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*"Inelastic Hard Spheres with Random Restitution Coefficient: a New  
Model for Heated Granular Fluids"*

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# Inelastic hard spheres with random restitution coefficient: a new model for heated granular fluids

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We consider a vertically shaken granular system interacting elastically with the vibrating boundary, so that the energy injected vertically is transferred to the horizontal degrees of freedom through inter-particle collisions only. This leads to collisions which, once projected onto the horizontal plane, become essentially stochastic and may have an effective restitution coefficient larger than 1. We therefore introduce the model of inelastic hard spheres with random restitution coefficient  $\alpha$  (larger or smaller than 1) to describe granular systems heated by vibrations. In the non-equilibrium steady state, we focus in particular on the single particle velocity distribution  $f(v)$  in the horizontal plane, and on its deviation from a Maxwellian. We use Molecular Dynamics simulations and Direct Simulation Monte Carlo (DSMC) to show that, depending on the distribution of  $\alpha$ , different shapes of  $f(v)$  can be obtained, with very different high energy tails. Moreover, the fourth cumulant of the velocity distribution (which quantifies the deviations from Gaussian statistics) is obtained analytically from the Boltzmann equation and successfully tested against the simulations.

## I. INTRODUCTION

Granular matter can exist in many very different states, all of which are currently subject of a large interest [1]. On the one hand, dense granular matter can be studied at rest, and in particular many open problems concern the transmission of forces through a sandpile. On the other hand, since thermal energy is negligible with respect to gravitational or kinetic energy, any dynamical behaviour has to be a response to a certain external energy input: for example, tapping leads to compaction [2], while a strong, continuous energy input by vibrations produces granular gases in continuous motion, for which kinetic energy is much larger than the gravitational one [3–8]. These vibrated systems are out of equilibrium but the energy input can compensate the dissipation due to inelastic collisions between grains and therefore lead to stationarity. While many experiments study the appearance of patterns or inhomogeneities, others, on which we will here concentrate, focus on the velocity distributions and its deviations from the Maxwell-Boltzmann distribution (which would correspond to a system with neither dissipation -i.e. elastic collisions- nor energy injection).

## II. SYSTEM STUDIED AND MODELISATION

We want to study a three-dimensional system of grains on a plate, which is shaken vertically (i.e. along the  $z$  direction): the energy is therefore injected by a vibrating elastic boundary only in the  $z$  direction (Figure 1). It is partly transferred to the other degrees of freedom, and also dissipated, through the inelastic collisions between grains. The velocities and their distribution are then studied in the horizontal ( $xy$ ) plane.

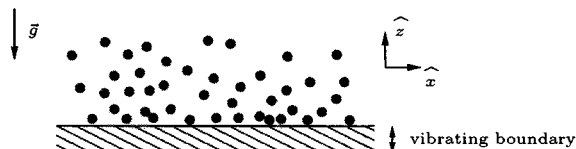


FIG. 1. Schematic view of the system under consideration: the grains are subject to gravity, and submitted to the vibration of an horizontal plate.

### A. Usual theoretical approach

The grains are modeled as smooth inelastic hard spheres (IHS) undergoing binary momentum-conserving collisions with a constant normal restitution coefficient  $\alpha < 1$ : a collision between two spheres 1 and 2, with velocities  $\mathbf{v}_1$  and

$\mathbf{v}_2$ , dissipates a fraction  $(1 - \alpha)$  of the component of the relative velocity  $\mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2$  along the center-to-center direction  $\hat{\sigma}$ . Once the dissipation has been described in this way, the problem is how to represent the energy injection. A possibility, used and studied by various authors [9–13], consists in submitting the spheres to a random force, i.e. to random “kicks” at a given frequency between collisions. Energy input then acts in all space directions.

### B. A new model

However, as previously noted, the real energy input occurs only in the vertical direction, and is not transferred *between* but *through* collisions to the horizontal plane. Indeed, a three-dimensional inelastic collision between two spheres globally dissipates energy, but its projection onto the  $xy$  plane can in fact gain energy (see fig 2 for an example). Therefore, the *effective* restitution coefficient of the *projected* collision can be larger than 1. This observation leads to the following effective (projected) simple model [14]:

- two-dimensional hard spheres (of diameter  $\sigma$ ) in the  $xy$ -plane
- binary momentum-conserving collisions
- *random* normal restitution coefficient  $\alpha$  ( $< 1$  or  $> 1$ ) with distribution  $\rho(\alpha)$  (the means over  $\rho(\alpha)$  will be denoted by an overline), uncorrelated with the velocities of the particles.

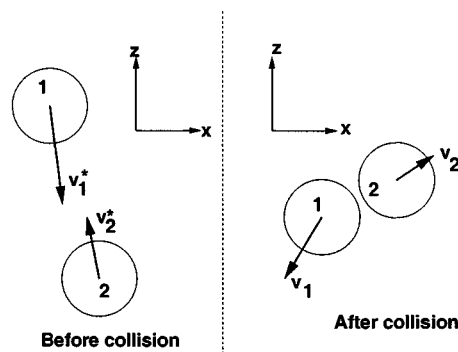


FIG. 2. Example of a globally dissipative collision leading to an energy increase in the horizontal plane.

Since, in a binary collision with restitution coefficient  $\alpha$ , the energy change is proportional to  $(\alpha^2 - 1)$ , we shall consider distributions with  $\overline{\alpha^2} = 1$  in order to ensure a stationary, constant temperature regime (at each collision, energy changes, but it is conserved on average). Since the average energy is constant, the granular temperature is also a constant determined by the initial velocity distribution. We will therefore study the distribution of *rescaled* velocities  $\mathbf{c} = \mathbf{v}/v_0$ , using analytical and numerical tools.

### III. KINETIC THEORY

The Molecular chaos approximation factorizes the two-point distribution function:

$$f^{(2)}(\mathbf{v}_1, \mathbf{v}_2, \underbrace{|\mathbf{r}_{12}| = \sigma, t}_{\text{contact}}) = \chi f(\mathbf{v}_1, t) f(\mathbf{v}_2, t) \quad (1)$$

where  $\chi$  accounts for excluded volume effects (for elastic hard spheres,  $\chi$  coincides with the density dependent pair correlation function at contact). We are then able to write the (Enskog-)Boltzmann equation in the steady state, averaged over the distribution of restitution coefficients:

$$\int' d\mathbf{v}_2 d\hat{\sigma} d\alpha (\mathbf{v}_{12} \cdot \hat{\sigma}) \rho(\alpha) \{ \alpha^{-2} f(\mathbf{v}_1^*) f(\mathbf{v}_2^*) - f(\mathbf{v}_1) f(\mathbf{v}_2) \} = 0 \quad (2)$$

The prime on the integration symbol is a shortcut for  $\int d\hat{\sigma} \Theta(\mathbf{v}_{12} \cdot \hat{\sigma})$  ( $\hat{\sigma}$  is the center-to-center direction and  $\Theta$  is the Heavyside function), and we consider collisions which yield  $(\mathbf{v}_1, \mathbf{v}_2)$  as postcollisional velocities, for precollisional velocities  $(\mathbf{v}_1^*, \mathbf{v}_2^*)$ :

$$\begin{aligned} \mathbf{v}_1^* &= \mathbf{v}_1 - \frac{1}{2} \left( 1 + \frac{1}{\alpha} \right) (\mathbf{v}_{12} \cdot \hat{\sigma}) \hat{\sigma} \\ \mathbf{v}_2^* &= \mathbf{v}_2 + \frac{1}{2} \left( 1 + \frac{1}{\alpha} \right) (\mathbf{v}_{12} \cdot \hat{\sigma}) \hat{\sigma} . \end{aligned} \quad (3)$$

From now on, we will be concerned with the study of the rescaled velocities  $\mathbf{c} = \mathbf{v}/v_0$  and of their distribution:

$$f(\mathbf{v}, t) = \frac{n}{v_0^d(t)} P(c) , \quad (4)$$

where  $n$  is the density and the thermal velocity  $v_0$  is by definition related to the temperature  $T(t)$  through  $\frac{m}{2} v_0^2(t) = T(t) \equiv \frac{2}{nd} \int d\mathbf{v} \frac{m}{2} v^2 f(\mathbf{v}, t)$  ( $d$  is the space dimension).

It is usual to look for solutions in the form of a Sonine expansion [15] around the Maxwell-Boltzmann distribution  $\Phi(c) = \pi^{-d/2} \exp(-c^2)$

$$P(c) = \Phi(c) \left[ 1 + \sum_{p=1}^{\infty} a_p S_p(c^2) \right] \quad (5)$$

where the polynomials  $\{S_p\}$  are orthogonal for the Gaussian weight  $\Phi$ .

Using the methods exposed in [11], we obtain the leading non Gaussian correction ( $a_1 = 0$  from the definition of temperature)  $a_2$ , which is related to the fourth cumulant:

$$a_2 \equiv \frac{\langle c^4 \rangle}{\langle c^4 \rangle_{\Phi}} - 1 = \frac{16 \left( 1 - 3\overline{\alpha^2} + 2\overline{\alpha^4} \right)}{9 + 24d + 32(d-1)\overline{\alpha} + (8d-11)\overline{\alpha^2} - 30\overline{\alpha^4}} \quad (6)$$

We will compare this result to numerical simulations in the next section, for  $d = 2$ . For the high energy tail, no analytical results have been obtained and we will investigate this issue numerically.

## IV. NUMERICAL SIMULATIONS

### A. Methods

We use two complementary approaches

- the Direct Monte Carlo Simulation method (DSMC) [16] generates a Markov chain with the same probabilities of transition as the Boltzmann equation: it produces therefore an “exact” numerical solution of the Boltzmann equation.
- Molecular Dynamics (MD) integrate the *exact* equations of motion of the hard spheres, with no reference to the Boltzmann equation: we consider  $N$  spheres of diameter  $\sigma$ , in a box of linear size  $L$  in dimension  $d$  (here  $d = 2$ ), with periodic boundary conditions [17,18]; the comparison with DSMC allows to test the molecular chaos approximation.

### B. Results

The first results show the validity of the Sonine expansion and of the theoretical values for  $a_2$ : figure 3 shows a comparison between DSMC results and the theoretical expansion: the agreement is perfect at small  $a_2$ , and satisfying at low velocities (note that the Sonine expansion is a low-velocities expansion) for larger  $a_2$ .

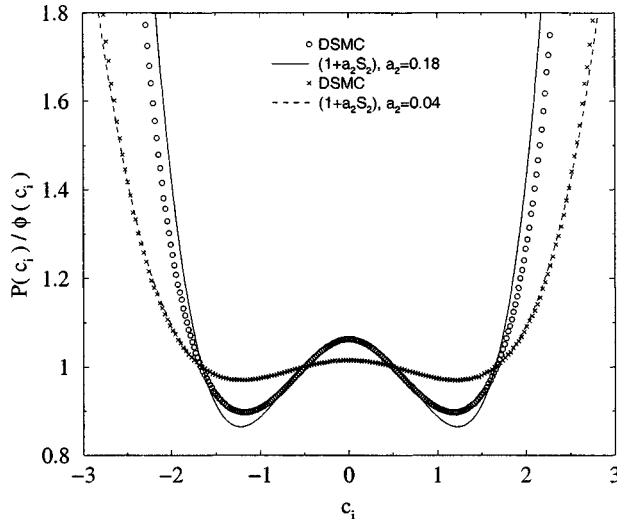


FIG. 3. Comparison of the  $P(c)/\Phi(c)$  measured in DSMC (symbols) with the Sonine expansion with the calculated  $a_2$  (lines), for two different  $\rho(\alpha)$ : flat distribution of  $\alpha^2 \in [0.5, 1.5]$  ( $a_2 = 0.04$ ), and flat distribution of  $\alpha^2 \in [0, 2]$  ( $a_2 = 0.18$ ).

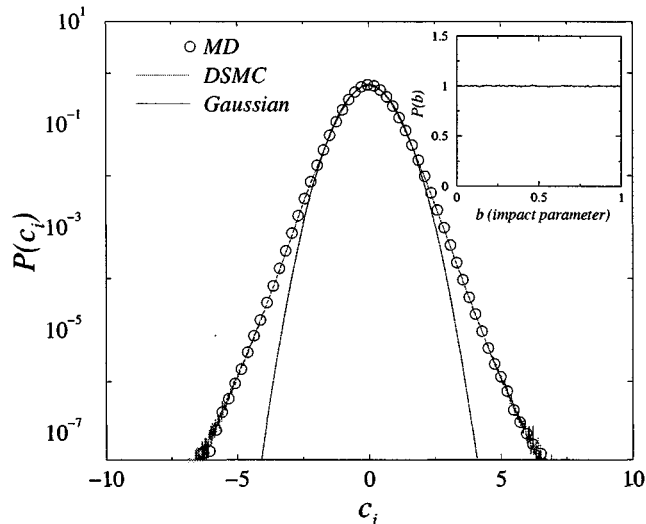


FIG. 4. Velocity distribution  $P(c)$ , for a flat distribution of  $\alpha^2 \in [0, 2]$ , for MD and DSMC. MD:  $50 \cdot 10^3$  particles (30 % packing fraction); DSMC:  $500 \cdot 10^3$  particles. A Gaussian is also shown for comparison. Inset: distribution of normalized impact parameters in MD

Moreover, figure 4 shows that MD and DSMC simulations are in perfect agreement (shown only for a particular choice of  $\rho(\alpha)$ , but checked for other choices of  $\rho(\alpha)$ ). Moreover, the curves obtained in MD simulations with small or large packing fractions (up to 40%) are indistinguishable (not shown). Important deviations from the Maxwell-Boltzmann distribution are obtained, but the inset shows that the distribution of impact parameters in Molecular Dynamics simulations is flat: this is a hint that no violation of molecular chaos is observed and that the factorization of the 2-particle correlation function Eq. (1) holds. In MD simulations, inhomogeneities and/or violations of molecular chaos could a priori appear, contrarily to DSMC. The fact that no such phenomenon is observed is in contrast with the phenomenology at constant  $\alpha$  [19] or with randomly driven IHS [20]: for a constant dissipative restitution parameter, colliding particles emerge with more parallel velocities than in the elastic case  $\alpha = 1$  and, when they recollide, their velocities are still more parallel. The possibility of having  $\alpha > 1$  seems to have removed this mechanism for the creation of velocity correlations violating molecular chaos, and to produce an efficient randomization of the velocities. This validates the theoretical approach based on the Boltzmann equation.

Let us now turn to the study of the large velocity tails: figure 5 shows fits to stretched exponentials (*over 6 orders*

of magnitude)

$$P(c) \propto \exp(-c^B)$$

with a wide range of possible values for  $B$ . In particular, a convenient choice of  $\rho(\alpha)$  is compatible with  $B = 1.6$ , which has been found in some experiments [6,7] (close to  $B = 3/2$  obtained in [11] for randomly driven IHS fluids). The possibility to obtain such different values of  $B$  may question the relevance of this exponent as an intrinsic quantity for granular gases in steady states.

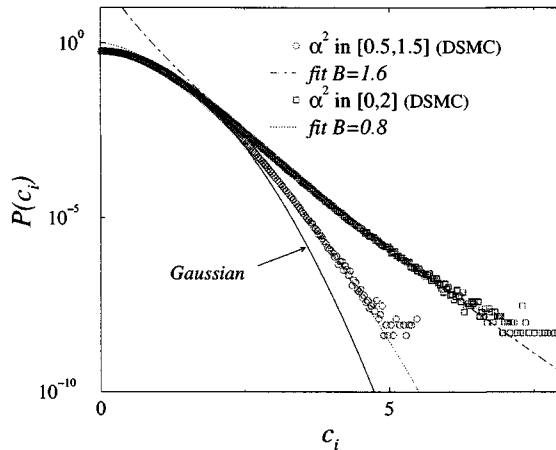


FIG. 5. Fits to stretched exponential forms  $\exp(-c^B)$  of the velocity distributions, for a flat distribution of  $\alpha^2 \in [0, 2]$  and  $\in [0.5, 1.5]$ .

## V. CONCLUSIONS AND PERSPECTIVES

We have introduced the idea of a random restitution coefficient in the IHS model, in order to account for the fact that, for a vertically vibrated layer of granular material, the energy is injected only along the vertical axis, and transferred through collisions in the horizontal directions: the projection in 2 dimensions of a 3-dimensional collision can correspond to a gain in the two-dimensional energy, and therefore to an effective restitution coefficient larger than 1, even if the genuine  $\alpha$  is necessarily smaller than 1, i.e. corresponds to a dissipative collision.

We have subsequently studied this model in 2 dimensions, with a probability distribution  $\rho(\alpha)$  for the restitution coefficient. We have focused on the velocity distributions, and in particular on the deviation from the Maxwellian:

- at low velocities, the Sonine expansion technique is used: we obtained analytically the expression of the fourth cumulant  $a_2$  and tested it against Molecular Dynamics (MD) and Monte Carlo Direct Simulations (DSMC). The theoretical predictions for  $a_2$  are quite accurate, with a slight overestimation for  $a_2$  that probably corresponds to the approximations made during the calculation (nonlinear terms  $\mathcal{O}(a_2^2)$  and higher order Sonine polynomials neglected); Moreover, the comparison between numerical data and the second order Sonine expansion shows a remarkable agreement for small values of  $a_2$ .
- the high energy tails, studied with DSMC simulations, can be fitted by functions of the form  $\exp(-Ac^B)$ , with  $B < 2$  depending on  $\rho(\alpha)$ . It would certainly be interesting to have theoretical predictions concerning  $B$ . Note that once a functional form has been chosen for  $\rho(\alpha)$ , very different tails can be observed depending on the range of variation for  $\alpha$ . This feature might question the relevance of the exponent  $B$  as an intrinsic quantity for granular gases in steady states.

The comparison of MD and DSMC results shows a remarkable agreement (even with a packing fraction as high as 40% in MD), and the study of the impact parameter in MD shows no violation of molecular chaos. This is to be compared with the situation of free cooling [19] but also with MD results on heated inelastic hard spheres with constant restitution coefficient [20], in which microscopic precollisional velocity correlations develop and molecular chaos is violated. A thorough investigation of short scale velocity correlations would require the computation of various precollisional averages involving moments of the relative velocities, and has not been performed. Our results however suggest that the dynamical correlations inducing recollisions [21] and responsible for the violation of molecular chaos may not be a generic feature of driven granular gases exhibiting a non equilibrium stationary state.

In the model introduced here, the random restitution coefficient is uncorrelated with the relative velocities of the particles; this somehow unrealistic feature could be improved in more refined models. Such correlations, which seem difficult to quantify from first principles, might affect the high energy tail or induce precollisional velocity correlations. It would be very interesting to be able to link a realistic energy injection mechanism with a precise distribution of restitution coefficients.

Finally, a hydrodynamic study of the present random  $\alpha$  model, in which the conservation of the energy is valid on average only, while density and momentum are conserved locally, is left for future investigations.

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# TRANSPARENCIES

## Heated granular fluids: the random restitution coefficient approach

(Eur. Phys. J. B 5, 161 (2001))

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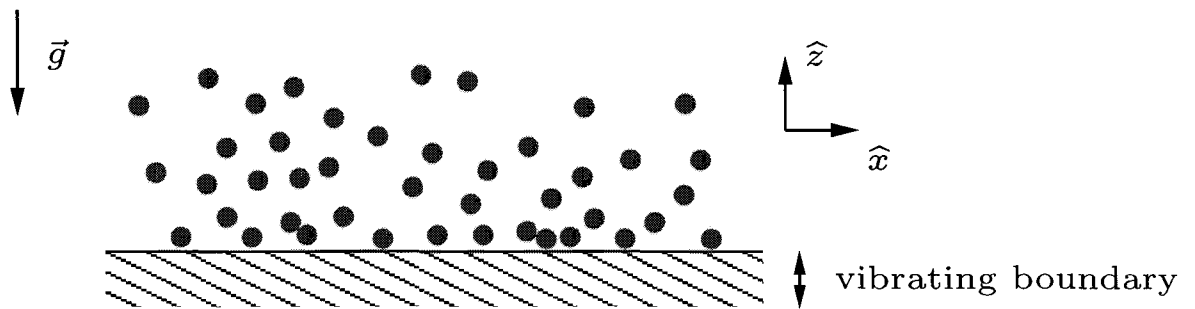
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- ◇ Collective behaviour of granular gases → ??
  - “ $T = 0$ ” media (particles of large mass)
  - dissipative collisions, unlike molecular gases
- vibrated layers of grains: important out of equilibrium but stationary model system where vibration compensates the energy loss due to friction and inelasticity
- ◇ focus on velocity statistics and deviations from Maxwell-Boltzmann distribution (observed in experiments).

## The system



vertical ( $z$ ) energy input but study of  
the horizontal ( $xy$ ) velocities

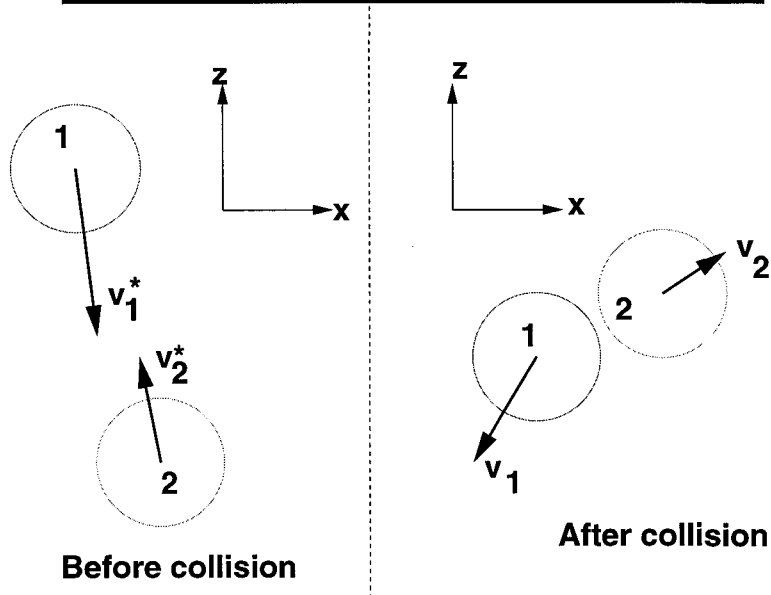
- ◇ Usual approach: inelastic hard spheres (IHS) with
    - constant normal restitution coefficient  $\alpha$
    - global energy injection through a random force $\Rightarrow$  Brownian “kicks” between collisions
- e.g. Williams et al, Puglisi et al, van Noije et al, Cafiero et al

- ◇ But... restricting to the horizontal plane:
  - $\longrightarrow$  projected 3D *dissipative* collisions lead to 2D *energy dissipation or injection* at each collision
  - $\longrightarrow$  stationary effective dynamics with a random restitution coefficient  $\alpha$

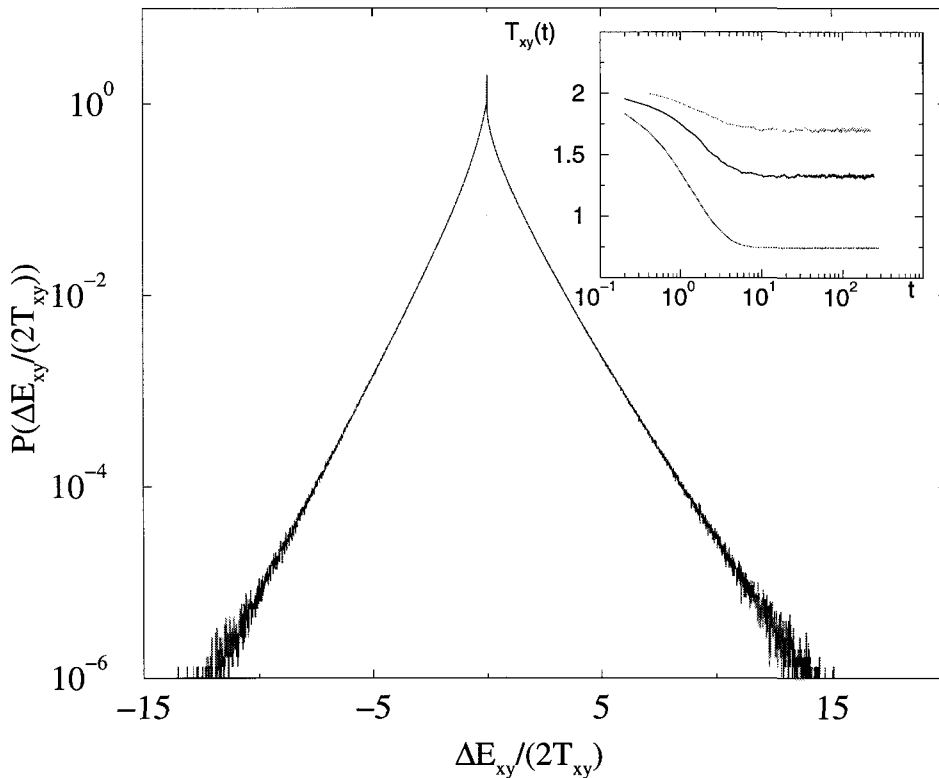
$\alpha > 1$  energy injection

$\alpha < 1$  energy dissipation

# Horizontal energy changes



Example of globally dissipative collision which leads to an energy gain in the horizontal plane



Histogram of the changes in the horizontal energy, for a DSMC simulation of a model with 3D collisions

## A new model

◇ Definition

smooth hard spheres in the  $xy$  plane

binary momentum-conserving collisions

random normal restitution  $\alpha$ , distribution  $\rho(\alpha)$

+ constraint to ensure a stationary state:

$$\overline{\alpha^2} = \int \alpha^2 \rho(\alpha) d\alpha = 1$$

◇ Study velocity distributions

- analytically (kinetic theory)
- numerically Monte Carlo (DSMC)  
Molecular Dynamics (MD)

## Kinetic theory

◇ Molecular chaos approximation:

$$f^{(2)}(\mathbf{v}_1, \mathbf{v}_2, \underbrace{|\mathbf{r}_{12}| = \sigma}_{\text{contact}}, t) = \chi f(\mathbf{v}_1, t) f(\mathbf{v}_2, t)$$

→ Boltzmann equation; in the steady state:

$$\int' d\mathbf{v}_2 d\hat{\sigma} d\alpha (\mathbf{v}_{12} \cdot \hat{\sigma}) \rho(\alpha) \{ \alpha^{-2} f(\mathbf{v}_1^*) f(\mathbf{v}_2^*) - f(\mathbf{v}_1) f(\mathbf{v}_2) \} = 0$$

where in a collision 1-2  $\{\mathbf{v}_1^*, \mathbf{v}_2^*\} \rightarrow \{\mathbf{v}_1, \mathbf{v}_2\}$

◇ Look for solutions in the form of a Sonine expansion

$$f(\mathbf{v}) = \mathcal{M}(\mathbf{v}) \left[ 1 + \sum_{p=1}^{\infty} a_p S_p(\mathbf{v}^2) \right]$$

the polynomials  $\{S_p\}$  are  $\perp$  for the Gaussian weight  $\mathcal{M}$

◇ Result: leading non Gaussian correction ( $a_1 = 0$ )

$a_2$  (kurtosis  $\sim$  fourth cumulant)

$$a_2 \equiv \frac{\langle \mathbf{v}^4 \rangle}{\langle \mathbf{v}^4 \rangle_{\mathcal{M}}} - 1 = \frac{16(1 - 3\overline{\alpha^2} + 2\overline{\alpha^4})}{9 + 24d + 32(d-1)\overline{\alpha} + (8d-11)\overline{\alpha^2} - 30\overline{\alpha^4}}$$

in dimension  $d$

## Numerical Simulations

*Two complementary approaches*

◇ Direct Monte Carlo Simulation method (DSMC)

Generate a Markov chain with the same probabilities of transition as the Boltzmann equation

→ “exact” numerical solution of the Boltzmann eq

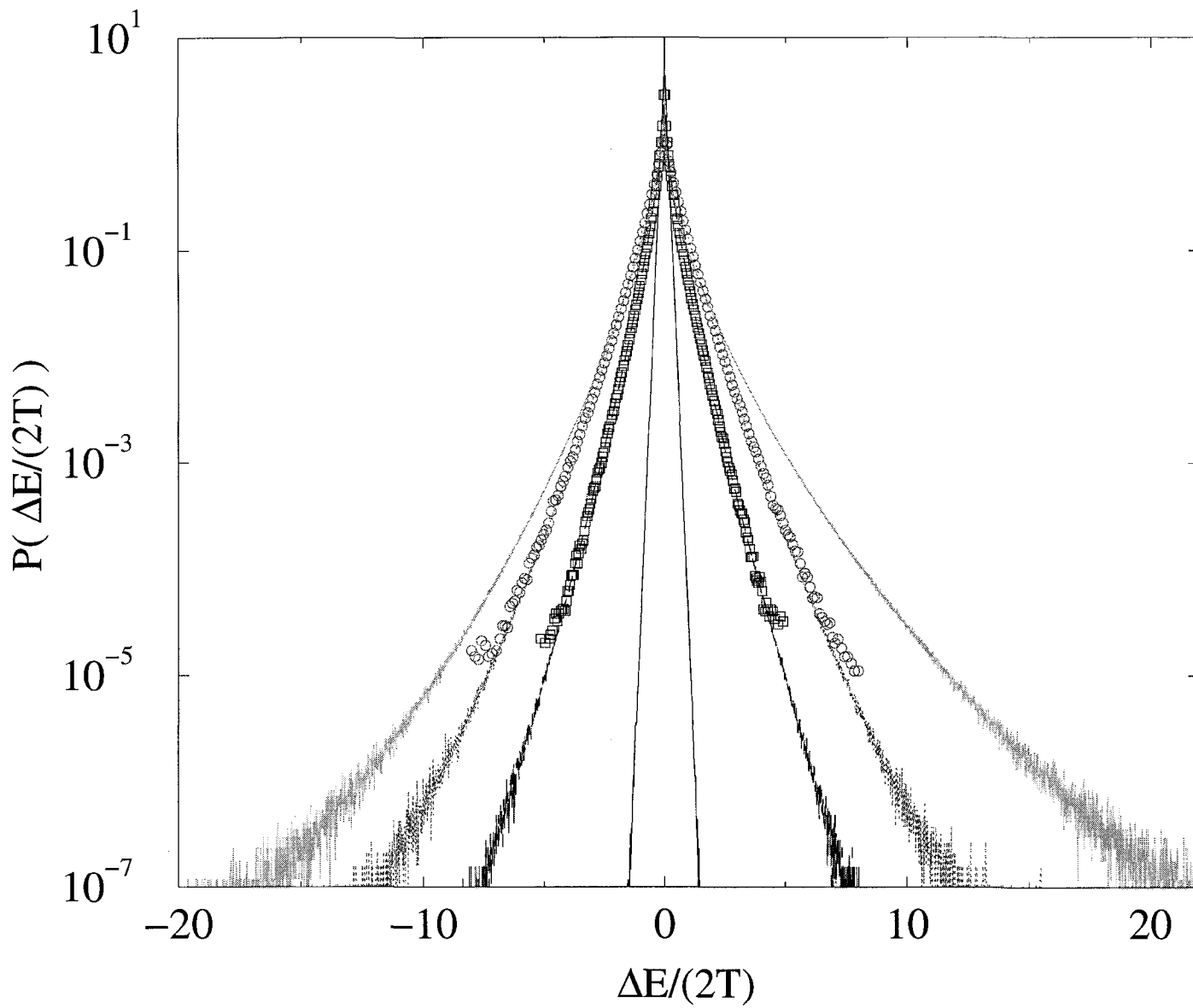
◇ Molecular Dynamics (MD)

Integrate the exact equations of motion

(with periodic boundary conditions)

→ tests the molecular chaos approximation

## Energy changes

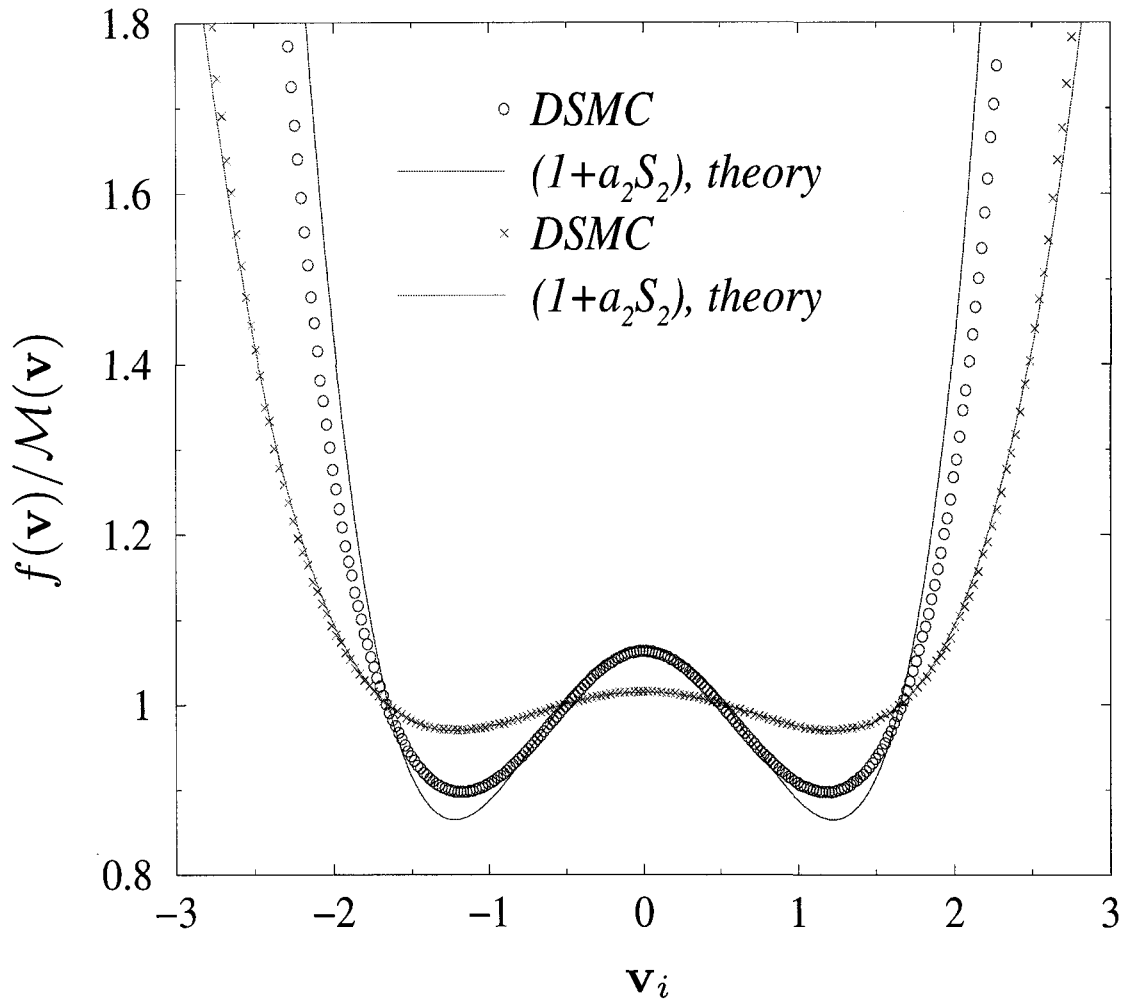


Histogram of the energy changes for various  $\rho(\alpha)$ .

Symbols: MD, lines: DSMC

# Velocity statistics I

Comparison theory/simulations

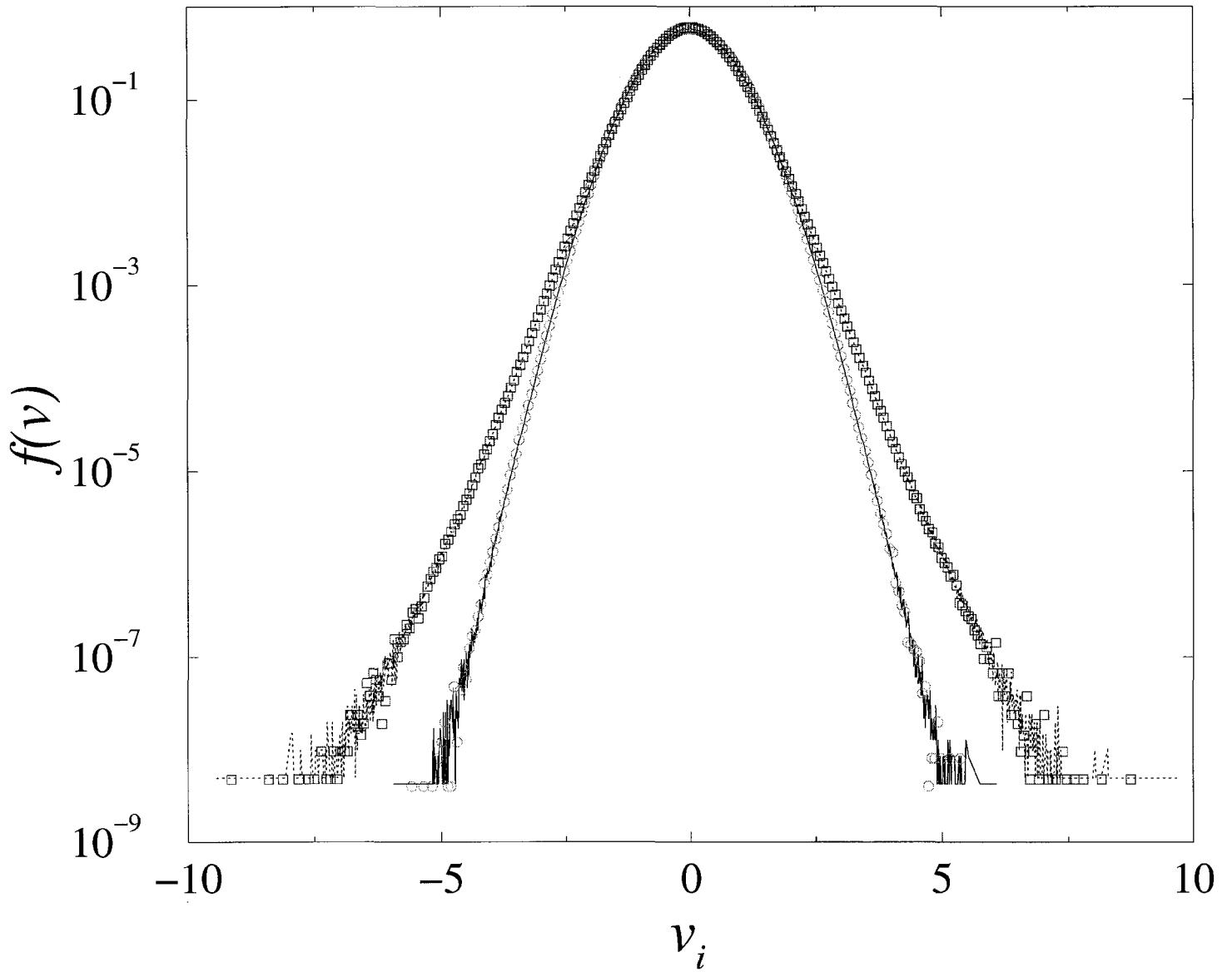


→ flat distribution of  $\alpha^2 \in [0.5, 1.5]$  ( $a_2 = 0.04$ )

→ flat distribution of  $\alpha^2 \in [0, 2]$  ( $a_2 = 0.18$ )



## Velocity statistics II

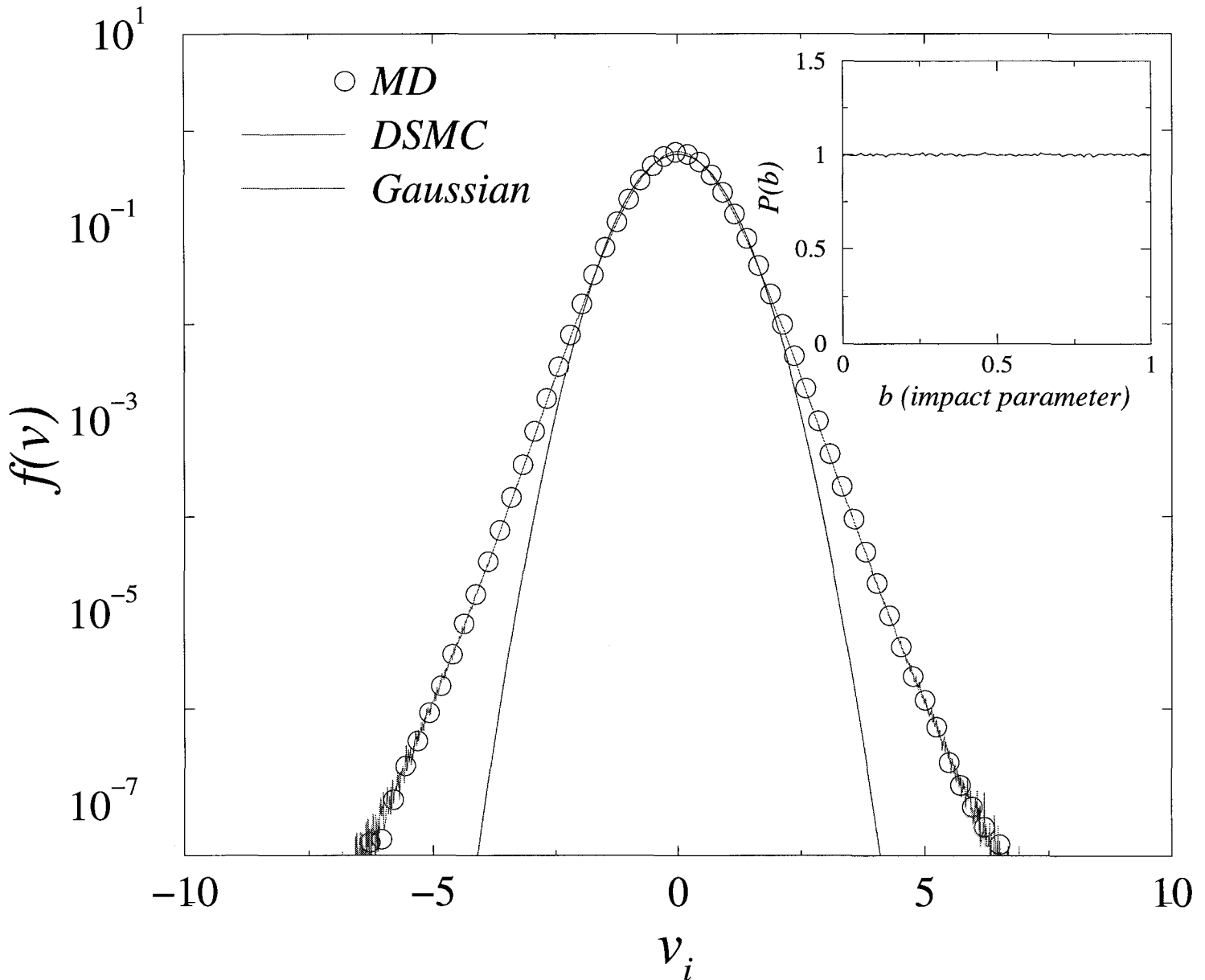


DSMC simulations ( $500 \cdot 10^3$  particles)

lines: flat distributions of  $\alpha^2 \in [0, 2]$  and  $\in [0.5; 1.5]$   
symbols: trimodal distributions with the same  $\bar{\alpha}$ ,  $\overline{\alpha^2}$ ,  $\overline{\alpha^4}$   
than the flat distributions

# Velocity statistics III

## Comparison MD/DSMC



flat distribution of  $\alpha^2 \in [0, 2]$

MD:  $50 \cdot 10^3$  particles (30 % packing fraction)

DSMC:  $500 \cdot 10^3$  particles (1 cell  $\leftrightarrow$  homogeneous solution)

Inset: distribution of normalized impact parameters in MD

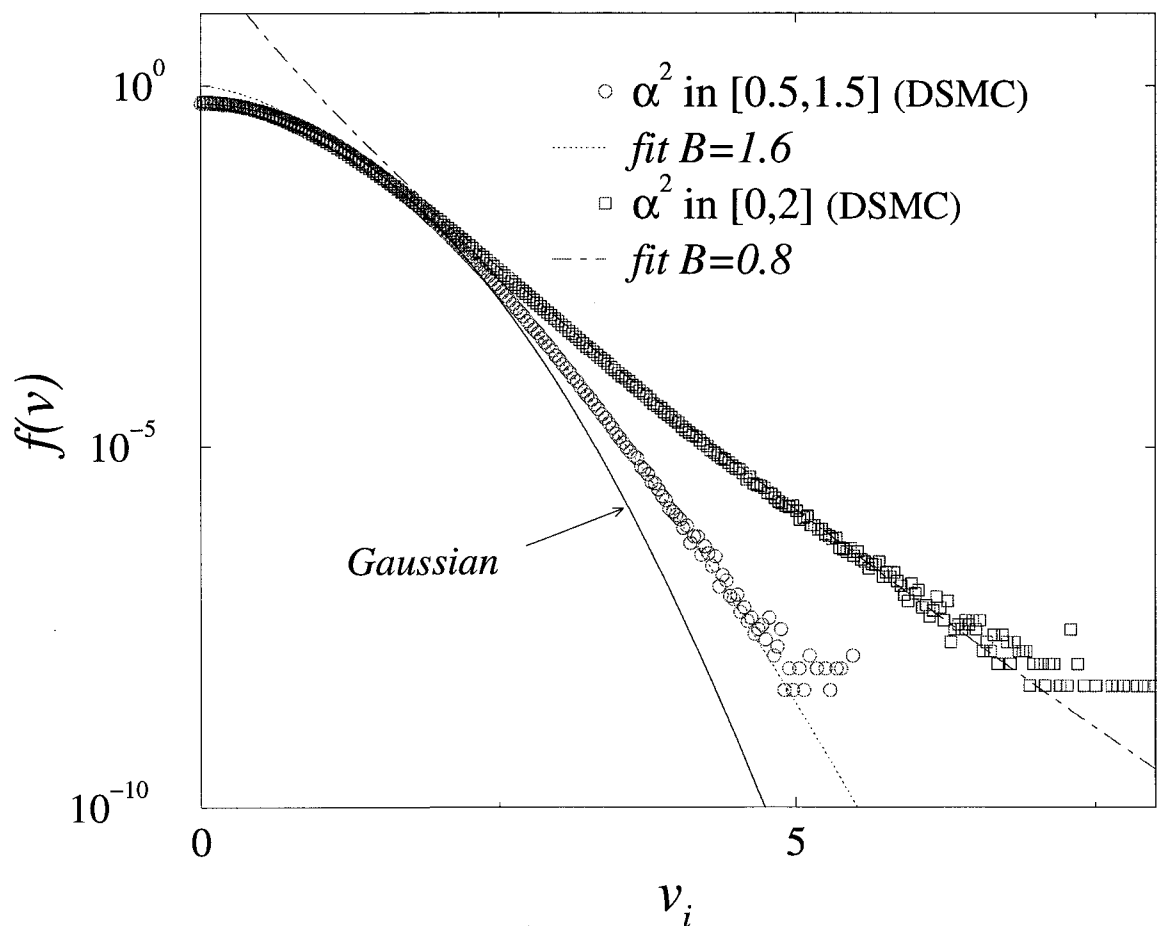
→ important deviations from Maxwell-Boltzmann

→ no violation of molecular chaos

## High energy tails

- ◇ Analytical predictions ??
- ◇ Fits to stretched exponentials (over 6 orders of magnitude)

$$f(\mathbf{v}) \propto \exp(-v^B)$$



→ may question the relevance of exponent  $B$  as an intrinsic quantity for granular gases in steady states.

## Perspectives

- ◇ Connection between  $\rho(\alpha)$  and experimentally relevant energy injection mechanisms ?  
correlations  $\alpha \leftrightarrow \mathbf{v}_{\text{impact}}$  ? (discarded here)
- ◇ Hydrodynamics of the random  $\alpha$  model ?  
(energy is globally conserved, whereas density and momentum are locally conserved)