Translations and Rotations Are Correlated in Granular Gases

N. V. Brilliantov,[1,2] T. Pöschel,[3] W. T. Kranz,[4] and A. Zippelius[4]
[1]*Institute of Physics, University of Potsdam, Am Neuen Palais 10, 14469 Potsdam, Germany*
[2]*Moscow State University, 119899 Moscow, Russia*
[3]*Charité, Augustenburger Platz 1, 13353 Berlin, Germany*
[4]*Institute of Theoretical Physics, University of Gottingen, 37073 Gottingen, Germany*
(Received 8 September 2006; published 23 March 2007)

In a granular gas of rough particles the axis of rotation is shown to be correlated with the translational velocity of the particles. The average relative orientation of angular and linear velocities depends on the parameters which characterize the dissipative nature of the collision. We derive a simple theory for these correlations and validate it with numerical simulations for a wide range of coefficients of normal and tangential restitution. The limit of smooth spheres is shown to be singular: even an arbitrarily small roughness of the particles gives rise to orientational correlations.

DOI: 10.1103/PhysRevLett.98.128001 PACS numbers: 45.70.−n, 45.70.Qj, 47.20.−k

Dilute systems of macroscopic particles, called granular gases, show many novel and surprising phenomena when compared to molecular gases. The particles of granular gases are macroscopic bodies which in general dissipate energy upon collision. As a consequence, such gases demonstrate features which drastically differ from molecular gases: The velocities are not distributed according to a Maxwell-Boltzmann distribution [1–7]; equipartition does not hold [8], and a homogeneous state is in general unstable [9–11]. In this Letter we present another unexpected result: The angular and linear velocities of rough particles are correlated in direction. In dependence on the coefficients of restitution, characterizing the dissipative particle properties, the rotational motion may be preferably perpendicular to the direction of linear motion, similar to a sliced (spinning) tennis ball, or in parallel to it, like a rifled bullet, Fig. 1. Surprisingly, the limit of vanishing dissipation of the rotational motion does not exist, that is, any arbitrarily small roughness leads to a macroscopic correlation between spin and velocity. We present a kinetic theory that quantifies this new effect and find good agreement with large scale numerical simulations. It is expected that the reported correlation between spin and linear velocity may have important consequences in understanding natural granular gases, such as dust clouds or planetary rings.

Model.—We consider a monodisperse granular gas consisting of N hard spheres of radius a, mass m, and moment of inertia $I = qma^2$. While the analytical results below are presented for general q, for the simulations we used $q = \frac{2}{5}$ as valid for homogeneous spheres. The degrees of freedom are the particles' position vectors $\{\mathbf{r}_i\}$, translational velocities $\{\mathbf{v}_i\}$, and rotational velocities $\{\boldsymbol{\omega}_i\}$ for $i = 1, 2, \ldots N$. The dynamic evolution of the system is governed by instantaneous two particle collisions, such that in general both translational and rotational energy is dissipated. Introducing the relative velocity at the point of contact, $\mathbf{g} = \mathbf{v}_1 - \mathbf{v}_2 + a\mathbf{n} \times (\boldsymbol{\omega}_1 + \boldsymbol{\omega}_2)$, the collision rules specify the change of $\mathbf{g}$ in the direction of $\mathbf{n} = (\mathbf{r}_1 - \mathbf{r}_2)/|\mathbf{r}_1 - \mathbf{r}_2|$ and perpendicular to $\mathbf{n}$: $(\mathbf{g} \cdot \mathbf{n})' = -\varepsilon_n(\mathbf{g} \cdot \mathbf{n})$ and $(\mathbf{g} \times \mathbf{n})' = +\varepsilon_t(\mathbf{g} \times \mathbf{n})$, where the primed values refer to the postcollision quantities. The coefficients of restitution in normal and tangential direction, $0 \le \varepsilon_n \le 1$ and $-1 \le \varepsilon_t \le 1$, characterize the loss of energy and, thus, describe the slowing down of the linear and rotational motion of the particles. These coefficients are the central quantities in the kinetic theory of granular gases [12]. For $\varepsilon_n = 1$ (elastic spheres) and $\varepsilon_t = \pm 1$ (perfectly smooth or rough spheres) the energy is conserved, while for $\varepsilon_n \to 0$ and $\varepsilon_t \to 0$ dissipation is maximal. Combining the above collision rules with conservation of angular and linear momentum, allows one to express the postcollision velocities in terms of the precollisional ones

$$\mathbf{v}_1' = \mathbf{v}_1 - \boldsymbol{\delta}, \qquad \boldsymbol{\omega}_1' = \boldsymbol{\omega}_1 + \left(\frac{1}{aq}\right)\mathbf{n} \times \boldsymbol{\delta},$$
$$\mathbf{v}_2' = \mathbf{v}_2 + \boldsymbol{\delta}, \qquad \boldsymbol{\omega}_2' = \boldsymbol{\omega}_2 + \left(\frac{1}{aq}\right)\mathbf{n} \times \boldsymbol{\delta}, \tag{1}$$

with $\boldsymbol{\delta} = \eta_t \mathbf{g} + (\eta_n - \eta_t)(\mathbf{n} \cdot \mathbf{g})\mathbf{n}$ and $\eta_n = (1 + \varepsilon_n)/2$, $\eta_t = q(1 - \varepsilon_t)/2(1 + q)$.

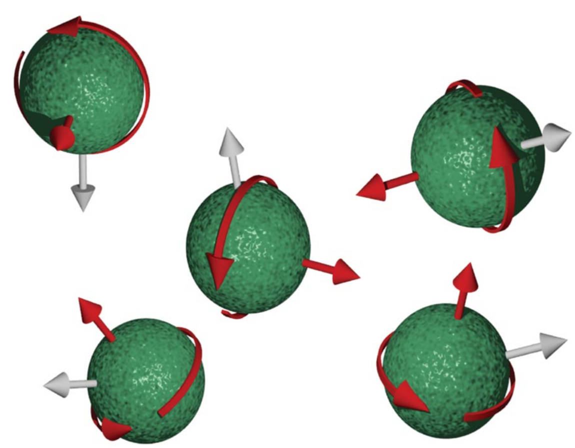

FIG. 1 (color). In granular gases, depending on the coefficients of restitution, spin (red arrow) and linear velocity (gray arrow) are oriented either preferably in parallel (cannon ball) or perpendicular (sliced tennis ball).

When particles collide according to the above laws, two processes take place: (i) dissipation of energy and (ii) exchange of energy between the rotational and translational degrees of freedom. The first process is described by two time-dependent granular temperatures

$$T_{\mathrm{tr}} = \frac{m}{3N}\sum_{i=1}^{N}\mathbf{v}_i^2 \quad \text{and} \quad T_{\mathrm{rot}} = \frac{I}{3N}\sum_{i=1}^{N}\boldsymbol{\omega}_i^2. \qquad (2)$$

The second process drives the system to a quasi−steady state, which is characterized by a constant ratio of the two temperatures, $r = T_{\mathrm{rot}}/T_{\mathrm{tr}} = \mathrm{const}$. In this state both temperatures continue to decay with their rates tied together by $\dot{T}_{\mathrm{rot}}/\dot{T}_{\mathrm{tr}} = r$. The ratio of temperatures, r, depends on the coefficients of restitution ε_n and ε_t and can take values smaller or larger than 1. If $r < 1$ collisions damp the translational motion more efficiently than the rotational one, $|\dot{T}_{\mathrm{tr}}| = |\dot{T}_{\mathrm{rot}}|/r > |\dot{T}_{\mathrm{rot}}|$, whereas for $r > 1$ the rotations are damped more efficiently.

At first glance there is no reason to expect that linear and angular velocities $\mathbf{v}$ and $\boldsymbol{\omega}$ are correlated. Nevertheless, the exchange of energy between the rotational and translational degrees of freedom may build up such correlations. We quantify them by the mean square cosine of the angle between $\mathbf{v}$ and $\boldsymbol{\omega}$:

$$K \equiv \frac{1}{N}\sum_{i=1}^{N}\frac{(\mathbf{v}_i\cdot\boldsymbol{\omega}_i)^2}{(v_i^2\omega_i^2)} = \frac{1}{N}\sum_{i=1}^{N}\cos^2\Theta_i. \qquad (3)$$

If there are no correlations between the rotational and translational motion, as in molecular gases, one obtains $K = \frac{1}{3}$; in granular gases we find that K in general deviates significantly from $\frac{1}{3}$.

The full quantitative understanding of these correlations requires detailed mathematical analysis of the collision rules Eq. (1) (see below). Nevertheless simple physical arguments are helpful for a qualitative understanding of these correlations. The transfer of energy from the translational to the rotational degrees of freedom (and vice versa) depends sensitively on the relative orientation of $\mathbf{v}_i - \mathbf{v}_j$ and $\boldsymbol{\omega}_i + \boldsymbol{\omega}_j$. To sustain a quasi−steady state with a fixed ratio, $r = T_{\mathrm{rot}}/T_{\mathrm{tr}}$ requires that fluctuations away from a given r are effectively suppressed. In the limit of nearly smooth particles, $\varepsilon_t \lesssim 1$ and $r \gg 1$ [13], the argument is particularly simple: For most of the collisions the relative velocity of the particles at the point of contact is dominated by rotations $\mathbf{g} = \mathbf{v}_i - \mathbf{v}_j + a\mathbf{n}\times(\boldsymbol{\omega}_i + \boldsymbol{\omega}_j) \approx a\mathbf{n}\times(\boldsymbol{\omega}_i + \boldsymbol{\omega}_j)$. For nearly smooth particles the rotational velocities change only slightly upon collision, $\boldsymbol{\omega}_i' \approx \boldsymbol{\omega}_i$ and $\boldsymbol{\omega}_j' \approx \boldsymbol{\omega}_j$, so that the collision rule Eq. (1) simplifies to

$$\mathbf{v}_i' - \mathbf{v}_i \approx -\eta_t\mathbf{g} \approx -\eta_t a(\mathbf{n}\times\boldsymbol{\omega}_i' + \mathbf{n}\times\boldsymbol{\omega}_j'), \qquad (4)$$

where $\eta_t \sim (1-\varepsilon_t) \ll 1$. The first term on the right-hand side gives a contribution to $\mathbf{v}_i'$ that is always perpendicular to the angular velocity $\boldsymbol{\omega}_i'$. The second term has no preferred orientation with respect to $\boldsymbol{\omega}_i'$,—the two vectors $\boldsymbol{\omega}_i'$ and $\boldsymbol{\omega}_j'$ being uncorrelated in a dilute gas. Hence, the sum of all contributions leads to $\mathbf{v}_i'$ being preferably perpendicular to $\boldsymbol{\omega}_i'$.

To describe these phenomena quantitatively beyond the limit of nearly smooth spheres, we develop an analytical theory which is based on an ansatz for the N-particle distribution function. We assume homogeneity, except for the excluded volume interaction, and molecular chaos, implying that the N-particle velocity distribution factorizes into a product of one particle distributions

$$\rho_1(\mathbf{v},\boldsymbol{\omega},t) \sim e^{-[mv^2/2T_{\mathrm{tr}}(t)]} \times e^{-[I\omega^2/2T_{\mathrm{rot}}(t)]}[1 + b(t)v^2\omega^2P_2(\cos\Theta)]. \qquad (5)$$

This ansatz takes into account for the first time orientational correlations between linear and angular velocities. To lowest order these correlations can be characterized by the second Legendre polynomial $P_2(x) \equiv \frac{3}{2}x^2 - \frac{1}{2}$. In general there will be higher-order terms in $(\cos\Theta)$, as well as non-Gaussian corrections for the velocity and angular velocity distribution [12,13]. The effects of these terms is not known *a priori*, but expected to be small, since the simplest ansatz already captures, even quantitatively, the correlations of interest. The strength of the orientational correlations is given by $b(t)$ which is related to the expectation value of $\langle\cos^2\Theta\rangle_t$ with the above distribution function

$$\langle\cos^2\Theta\rangle_t = \frac{1}{3} + b(t)\frac{6T_{\mathrm{tr}}(t)T_{\mathrm{rot}}(t)}{5qm^2a^2} \qquad (6)$$

Our ansatz (5) contains three functions, $T_{\mathrm{tr}}(t)$, $T_{\mathrm{rot}}(t)$, and $b(t)$, which have been calculated self-consistently using the Pseudo Liouville operator.

Results.—We find that very strong dynamic correlations may develop, depending on the initial conditions. After a transient period, the correlation factor K reaches a steady-state value which is independent of the initial conditions. In Fig. 2 we show this steady-state value as a function of the coefficient of tangential restitution ε_t for several values of

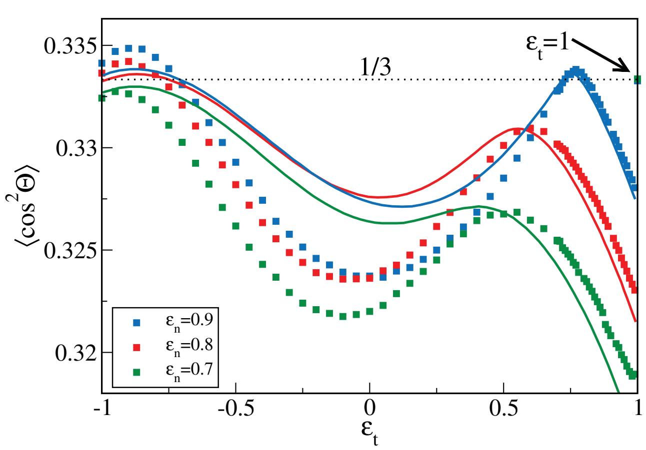

FIG. 2 (color). Steady-state value of the correlation factor $K = \langle\cos^2\Theta_i\rangle$ as a function of ε_t, for different values of ε_n. Lines: analytical theory. Points: DSMC simulations. The isolated point at $\varepsilon_t = 1$ indicates vanishing correlations for perfectly smooth particles.

the normal coefficient ε_n. We compare results from the analytical theory with data obtained with direct simulation Monte Carlo (DSMC) [14] of $N = 2 \times 10^7$ particles. The analytical results are in qualitatively good agreement with simulations, especially for small dissipation. As can be seen in the figure, pronounced correlations are observed for $\varepsilon_t = 0$, that is, for maximal damping of the tangential motion. The correlations weaken when the damping decreases with growing $|\varepsilon_t|$ and become less pronounced for comparable tangential and normal dissipation, $|\varepsilon_t| \sim \varepsilon_n$. With still increasing magnitude of ε_t, for $\varepsilon_t > 0$, the correlations rise again, driving K away from the uncorrelated value $\frac{1}{3}$.

The complete dependence of the correlation factor K on both coefficients of restitution is shown in Fig. 3 along with the contour plots of the temperature ratio r. In agreement with the qualitative argument discussed above, we see that translational and rotational velocities are preferentially perpendicular ($K < \frac{1}{3}$) in those regions where r strongly deviates from 1.

The right-hand side of Fig. 2 reveals that the limit of smooth spheres, is not continuous—contrary to naive expectations. For perfectly smooth particles $\varepsilon_t = 1$, we obtain $K = \frac{1}{3}$, as expected for a molecular gas. This happens, because translational and rotational motion decouple, so that all spins simply persist in time. Hence, trivially, angular and linear velocities are not correlated for $\varepsilon_t = 1$. Nevertheless, even for vanishingly small roughness $\varepsilon_t \to 1$ the correlation factor K noticeably deviates from $\frac{1}{3}$. Our analytic theory predicts

$$\lim_{\varepsilon_t \to 1} \langle \cos^2\Theta \rangle_\infty = \frac{1}{3} - \frac{3}{8}\frac{(1-\varepsilon_n)}{(7-\varepsilon_n)}, \tag{7}$$

in good agreement with DSMC calculations. In the limit $\varepsilon_t \to 1$ the relaxation time to the quasi–steady state diverges, because the exchange of energy between rotational and translational degrees of freedom becomes more and more inefficient as their mutual coupling vanishes.

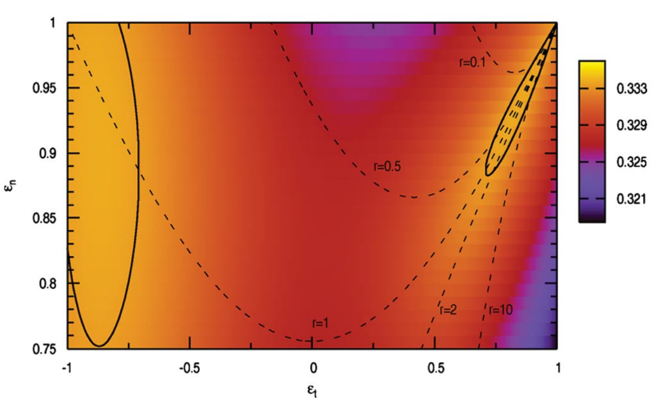

FIG. 3 (color). Color encoded steady-state value of K as predicted by analytical theory as a function of ε_n and ε_t. The full lines show the manifold $K = \frac{1}{3}$ (no correlations); the dashed lines are the contour plots for $r = T_{\rm rot}/T_{\rm tr}$.

Figure 4 gives an illustrative example, how correlations develop in time. We have chosen parameter values and initial conditions such that both regimes—dominance of translational motion $r \ll 1$ and dominance of rotational motion $r \gg 1$—are visible. Initially $K = \frac{1}{3}$ and $r \to 0$, which means that correlations are lacking and the particles' spins are vanishingly small. The evolution proceeds in three stages. In the initial stage rotational motion is generated mainly in grazing collisions so that the particles rotate around an axis perpendicular to their linear velocity, like a spinning tennis ball, implying $\langle \cos^2(\theta) \rangle < \frac{1}{3}$. Once the rotational motion has become comparable in magnitude to the translational motion, correlations are small, because both translational and rotational velocities contribute about equally to the momentum transfer in collision. Finally in the asymptotic stationary state the rotational motion is considerably more intense than the translational motion, so that the quasi–stationary state with $r \gg 1$ is characterized by significant correlations $K < \frac{1}{3}$.

Methods.—Two different numerical methods were used: Direct simulation Monte Carlo (DSMC) [14] and event-driven molecular dynamics (MD) [15]. In contrast to the latter method, where the trajectory of each particle of the ensemble is directly computed according to the basic kinematics and collision rules, the DSMC is based on the solution of the kinetic Boltzmann equation. Because the gas is explicitly treated as uniform in this method, and spatial correlations between grains are ignored, it allows one to handle up to $\sim 10^8$ particles, which is necessary for

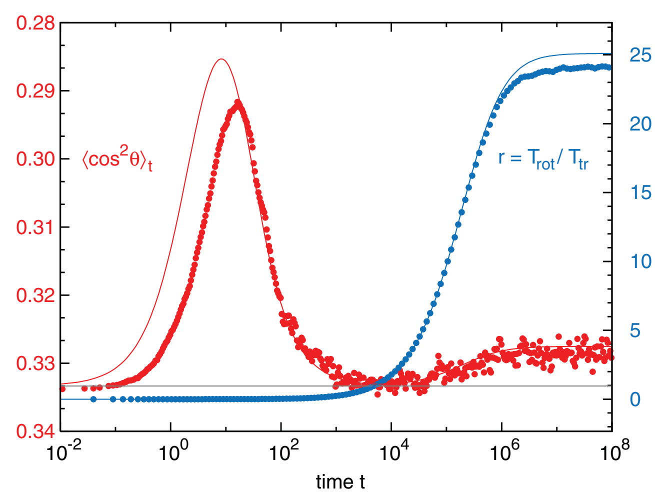

FIG. 4 (color). Relaxation of temperature ratio r and correlation factor $K = \langle \cos^2(\Theta) \rangle_t$ to their steady-state values for $\varepsilon_n = 0.8$, $\varepsilon_t = 0.8$ and initial conditions $T_{\rm rot} = 0$, $T_{\rm tr} = 1$. Full lines: analytical theory. Dots: simulations of $N = 8000$ particles. The vertical axes are chosen such that $r = 1$ coincides with $K = \frac{1}{3}$ as indicated by the gray line. Note the three different time regimes: First, from $r = 0$ to $r = 1$, very strong correlations develop; second, for $r \sim 1$ correlations are small, i.e., $K \sim \frac{1}{3}$; finally in the quasi–steady state with $r \gg 1$, correlations acquire a stationary value $K < \frac{1}{3}$.

the precise measurement of the effect of interest. While the MD method is more appealing from a physical point of view, the DSMC method is much more powerful for a homogeneous granular gas; in the limit of low density the two methods are, in principle, identical [15].

In the analytic approach we have used the pseudo Liouville operator technique to compute the rates of change $\dot{T}_{\rm tr}(t)$, $\dot{T}_{\rm rot}(t)$, and $\dot{b}(t)$ (see, e.g., [13] for details of similar computations). Given our ansatz for the distribution function, Eq. (5), these can be expressed in terms of $T_{\rm tr}(t)$, $T_{\rm rot}(t)$, and $b(t)$ so that a closed set of three first order nonlinear differential equations results. These allow for a quasi–stationary state, where the ratio of temperatures and the orientational correlations are independent of time. The latter are described by

$$\langle\cos^2\Theta\rangle_\infty - \frac{1}{3} = -\frac{6}{5}\,\frac{A^{(0)} + (A-C)\frac{B^{(0)}}{B} + (B^{(0)} + C^{(0)})r^{*-1}}{A^{(1)} - 40C + (A-C)\frac{B^{(1)}}{B} + (40B + B^{(1)})r^{*-1}}. \quad (8)$$

Here r^* is the stationary ratio of temperatures which is given in [8] together with the coefficients A, B, and C. The remaining coefficients are explicitly given by

$$A^{(0)} = \frac{16}{3}\frac{\eta_t^3}{q}\left(\frac{2\eta_t}{q} - 1\right) - \frac{2}{3}\frac{\eta_t^2}{q}\left(\frac{8\eta_t}{q} - 3\right) + \frac{1}{3}\frac{\eta_t}{q}\left(\frac{\eta_t}{q} - 1\right) + \frac{8}{3}\frac{\eta_t}{q}\left(\frac{\eta_t}{q} - 1\right)\eta_n(\eta_n - 1)$$

$$A^{(1)} = -\frac{4\eta_t\eta_n^2}{q}\left(\frac{\eta_t}{q} - 1\right) + \frac{1}{3}\frac{\eta_t^2}{q}\left(\frac{24\eta_t}{q} - 37\right) - \frac{5}{6}\frac{\eta_t}{q}\left(\frac{9\eta_t}{q} - 29\right) - \frac{8\eta_t^3}{q}\left(\frac{2\eta_t}{q} - 1\right) + \frac{4}{3}\frac{\eta_t\eta_n}{q}\left(\frac{3\eta_t}{q} - 14\right) - 12\eta_t\eta_n + 22(\eta_t + \eta_n) - 6(\eta_t^2 + \eta_n^2)$$

$$B^{(0)} = \frac{1}{3}\frac{\eta_t^2}{q}\left(\frac{16\eta_t}{q}\left(\frac{\eta_t}{q} - 1\right) + 5\right) \qquad B^{(1)} = -\frac{2}{3}\frac{\eta_t^2}{q}\left(\frac{8\eta_t}{q}\left(\frac{\eta_t}{q} - 1\right) + 1\right) \qquad C^{(0)} = \frac{2}{3}\frac{\eta_t^2}{q}(8\eta_t(\eta_t - 1) + 4\eta_n(\eta_n - 1) + 3)$$

Details of the calculation will be published elsewhere.

Conclusions.—In conclusion, we reveal a novel phenomenon, which is unique for granular gases and surprising in two respects: (a) Except for very special values of the coefficients of restitution $(\varepsilon_n, \varepsilon_t)$ the linear and angular velocities are noticeably correlated. For most of the parameter values $\mathbf{v}$ and $\boldsymbol{\omega}$ are preferably perpendicular and $K < \frac{1}{3}$ like for a sliced tennis ball. In a small region of low dissipation they are preferably parallel, so that $K > \frac{1}{3}$ like for a rifled bullet. (b) The limit of vanishing tangential dissipation, $\varepsilon_t \to 1$ is not continuous.

These results have important consequences for the hydrodynamic theory of dilute granular flows. It was recently shown [7] that the angular velocity needs to be included in the set of hydrodynamic fields. In view of the singular nature of the limit of vanishing roughness, perturbation expansions around the smooth limit are questionable. Orientational correlations between spin and linear velocity presumably also affect the stability of the system towards shear fluctuations which constitute the dominant instability of granular flows of smooth particles.

This research was supported by a grant from the GIF, the German-Israeli Foundation for Scientific Research and Development.

[1] A. Goldshtein and M. Shapiro, J. Fluid Mech. **282**, 75 (1995).

[2] T. P. C. van Noije and M. H. Ernst, Granular Matter **1**, 57 (1998).

[3] S. E. Esipov and T. Pöschel, J. Stat. Phys. **86**, 1385 (1997).

[4] J. J. Brey, D. Cubero, and M. J. Ruiz-Montero, Phys. Rev. E **59**, 1256 (1999).

[5] P. Deltour and J.-L. Barrat, J. Phys. I (France) **7**, 137 (1997).

[6] M. Huthmann, J. Orza, and R. Brito, Granular Matter **2**, 189 (2000).

[7] I. Goldhirsch, S. H. Noskowicz, and O. Bar-Lev, Phys. Rev. Lett. **95**, 068002 (2005).

[8] M. Huthmann and A. Zippelius, Phys. Rev. E **56**, R6275 (1997); S. Luding, M. Huthmann, S. McNamara, and A. Zippelius, Phys. Rev. E **58**, 3416 (1998).

[9] I. Goldhirsch and G. Zanetti, Phys. Rev. Lett. **70**, 1619 (1993).

[10] S. McNamara and W. R. Young, Phys. Fluids A **4**, 496 (1992).

[11] R. Brito and M. H. Ernst, Europhys. Lett. **43**, 497 (1998).

[12] N. V. Brilliantov and T. Pöschel, *Kinetic Theory of Granular Gases* (Oxford University Press, Oxford, 2004).

[13] T. Aspelmeier, M. Huthmann, and A. Zippelius, in *Granular Gases*, edited by S. Luding and T. Pöschel, Lecture Notes in Physics Vol. 425 (Springer, Berlin, 2000), p. 680.

[14] G. A. Bird, *Molecular Gas Dynamics and the Direct Simulation of Gas Flows* (Oxford University Press, New York, 1994).

[15] T. Pöschel and T. Schwager, *Computational Granular Dynamics* (Springer, New York, 2005).