stochastic dynamics on a mesoscopic level: The time evolution of  $E_{tr}$  upon successive collisions (cf. Sec. III) is described as a Markov process and  $p(\epsilon^2)$  is interpreted as the transition probability between two “states”  $E_{tr}$  and  $E'_{tr}$ . The basic ingredients of the mesoscopic dynamics are the Markov assumption for the stochastic process and the fast achievement of equipartition among the internal modes.

In detail, we proceed as follows. Led by the numerical solution of the full dynamics (Sec. III) we regard the time evolution of  $E_{tr}$  as a stochastic process in discrete time  $(1, 2, \dots, n)$

$$E_{tr(1)} \rightarrow E_{tr(2)} \rightarrow \dots \rightarrow E_{tr(n)} \quad (27)$$

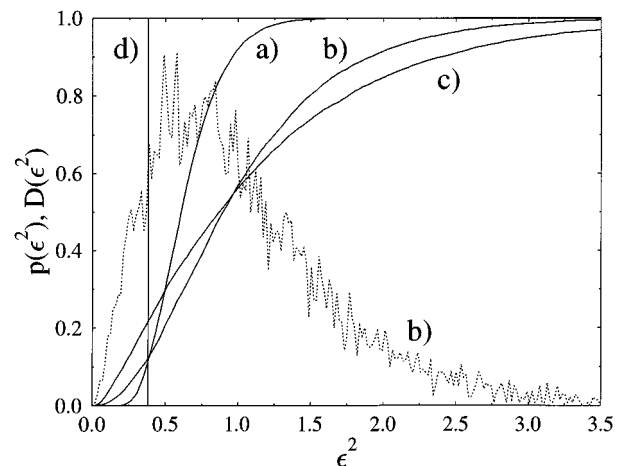


FIG. 9. The probability density  $p(\epsilon^2)$  (dotted line) and its integral, the distribution function  $D(\epsilon^2)$  (full line), for different energy and length ratios: (a)  $E_{tr}/T_{bath}=10$ ,  $\gamma=0.6173$ , (b)  $E_{tr}/T_{bath}=1$ ,  $\gamma=0.6173$ , and (c)  $E_{tr}/T_{bath}=1$ ,  $\gamma=0.2173$ . (d) displays the distribution function for  $\gamma=0.6173$  in the deterministic limit  $\kappa \rightarrow \infty$ . Data were obtained from 8000 realizations of  $W(\tau)$  with  $\kappa=100$ .

with each time step representing one collision. We assume that this stochastic process is a Markov process, because subsequent collisions are approximately independent (see Fig. 3). The Markov assumption implies that the noise, which models the effect of the internal oscillators, is chosen independently after each collision.

Changes in the bath temperature are not independent, but determined by energy conservation:

$$E_{tr(j+1)} = \epsilon_{(j)}^2 E_{tr(j)}, \quad (28)$$

$$T_{B(j+1)} = T_{B(j)} + \frac{1 - \epsilon_{(j)}^2}{2N_{mod}} E_{tr(j)}.$$

The transition probability from a state  $E_{tr}$  before collision to a state  $E'_{tr} = \epsilon^2 E_{tr}$  after collision is then determined by the probability density  $p_{E'_{tr}/T_B}^\gamma(\epsilon^2)$  according to

$$p_{T_B}(E_{tr} \rightarrow E'_{tr}) = \frac{1}{E_{tr}} p_{E'_{tr}/T_B}^\gamma(\epsilon^2) \Big|_{\epsilon^2 = E'_{tr}/E_{tr}}. \quad (29)$$

The stationary state of the Markov process is known: after cooling, the system of two particles, each equipped with an internal bath, evolves into a stationary state with a Boltzmann distribution for  $E_{tr}$ ,

$$p_{T_B^0}^{stat}(E_{tr}) = \frac{1}{T_B^0} \exp\left(-\frac{E_{tr}}{T_B^0}\right) \quad (30)$$

with the bath temperature

$$T_B^0 = \frac{E_{tot}}{2N_{mod} + 1}. \quad (31)$$

This implies for the transition rates of the Markov process

$$p_{T_B^0}^{stat}(E) = \int_0^\infty dE' p_{T_B^0}(E' \rightarrow E) p_{T_B^0}^{stat}(E'). \quad (32)$$

Here we neglect changes in the bath temperature, which are of  $O(1/N_{mod})$  as compared to  $O(1)$  changes in  $E_{tr}$ . A more stringent constraint on the transition probabilities is the requirement of detailed balance, i.e., equal probability currents between two microstates  $E_{tr}$  and  $E'_{tr}$ ,

$$p_{T_B^0}(E_{tr} \rightarrow E'_{tr}) p_{T_B^0}^{stat}(E_{tr}) = p_{T_B^0}(E'_{tr} \rightarrow E_{tr}) p_{T_B^0}^{stat}(E'_{tr}). \quad (33)$$

This implies for the transition probability density of  $\epsilon^2$

$$\frac{p_{E'_{tr}/T_B^0}^\gamma(\epsilon^2)}{p_{\epsilon^2 E_{tr}/T_B^0}^\gamma\left(\frac{1}{\epsilon^2}\right)} = \frac{1}{\epsilon^2} \exp\left(\frac{E_{tr}}{T_B^0} (1 - \epsilon^2)\right). \quad (34)$$

We have checked the above considerations by a numerical simulation of the Markov process. To simulate the transition probabilities, which are not known analytically, we produce a random  $\epsilon^2$  by solving the stochastic differential equation for the momentary value of  $E_{tr}$  and a fixed equilibrium temperature  $T_B^0$ . The distribution of  $E_{tr}/T_B^0$  based on 10 000

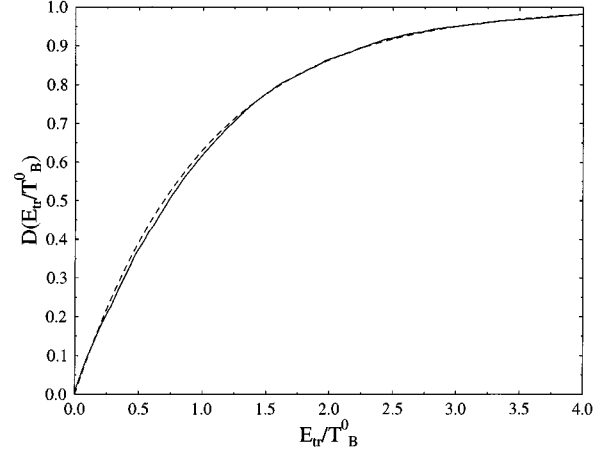


FIG. 10. Result of a simulation of the Markov process (27) in the stationary state with fixed  $T_B^0$ . The transition densities  $p_{T_B^0}(E_{tr} \rightarrow E'_{tr})$  were simulated by numerical integration of Eq. (16) with  $\gamma = 0.6$ . The distribution function  $D(\epsilon^2)$  (full line) is calculated from 10 000 simulation steps and compared with the Boltzmann distribution [dashed line, cf. Eq. (30)].

steps in the Markov process is shown in Fig. 10. As expected, the distribution approximates a Boltzmann statistics rather well. The statistics for  $p(\epsilon^2)$  that we have obtained so far is not sufficient to test detailed balance numerically, however.

Detailed balance is not enough to uniquely specify a transition probability. As for the dynamics of Ising spins, one may construct many different transition probabilities, which all satisfy detailed balance and hence relax to the same stationary state. In particular, Glauber's choice [21] would correspond to

$$p_{E'_{tr}/T_B}^{(G)}(\epsilon^2) = \frac{E_{tr}}{T_B} \exp\left(-\epsilon^2 \frac{E_{tr}}{T_B}\right). \quad (35)$$

However, this expression has the wrong deterministic limit

$$\lim_{E'_{tr}/T_B \rightarrow \infty} p_{E'_{tr}/T_B}^{(G)}(\epsilon^2) = \delta(\epsilon^2). \quad (36)$$

Collisions, where the internal vibrations are not excited, would be completely inelastic. It is an open question whether detailed balance, together with the right deterministic limit, uniquely specifies the transition probabilities.

Also we want to stress the following point: In contrast to most Monte Carlo simulations we are not interested in the stationary state, which is trivial, but rather in the cooling dynamics. At present it is not clear at all how sensitive the cooling dynamics is with respect to variations in the transition probabilities. However, our approach allows for a systematic investigation of this point. For that purpose it would be helpful to have a simple analytical expression for the transition probabilities. Detailed balance and the deterministic limit may serve as guidelines in the search of such approximations.



### VIII. OUTLOOK

The stochastic dynamics of Sec. VII is easily generalized to a dilute gas of many granular particles, each characterized by its center-of-mass position and velocity and by the temperature of its own bath. As long as the rods do not interact, they move freely and integration of the equations of motion is trivial. In particular, one can calculate the time of the next collision, as is done in event-driven simulations. The collision event is then treated statistically, as discussed in Sec. VII: For the colliding pair the kinetic energy and the temperatures are updated with a randomly chosen  $\epsilon^2$ , whose distribution is given by  $p(\epsilon^2)$ . This part of the dynamics resembles a Monte Carlo procedure,  $p(\epsilon^2)$  being interpreted as the transition probability between two states. An interesting open question is whether this algorithm is able to avoid the inelastic collapse, which is observed in event-driven algorithms. In this context dissipation of the internal vibrations may become important. In the simplest model dissipation can be taken into account by a time-dependent bath temperature, as discussed in the Introduction. Work along these lines is in progress.

One may also try to extend our analysis to higher dimensional objects like disks or spheres. Frequently a quasistatic potential due to Hertz is used for two colliding spheres. However, in a real collision the quasistatic approximation is not expected to hold. For the above example of two colliding rods, the dynamic theory yields results that are completely different from the static approximation. The latter implies that the repulsive force depends linearly on the relative distance of the two rods. The dynamic theory, which is based on the propagation of elastic waves inside the rods, predicts a constant force during collision.

### ACKNOWLEDGMENTS

We gratefully acknowledge stimulating discussions with Reiner Kree, Kurt Broderix, and Timo Aspelmeier. This work has been supported by the Deutsche Forschungsgemeinschaft through SFB 345.

### APPENDIX A: DERIVATION OF THE STOCHASTIC EQUATION (16)

Starting from the equations of motion (14) we integrate the internal coordinates by means of the Green function for harmonic oscillators:

$$q_i^{(\nu)}(t) = \sqrt{2} \frac{\mu}{m_i} \int_0^t dt' \frac{\sin \omega_{i,\nu}(t-t')}{\omega_{i,\nu}} \ddot{R}_{2,1}(t') + q_i^{(\nu)}(0) \cos \omega_{i,\nu} t + \frac{p_i^{(\nu)}(0)}{m_i \omega_{i,\nu}} \sin \omega_{i,\nu} t. \quad (\text{A1})$$

Next we introduce a dimensionless time variable  $\tau = ct/l$  such that mass ratios are given by the corresponding wave propagation times

$$\frac{m_i}{\mu} = \Gamma_i \quad (\text{A2})$$

and define the scaled center of mass distance  $Z(\tau) = \alpha R_{2,1}(\tau l/c)$  and the total displacement

$$U(\tau) = \alpha u_2 \left( -\frac{l_2}{2}, \frac{l}{c} \tau \right) - \alpha u_1 \left( \frac{l_1}{2}, \frac{l}{c} \tau \right) = \alpha \sqrt{2} \sum_{i,\nu} q_i^{(\nu)}. \quad (\text{A3})$$

If we denote derivatives with respect to  $\tau$  by primes and set the arbitrary constant  $B = \mu c^2 / (\alpha^2 l^2)$ , the translational equation of motion reads

$$Z''(\tau) = e^{-(Z+U)}, \quad (\text{A4})$$

where

$$U(\tau) = \sum_{i=1}^2 \int_0^{\tau} ds \sum_{\nu} \frac{1}{\pi} \sin \left( \frac{2\pi\nu}{\Gamma_i} (\tau-s) \right) Z''(s) + Q(\tau). \quad (\text{A5})$$

Here  $Q(\tau)$  corresponds to displacements that result from the initial conditions [cf. Eq. (17)]. We now use the identities

$$\frac{1}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \sin(2\pi n x) = \frac{1}{2} - x + \sum_{n=1}^{\infty} \theta(x-n) \quad \text{for } x \geq 0 \quad (\text{A6})$$

[ $\theta(x)$  denotes the step function] and  $1/\Gamma_1 + 1/\Gamma_2 = 1$  and get after integration by parts

$$U(\tau) = Z'(\tau) - Z'(0) + Z'(0)\tau - Z(\tau) + Z(0) + \sum_{n=1}^{\infty} \theta(\tau - n\Gamma_i) [Z'(\tau - n\Gamma_i) - Z'(0)] + Q(\tau). \quad (\text{A7})$$

After inserting Eq. (A7) into Eq. (A4),  $Z''(\tau)$  becomes independent of  $Z$  and we obtain the *first-order* differential equation (16) for the velocity increase

$$W(\tau) \equiv Z'(\tau) - Z'(0) \quad (\text{A8})$$

[note that  $Z(0) = \alpha R_0$  and  $Z'(0) = -\kappa$ ].

### APPENDIX B: DETERMINISTIC SOLUTION

In the following we consider Eq. (16) in the limit  $Q(\tau) \equiv 0$ :

$$W'(\tau) = \exp \left\{ \kappa(\tau - \tau_{free}) - W(\tau) - \sum_{i=1}^2 \sum_{n=1}^{\infty} W(\tau - n\Gamma_i) \right\} \quad (\text{B1})$$

$$W(\tau) = 0 \quad \text{for } \tau \leq 0.$$

We confine ourselves to the case  $0.5 \leq \gamma < 1$ , i.e.,  $\Gamma_1 < \Gamma_2 \leq 2\Gamma_1$  and look for an approximate solution of Eq.

(B1) that is correct up to terms of order  $o(e^{-\kappa\delta})$ ,  $\delta > 0$ . As a first step, the solution of (B1) *without* memory terms is

$$W(\tau) \sim \ln \left[ 1 + \frac{1}{\kappa} e^{\kappa(\tau - \tau_{free})} \right]. \quad (\text{B2})$$

Apparently, this solution decays exponentially fast for  $\tau < \tau_{free}$  and grows — essentially linearly in  $\tau$  and  $\kappa$  — for  $\tau > \tau_{free}$ . This means that all memory terms that are obtained from Eq. (B2) at times *smaller* than  $\tau_{free}$  can be neglected. Consequently, (B2) is a consistent solution of (B1) in the entire time interval  $[0 \leq \tau \leq \tau_{free} + \Gamma_1 - \delta]$ , where  $\delta$  is small and positive. In the interval  $[\tau_{free} - \delta, \tau_{free} + 2\Gamma_1 - \delta]$  only two memory terms need to be considered, each evaluated with the help of Eq. (B2), so that we have to solve the equation

$$W'(\tau) = \frac{\exp\{\kappa(\tau - \tau_{free}) - W(\tau)\}}{\left[ 1 + \frac{1}{\kappa} e^{\kappa(\tau - \Gamma_1 - \tau_{free})} \right] \left[ 1 + \frac{1}{\kappa} e^{\kappa(\tau - \Gamma_2 - \tau_{free})} \right]} \quad (\text{B3})$$

with initial condition  $W(\tau_{free} - \delta) \sim 0$ . This equation can be solved by elementary integration, yielding

$$e^{W(\tau)} = 1 + e^{\kappa\Gamma_1} \left[ \ln \left( \frac{1+r}{1+e^{-D}r} \right) \right]_{r(\tau_{free}-\delta)}^{r(\tau)} + O(e^{-D}), \quad (\text{B4})$$

where  $D = \kappa(\Gamma_2 - \Gamma_1)$  and

$$r(s) = \frac{1}{\kappa} e^{\kappa(s - \Gamma_1 - \tau_{free})}. \quad (\text{B5})$$

Neglecting the lower boundary term in Eq. (B4) we obtain Eq. (22). For  $\tau < \tau_{free} + \Gamma_1$  this solution differs from Eq. (B2) only by exponentially small terms. Hence it is an approximate solution of Eq. (B1) in the entire range  $\tau < \tau_{free} + 2\Gamma_1$ . [If  $\gamma < 0.5$  one has to replace  $\Gamma_2$  in Eq. (22) by  $2\Gamma_1$ , whereas for the derivation of Eq. (21) only a single memory term has to be considered.]

In order to prove that Eq. (22) also gives the correct behavior in the limit  $\tau \rightarrow \infty$  one still has to show that  $W' \sim 0$  for  $\tau \geq \tau_{free} + 2\Gamma_1$ , i.e., that there is no relevant contribution to  $W(\tau)$  from other memory terms. Again, this can be done [18] by feeding the solution into the right-hand side of Eq. (B1).

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