Stochastic Coefficient of Restitution — a New Approach to the Dynamics of Granular Media

Götz Giese
Institut für Theoretische Physik, Universität Göttingen,
Bunsenstr. 9, 37073 Göttingen, Germany

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Abstract

We consider a one-dimensional "gas" of inelastically colliding particles where kinetic energy is dissipated by the excitation of vibrational degrees of freedom. In our model the coefficient of restitution is a stochastic quantity whose distribution can be calculated from an exact stochastic equation of motion. We investigate the equipartition properties of the system and propose a new algorithm for computer simulations, that is a combination of event-driven (ED) and Monte-Carlo methods.

Numerical and theoretical approaches to the dynamics of granular materials frequently adopt the concept of a coefficient of restitution that determines the energy loss during collisions of granular particles. Event-driven (ED) simulations\cite{1,2,3} have shown that model systems with 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\cite{4}. On the other hand, molecular-dynamics simulations\cite{5} have the difficulty that ad hoc assumptions about microscopic interaction laws have to be made. An inadequate choice of the interaction parameters can lead\cite{6} to spurious effects in the simulations.

Here we present a one-dimensional model where colliding particles interact via an exponential potential. A control parameter is introduced that allows to perform the limit of a hard core interaction. On collision particles lose kinetic energy by the excitation of internal vibrational modes. In a statistical description we characterize the energy contained in this bath of internal oscillators by a bath temperature $T_{bath}$. Our main aim is to investigate the cooling properties of the system: Starting from an initial distribution of center of mass velocities we would like to understand in detail, how energy is transferred from the translational to the internal degrees of freedom.

The principal results of this Letter are as follows: (1) Granular cooling can be understood as energy equipartition among all (translational and vibrational) modes of the system. (2) At a single collision the coefficient of restitution $\epsilon$ is a stochastic quantity. We derive an exact stochastic equation of motion for the relative coordinates, from which $\epsilon$...
can be calculated. For the special case of "cold" particles \( T_{\text{bath}} = 0 \) we recover a classical result of the wave theory of impact. (3) We give a statistical interpretation of the probability density of \( \epsilon \) and propose a new algorithm for simulations of granular particles.

### The model

We consider a one–dimensional system of \( N \) elastic rods with mass density \( \rho \) and elastic module \( E \). The elastic state of the \( i \)th particle at time \( t \) is described by the longitudinal strain field \( u(s, t) \), \(-\frac{l_i}{2} \leq s \leq \frac{l_i}{2}\), where \( s \) is the internal position coordinate and \( l_i \) is the length of the one–dimensional rod. In order to separate internal and translational degrees of freedom the strain field contains only fluctuations, i.e. \( \int_{-\frac{l_i}{2}}^{\frac{l_i}{2}} ds \ u_i(s, t) \equiv 0 \), while homogeneous distortions contribute to the center of mass coordinate \( R_i \) of the particle. On collision adjacent particles interact via a potential \( V_{hc}(r) \), which depends only on the current end–to–end distance of the distorted rods \( r = R_{i+1,i} + u_{i+1}(-\frac{l_{i+1}}{2}, t) - u_i(\frac{l_i}{2}, t) \), where \( R_{i+1,i} := R_{i+1} - R_i - \frac{l_i + l_{i+1}}{2} \). In the present calculations we investigate an exponential interaction potential with characteristic length scale \( \frac{1}{\alpha} \)

\[
V_{hc}(r) = Be^{-\alpha r},
\]

which includes for large \( \alpha \) the limit of a hard core potential. The constant \( B \) can be chosen arbitrarily, since changing its value merely corresponds to a rescaling of the relativ coordinates \( R_{i+1,i} \). We expand the strain fields \( u_i \) in sine and cosine normal modes with amplitudes \( q_{i,\nu}(t) \) and normal frequencies \( \omega_{i,\nu} = \nu \pi c_{li} \), where \( c = \sqrt{\frac{E}{\rho}} \) is the speed of sound.

If we denote conjugate moments by \( p_i \) and \( p_{i,\nu} \), respectively, and treat the elastic energy in harmonic approximation, the Hamiltonian reads

\[
H = H_{\text{bath}} \left\{ p_i^{\nu}, q_i^{\nu} \right\} + H_{\text{trans}} + H_{\text{int}}
\]

\[
= \sum_{i=1}^{N} \sum_{\nu=1}^{\infty} \left\{ \frac{p_i^{\nu 2}}{2m_i} + m_i \omega_{i,\nu}^2 q_i^{\nu 2} \right\} + \sum_{i=1}^{N} \frac{p_i^2}{2m_i} + \sum_{i=1}^{N} B \exp \left\{ -\alpha \left( R_{i+1,i} + \sqrt{2} \sum_{\nu} (q_{i+1,\nu} - (-1)^\nu q_{i,\nu}^*) \right) \right\} .
\]

Here we assume periodic boundary conditions, i.e. place the particles on a ring with perimeter \( P \), so that \( R_{N+1,N} := P + R_1 - R_N \) and \( q_{N+1,\nu} := q_1^{\nu} \). Because of the non-linear coupling between oscillator modes our model has some resemblance with the classical Fermi–Pasta–Ulam (FPU) problem. The important difference is that here the interaction is "switched" on and off depending on the relative distance of the translational coordinates: As long as a particle is not involved in a collision, all its vibrational modes are effectively decoupled.

### Equipartition properties

We now confine ourselves to two–particle collisions and consider the case \( N = 2 \): In the center of mass frame we introduce the reduced mass \( \mu \) and an effective length scale
$l=2l_1l_2/(l_1+l_2)$. Taking $N_{\text{modes}}$ normal modes for each particle we numerically integrate the equations of motion resulting from the Hamiltonian (2). The following scenario is considered: We start with an initial relative velocity $\dot{R}_{2,1}(0)=-V_0$ and place the particles at maximum distance, $R_{2,1}(0)=P/2 \gg \frac{1}{l}$. We concentrate on the hard core limit $\alpha \gg \frac{1}{l}$ and set the initial temperature of the bath of oscillators equal to zero: $q_i^{(v)}(0)=p_i^{(v)}(0)=0$. The system now undergoes an infinite series of collisions with the two particles colliding alternately at either ends. We observe a rapid decrease of $E_{\text{tr}}=\frac{1}{2}\dot{R}_{2,1}^2$, the kinetic energy of the relative coordinate. Fig. 1 displays a decay of $E_{\text{tr}}$ over a range of approximately 100 collisions until a stationary state is reached with the kinetic energy fluctuating around an equilibrium value $\mu V_0^2/2(2N_{\text{modes}}+1)$, that is, of course, essentially zero for large $N_{\text{modes}}$. We interprete this phenomenon as a spreading of the translational energy among all degrees of freedom of the system.

This view is supported by a statistical analysis of the distribution of vibrational energies: Denoting modal energies by $E_i^{(v)}$ we define the energy of the oscillator bath as $E_{\text{bath}} = \sum_{\nu=1,2} \sum_i E_i^{(v)}$. After a transient time we calculate the relative modal energies $w_i^{(v)} = E_i^{(v)}/E_{\text{bath}}$ after each collision and take the average. (Due to the continuous interchange of energy between translational and vibrational modes $E_{\text{bath}}$ itself is a dynamical quantity.) The resulting energy spectrum (inset of Fig. 1) shows a homogeneous partition of vibrational energies. This is what we shall call modal equipartition regime in the following. (For particular values of $\gamma = l_1/l_2$, the length ratio of the rods, we found a periodic structure underlying the spectra. This subtlety does not affect the main results of this section, however.) We have also investigated the distribution function of $w_i^{(v)}$ ($i$ and $v$ fixed) and always observed an excellent agreement with the Boltzmann distribution.

An important question is, how fast the modal equipartition regime is reached. Does the relaxation time (measured by the number of collisions) scale with $N_{\text{modes}}$? A sensitive probe of equipartition is the normalized spectral entropy $\eta = 1-h/h_{\text{max}}$, where $h = -\sum_{i,v} w_i^{(v)} \ln w_i^{(v)}$ and $h_{\text{max}} = \ln(2N_{\text{modes}})$, which was first introduced in numerical studies on the FPU problem (3). If equipartition takes place, $\eta$ will decay from its initial value $\eta = 1$ to its equilibrium value $\eta_{eq}$ (for Boltzmann distributed $w_i^{(v)}$ one finds $\eta_{eq} \approx 0.423/\ln(2N_{\text{modes}})$). Our plot of $\eta$ for different numbers of modes (Fig. 2) suggests a relaxation time of approximately 20 collisions, essentially independent of $N_{\text{modes}}$. Comparison with Fig. 1 shows that the time scale for modal equipartition is considerably shorter than the relaxation time of the granular cooling process.

**Stochastic coefficient of restitution**

We are now going to discuss in detail a single two–particle collision in the modal equipartition regime. Let us denote the precollisional and post–collisional relative velocity of the particles by $-V$ and $V'$, respectively. In our model the coefficient of restitution $\epsilon = V'/V$ is a stochastic quantity (cf. Fig. 1) and the collision process is described by a stochastic differential equation. If modal equipartition is valid, we can apply the usual concepts of statistical physics and consider the precollisional values of the internal coordinates as independent, Boltzmann distributed variables (with bath temperature $T_{\text{bath}} = E_{\text{bath}}/2N_{\text{modes}}$). Note that this choice of initial conditions is equivalent to imposing a Markov approxi-
mation on the collisional dynamics, since correlations with preceding collision events are neglected.

Obviously, the coefficient of restitution contains the complete information about the energy transfer between \( E_{tr} = \frac{1}{2} V^2 \) and \( T_{bath} \): Due to conservation of total energy we have \( E_{tr}' = \epsilon^2 E_{tr} \) and \( T_{bath}' = T_{bath} + \frac{1}{2} \epsilon^2 E_{tr} \) after collision. In order to derive the equation of motion for the translational coordinate it is convenient to introduce the following scaled variables: \( \tau = \gamma t \) (scaled physical time), \( z(\tau) = \alpha R_{2,1} \), \( z_0 = z(\tau_0) \) (initial distance), and \( \kappa = \alpha \sqrt{\frac{2}{\gamma}} \) (= \(- \frac{d}{d\tau} (\tau_0) \), scaled initial velocity). Again we are mainly interested in the hard core limit so that now \( \kappa \gg 1 \) is our large control parameter. Furthermore we set the free constant \( B = \mu \frac{\epsilon^2}{(\alpha \gamma)^2} \). The internal coordinates in Hamilton’s equations of motion can be integrated out using Green’s function method and we arrive at the following equation for \( W(\tau) = \frac{dW}{d\tau} + \kappa \), the velocity increase throughout collision:

\[
\frac{dW}{d\tau} = \exp \left\{ \kappa \tau - z_0 - W(\tau) - \sum_{i=1,2} \sum_{n=1}^{\infty} W(\tau - n \Gamma_i) + Q_1(\tau) + Q_2(\tau) \right\} ,
\]

with \( W(\tau) := 0 \) for \( \tau \leq \tau_0 \). The coefficient of restitution is then obtained from the asymptotics of \( W \):

\[
\epsilon = \lim_{\tau \rightarrow \infty} \frac{W(\tau)}{\kappa} - 1 .
\]

In Eq. (3) \( \Gamma_1 = 1 + \gamma \) and \( \Gamma_2 = 1 + 1/\gamma \) are the periods of the lowest normal modes in scaled time and \( Q_1, Q_2 \) are Gaussian stochastic processes resulting from the initial conditions. They take on the form of stochastic Fourier series \( Q_i(\tau) = \sum_{n=1}^{\infty} \frac{a_{in}}{n} \sin(n2\pi \tau / \Gamma_i) + \sum_{n=1}^{\infty} \frac{b_{in}}{n} \cos(n2\pi \tau / \Gamma_i) \) with independent and identically distributed Gaussian coefficients \( a_{in}, b_{in} \). As a consequence, we have

\[
< Q_i(\tau) > = 0
\]

and

\[
< Q_i(\tau) Q_j(\tau') > = \delta_{ij} \kappa^2 \frac{T_{bath} \Gamma_i}{E_{tr}} \left\{ \frac{(\tau - \tau')}{1_i} - \frac{1}{2} - \frac{1}{12} \right\}
\]

for \( 0 \leq \tau - \tau' \leq \Gamma_i \) and periodic continuation everywhere else. The periodicity of the correlation function and the memory terms in Eq. (3) reflect the fact, that we consider a system of ideal oscillators that never forgets its collision history. Note that typical fluctuations of the noise processes are of the same order as \( W(\tau) \), which makes an analytical treatment even more difficult.

However, it is possible to solve the deterministic equation \( T_{bath} = 0 \): In the large \( \kappa \) regime the coefficient of restitution is essentially given by the length ratio \( \gamma \): \( \epsilon = \min(\gamma, 1/\gamma) + \ln(\kappa(\Gamma_2 - \Gamma_1)/\kappa) \), and the actual collision takes place in the time interval \([\frac{\tau_0}{\kappa}, \frac{\tau_0}{1\kappa} + \min(\Gamma_1, \Gamma_2)]\), i.e. the duration of the collision is equal to the wave propagation time of the shorter rod. These results are in agreement with the wave theory of impact [11], that 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.

For \( T_{bath} \neq 0 \) we had to integrate Eq.(3) numerically and average over many realizations of the noise processes. We have focussed on the statistics of \( \epsilon^2 \), since it is the relevant
quantity for energy transfer. In the hard core regime ($\kappa$ larger than $\approx 30$) the probability density of $\epsilon^2$, $p(\epsilon^2)$, does not significantly depend on $\kappa$, but it is still a function of $E_{tr}/T_{bath}$ and $\gamma$. Recall that Eq. (3) describes a single collision, given the current values of $E_{tr}$ and $T_{bath}$. After collision the energy ratio has changed to $E'_{tr}/T'_{bath}$ (see above) and in turn there is a different distribution of $\epsilon^2$ at the next collision. Fig. 3 displays plots of the distribution function for different values of the parameters.

The important point is that $p(\epsilon^2)$ has to be interpreted as a transition density: In the context of the Markov approximation leading to Eqs. (3), (5), the time evolution of $E_{tr}$ (cf. Fig. 1) is simply a Markovian jump process in discrete "time" (i.e. cumulative number of collisions). If the system is in a state with energy $E_{tr}$, the probability density for a transition to energy $E'_{tr}$ is determined by

$$p(E_{tr} \rightarrow E'_{tr}) = \frac{1}{E_{tr}} p\left(\epsilon^2 = \frac{E'_{tr}}{E_{tr}}\right). \quad (6)$$

As expected, the transition density resulting from Eq. (3) can be shown numerically to yield a stationary energy density $p^{\text{stat}}(E_{tr}) \propto \exp\left(-\frac{E_{tr}}{T_{bath}}\right)$. In view of the many–particle problem (see below) it seems reasonable to replace the exact distribution of $\epsilon^2$ by a simpler one, that obeys detailed balance and leads to the same stationary density $p^{\text{stat}}(E_{tr})$. A possible choice, for example, is the analog of Glauber dynamics [12] for Ising spin systems:

$$p^{(G)}(\epsilon^2) = \frac{E_{tr}}{T_{bath}} \exp\left(-\epsilon^2 \frac{E_{tr}}{T_{bath}}\right). \quad (7)$$

Many–particle problem

For the many–particle system translational energy and bath temperature become functions of time and position. From the preceding sections it is clear that each two–particle collision tends to establish a state where locally $E_{tr} \approx T_{bath}$. As in the case $N = 2$, we assume modal equipartition for each particle and treat collisions in the Markov approximation. Furthermore, we expect that the cooling properties of the system will not sensitively depend on the detailed form of the probability density $p(\epsilon^2)$.

For computer simulations we therefore suggest an algorithm that is a combination of ED and Monte Carlo methods: Each of the $N$ particles is assigned an individual bath temperature $T^{(i)}_{bath}$ that characterizes its vibrational state. For each collision the following steps have to be performed: (1) Calculate the next collision event by the ED procedure. (2) For the colliding pair determine $E_{tr}$ and an averaged local bath temperature $T_{bath}$. With these parameters choose $\epsilon$ randomly from a simple distribution, e.g. $p^{(G)}(\epsilon^2)$. (4) Update the relative velocities and the post–collisional values of $T^{(i)}_{bath}$; go back to (1).

Another possible extension of our study would be a generalization of the inelastic Boltzmann equation [4, 11] to a stochastic coefficient of restitution. Work along these lines is in progress.

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Figure captions

**Figure 1:** Time evolution of the relative kinetic energy for a two–particle system with length ratio $\gamma = l_1/l_2 = 0.6173$, $\alpha V_0/c l = 4000$, and $N_{\text{modes}} = 75$. The dashed line is the equilibrium value resulting from energy equipartition. 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. Grey and black bars correspond to particle 1 and 2, respectively.

**Figure 2:** Time behaviour of the spectral entropy $\eta$ for different numbers of modes. Again, $\gamma = 0.6173$ and $\alpha V_0/c l = 4000$.

**Figure 3:** The probability density $p(\epsilon^2)$ (dotted line) and its integral, the distribution function (full line), for different energy and length ratios: a) $E_{\text{tr}}/T_{\text{bath}} = 10$, $\gamma = 0.6173$, b) $E_{\text{tr}}/T_{\text{bath}} = 1$, $\gamma = 0.6173$, and c) $E_{\text{tr}}/T_{\text{bath}} = 1$, $\gamma = 0.2173$. Data were obtained from the numerical integration of 8000 realizations of Eq. (3) in the hard core regime ($\kappa = 100$).
Goetz Giese, Fig. 3

\[ p(\epsilon^2), D(\epsilon^2) \]

\[ \epsilon^2 \]
Goetz Giese, Fig. 2

Collision no.

\[ \eta \]

\begin{align*}
&\text{75 modes} \\
&\text{50 modes} \\
&\text{25 modes}
\end{align*}
Goetz Giese, Fig. 1