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Role of roughness on the hydrodynamic homogeneous base state of inelastic spheres

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A gas of inelastic rough spheres admits a spatially homogeneous base state which turns into a hydrodynamic state after a finite relaxation time. We show that this relaxation time is hardly dependent on the degree of inelasticity but increases dramatically with decreasing roughness. An accurate description of translational-rotational velocity correlations at all times is also provided. At a given inelasticity, the roughness parameter can be tuned to produce a huge distortion from the Maxwellian distribution function. The results are obtained from a Grad-like solution of the Boltzmann-Enskog equation complemented by Monte Carlo and molecular dynamics simulations.

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The extension of statistical and fluid mechanics concepts to fluidized granular matter systems has allowed for a better understanding of the discrete-to-continuum description of matter by placing it into a more general theoretical framework [1–4].

Granular systems may exist in fluidized states at densities low enough to make a description by means of the (inelastic) Boltzmann and Enskog equations [2,3,5–7] possible. In that context, an immediate question arises: Do the inelastic versions of these kinetic equations support an accurate hydrodynamic description for granular gases as the elastic one [8] does for molecular gases? A variety of interesting kinetic theory studies have successfully modeled granular gas dynamics, proving additionally that granular gases may admit a hydrodynamic description [2–4,9–11]. However, most granular transport theories do not take into account the effects of particle roughness, which is inherently present in all real granular systems [12,13], or do it in the quasismooth regime [5,6]. Thus, the debate on the limits of applicability of granular hydrodynamics is still not closed.

The existence of a hydrodynamic regime relies on scale separation [14], i.e., individual particle (microscopic) dynamics variations (both in time and space) should be much shorter than those for the (macroscopic) average fields [2,8,14]. For molecular fluids, hydrodynamic states exist if the system is not subject to large gradients from the boundaries. However, for granular gases, even if no gradients are applied at all, the inelastic cooling sets an inherent decay time rate for the kinetic energy which is not necessarily slow compared to the characteristic microscopic time. This makes the proof of existence of a hydrodynamic solution in granular gases be not trivial [15], even for homogeneous states. The more realistic case of rough spheres seems to be much more complex [12]. For instance, energy nonequipartition [16,17], non-Maxwellian behavior [5–7], and correlations between translational and angular velocities [18–20] appear.

Taking the homogeneous cooling state (HCS) [4] as the base state for hydrodynamics, we address in this Rapid Communication questions such as the following: Is the ability of a homogeneous gas of rough spheres to reach a hydrodynamic state related to the degrees of inelasticity and/or roughness? How does the degree of roughness affect the aging time needed to reach the hydrodynamic HCS state? Is the HCS marginal probability distribution of angular velocities close to a Maxwellian? For this, both theoretical and simulational routes are followed. We develop a perturbative, Grad-like solution of the Boltzmann-Enskog (BE) equation that takes into account the effects of translational-rotational velocity correlations and non-Maxwellian features of the velocity distribution function. Moreover, we confirm our theory results by numerical solutions of the BE equation by means of the direct simulation Monte Carlo (DSMC) method [4]. In order to check that eventual violations of molecular chaos are not relevant, we carry out additional molecular dynamics (MD) simulations, using an event-driven algorithm [21,22].

The BE equation for a homogeneous state reads

$$\frac{\partial f}{\partial t} = \sigma^2 \chi K[\mathbf{v},\boldsymbol{\omega}|f], \tag{1}$$

where $f(\mathbf{v},\boldsymbol{\omega},t)$ is the one-body distribution function, $\mathbf{v}$ and $\boldsymbol{\omega}$ being the particle translational and angular velocities, respectively, σ is the sphere diameter, χ is the pair correlation function at contact (Enskog factor), which accounts for finite-density effects [23], and $\sigma^2\chi K \equiv J$ is the usual collision operator for inelastic and rough hard spheres [24,25]. The collision rule involves the normal (α) and tangential (β) coefficients of restitution [24,26]. While α ranges from 0 (perfectly inelastic) to 1 (perfectly elastic), β ranges from -1 (perfectly smooth) to 1 (perfectly rough). A more detailed description on the mechanics of collisions of rough hard spheres may be found elsewhere [12,18,26,27].

While the two-parameter (α,β) model neglects sliding effects that can be relevant in grazing collisions [27], a more sophisticated collision model with a Coulomb friction constant [28] may hinder the possibility of analytical treatments outside of the quasielastic and/or quasismooth limits [5,29]. Moreover, the (α,β) model still captures the basic features of the collision

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process and of the hydrodynamic issue [18,19,30] without compromising its physical content as a granular fluid model.

The translational and rotational temperatures are defined in the usual way [18,26] as $T_t = \frac{m}{3}\langle(\mathbf{v}-\mathbf{u}_f)^2\rangle$ and $T_r = \frac{I}{3}\langle\omega^2\rangle$, respectively, where m and I are the mass and moment of inertia, respectively, of the particles, and $\mathbf{u}_f = \langle\mathbf{v}\rangle$ is the flow velocity. The total temperature $T = \frac{1}{2}(T_t + T_r)$ decays monotonically with time (unless $\alpha = \beta^2 = 1$). Since both $\mathbf{u}_f$ and the density n are constant in homogeneous states, T is the only relevant hydrodynamic quantity of the system. Thus, if a hydrodynamic regime does exist, the whole temporal dependence of f must occur through a dependence on T [31].

The investigation of this scenario calls for the introduction of the reduced translational and angular velocities $\mathbf{c}(t) \equiv (\mathbf{v}-\mathbf{u}_f)/\sqrt{2T_t(t)/m}$, $\mathbf{w}(t) \equiv \boldsymbol{\omega}/\sqrt{2T_r(t)/I}$, and the reduced distribution function $\phi(\mathbf{c},\mathbf{w},t) \equiv n^{-1}[4T_t(t)T_r(t)/mI]^{3/2} f(\mathbf{v},\boldsymbol{\omega},t)$. In terms of these reduced quantities, the evolution equation for the temperature ratio $\theta(t) \equiv T_r(t)/T_t(t)$ and the BE equation (1) become

$$\partial_\tau \ln\theta = -\frac{2}{3}\left(\mu_{02}^{(0)} - \mu_{20}^{(0)}\right), \tag{2}$$

$$\partial_\tau\phi + \frac{\mu_{20}^{(0)}}{3}\frac{\partial}{\partial\mathbf{c}}\cdot(\mathbf{c}\phi) + \frac{\mu_{02}^{(0)}}{3}\frac{\partial}{\partial\mathbf{w}}\cdot(\mathbf{w}\phi) = \mathcal{J}[\mathbf{c},\mathbf{w}|\phi], \tag{3}$$

where $\partial_\tau \equiv [\nu(t)]^{-1}\partial_t$ is a time derivative scaled by the effective collision frequency $\nu(t) = 2n\sigma^2\chi\sqrt{\pi T_t(t)/m}$, $\mathcal{J} \equiv \nu^{-1}n^{-1}(4T_tT_r/mI)^{3/2}J$ is the reduced collision operator [25], and

$$\mu_{pq}^{(r)} \equiv -\int d\mathbf{c}\int d\mathbf{w}\, c^p w^q (\mathbf{c}\cdot\mathbf{w})^r \mathcal{J}[\mathbf{c},\mathbf{w}|\phi] \tag{4}$$

are reduced collisional moments. Taking moments on both sides of Eq. (3) we get the equations

$$\partial_\tau \ln M_{pq}^{(r)} - \frac{p+r}{3}\mu_{20}^{(0)} - \frac{q+r}{3}\mu_{02}^{(0)} = -\mu_{pq}^{(r)}/M_{pq}^{(r)}, \tag{5}$$

where $M_{pq}^{(r)} \equiv \langle c^p w^q (\mathbf{c}\cdot\mathbf{w})^r\rangle$. If a hydrodynamic description applies, it is expected that, after a certain transient period (kinetic stage), the system reaches an asymptotic regime (hydrodynamic stage) where θ and $\phi(\mathbf{c},\mathbf{w})$ (or, equivalently, its moments $M_{pq}^{(r)}$) become independent of time.

In isotropic conditions, $\phi(\mathbf{c},\mathbf{w})$ is actually a function of the three scalar quantities $c^2 = \mathbf{c}\cdot\mathbf{c}$, $w^2 = \mathbf{w}\cdot\mathbf{w}$, and $(\mathbf{c}\cdot\mathbf{w})^2$. As a consequence, one can formally represent the ratio $\phi(\mathbf{c},\mathbf{w})/\phi_M(\mathbf{c},\mathbf{w})$, where $\phi_M(\mathbf{c},\mathbf{w}) = \pi^{-3}e^{-c^2-w^2}$ is the (reduced) two-temperature Maxwellian distribution, as an infinite series of *polynomials* in c^2, w^2, and $(\mathbf{c}\cdot\mathbf{w})^2$:

$$\phi(\mathbf{c},\mathbf{w}) = \phi_M(\mathbf{c},\mathbf{w})\sum_{j=0}^{\infty}\sum_{k=0}^{\infty}\sum_{\ell=0}^{\infty} a_{jk}^{(\ell)}\Psi_{jk}^{(\ell)}(\mathbf{c},\mathbf{w}), \tag{6}$$

where $\Psi_{jk}^{(\ell)}(\mathbf{c},\mathbf{w}) = L_j^{(2\ell+\frac{1}{2})}(c^2)L_k^{(2\ell+\frac{1}{2})}(w^2)(c^2w^2)^\ell P_{2\ell}(u)$ is a polynomial of total degree $2(j+k+2\ell)$ in velocity. Here, $L_j^{(2\ell+\frac{1}{2})}(x)$ and $P_{2\ell}(x)$ are Laguerre and Legendre polynomials, respectively, and $u \equiv (\mathbf{c}\cdot\mathbf{w})/cw$ is the cosine of the angle made by $\mathbf{v}$ and $\boldsymbol{\omega}$. The set of polynomials $\{\Psi_{jk}^{(\ell)}\}$ is a complete orthogonal basis for the solution of Eq. (3) [25]. The expansion coefficients $a_{jk}^{(\ell)} \propto \langle\Psi_{jk}^{(\ell)}\rangle$ are linear combinations of the moments $M_{pq}^{(r)}$ with $p,q,r =$ even and $p+q+2r \leqslant 2(j+k+2\ell)$. By normalization, $a_{00}^{(0)} = 1$, $a_{10}^{(0)} = a_{01}^{(0)} = 0$, so the first nontrivial coefficients are those of degree four, namely, the fourth-degree *cumulants*

$$a_{20}^{(0)} = \tfrac{4}{15}\langle c^4\rangle - 1, \quad a_{02}^{(0)} = \tfrac{4}{15}\langle w^4\rangle - 1, \tag{7a}$$

$$a_{11}^{(0)} = \tfrac{4}{9}\langle c^2w^2\rangle - 1, \quad a_{00}^{(1)} = \tfrac{8}{15}\left[\langle(\mathbf{c}\cdot\mathbf{w})^2\rangle - \tfrac{1}{3}\langle c^2w^2\rangle\right]. \tag{7b}$$

In our theoretical approach we apply a Grad-Sonine (GS) methodology [31,32]. First, the expansion (6) is *truncated* after $j+k+2\ell = 2$ [7], so that the only retained coefficients are $a_{00}^{(0)} = 1$ and those in Eqs. (7). Next, the collisional moments $\mu_{20}^{(0)}, \mu_{02}^{(0)}, \mu_{40}^{(0)}, \mu_{04}^{(0)}, \mu_{22}^{(0)}$, and $\mu_{00}^{(2)}$ are evaluated by inserting the truncated expansion into the collision operator $\mathcal{J}$, neglecting terms that are quadratic in the cumulants, and performing the velocity integrals. The resulting expressions (with coefficients being nonlinear functions of the temperature ratio θ, the two coefficients of restitution α and β, and the dimensionless moment of inertia $\kappa \equiv 4I/m\sigma^2$) can be found in Ref. [25]. Finally, the coupled set of five equations (2) and (5) with $p+q+2r = 4$ are numerically solved to obtain the time evolution of θ and the cumulants (7) [25]. Setting $\partial_\tau \to 0$, the solution to the corresponding set of algebraic equations gives the stationary values of those quantities. To check the stability of the stationary values, we have analyzed the associated linearized problem and observed that all the eigenvalues indeed have a negative real part. The characteristic relaxation period (in units of the accumulated number of collisions per particle) is $-1/\mathrm{Re}(s)$, where s is the eigenvalue with the real part closest to the origin. It strongly increases when the roughness parameter decreases from $\beta \approx 0$ to $\beta \gtrsim -1$ but is hardly dependent on the inelasticity parameter α [25].

In order to check the accuracy of our GS approximation, we have performed DSMC and MD simulations in the case of uniform spheres ($\kappa = \frac{2}{5}$), starting from an initial equilibrium state, for a large number of (α,β) pairs. As a particularly unfavorable case (see below), in Fig. 1 we plot the temporal evolution (as measured by the accumulated number of collisions per particle $\mathcal{N}$) of the cumulants for $\alpha = 0.7$ and $\beta = -0.575$. As we see, MD and DSMC results are hardly distinguishable, which reinforces the validity of the BE (1) for dilute granular gases. Moreover, both theory and simulation results agree very well in the first stages of development (up to $\mathcal{N} \approx 10$ collisions per particle). Beyond that stage, the angular velocity kurtosis $a_{02}^{(0)}$ becomes larger than about 0.3 and the GS theory (being based on truncation and linearization around the Maxwellian) underestimates the magnitude of the cumulants. However, the theory successfully captures the qualitative later evolution and the duration of the total relaxation period. The discrepancies between theory and simulations observed in Fig. 1 for $\mathcal{N} \gtrsim 10$ are not due to an inherent limitation of the GS theory to the early stages of evolution but to the high values reached by the cumulant $a_{02}^{(0)}$ in this particularly stringent case. In fact, a good agreement is found at all times for most combinations of (α,β) since in those cases the magnitudes of the cumulants are smaller than about 0.3 [25].

To characterize the duration ($\mathcal{N}_r$) of the relaxation period, we adopt the practical criterion that the values of θ and $a_{jk}^{(\ell)}$

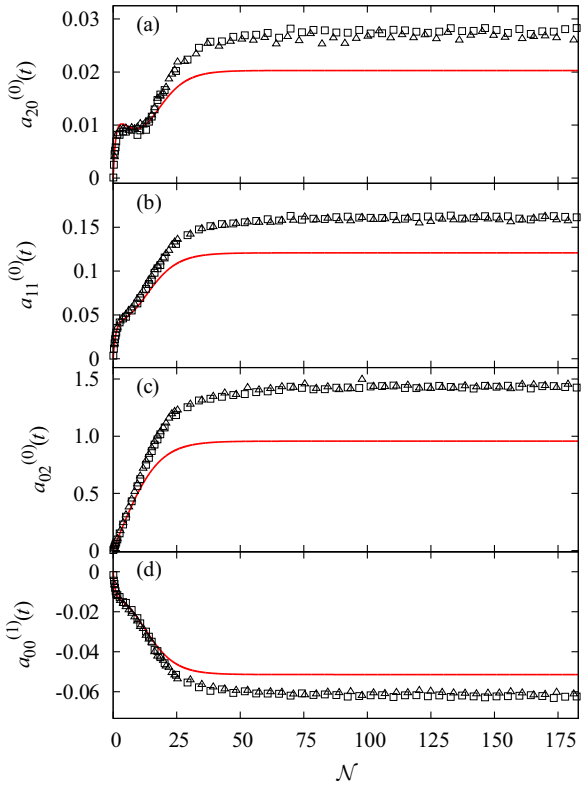

FIG. 1. (Color online) Temporal evolution of the velocity cumulants for $\alpha = 0.7$ and $\beta = -0.575$. Henceforth, lines stand for theoretical results and symbols for simulation data (DSMC: □; MD: △).

(with $j + k + 2\ell = 2$) must differ from their stationary values by less than 5% if $\mathcal{N} > \mathcal{N}_r$. The theoretical and simulation results are presented in Fig. 2, where a good agreement is found. Since each quantity satisfies the 5% criterion after a different relaxation period, what is plotted in Fig. 2 is the maximum of the five particular relaxation times [25]. This, together with the cases where the relaxation is not monotonic, explains the nonsmooth shape of $\mathcal{N}_r$ at some points. We may

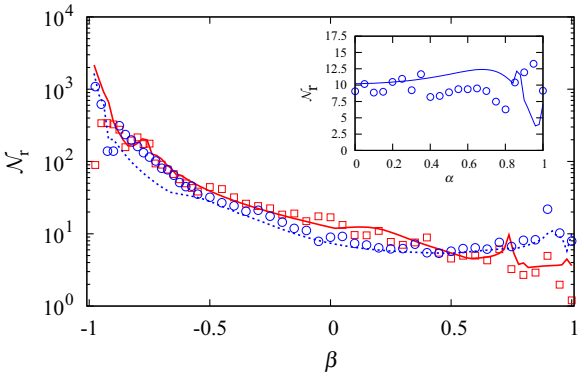

FIG. 2. (Color online) Relaxation time $\mathcal{N}_r$ (in units of collisions per particle) as a function of β for constant $\alpha = 0.7$ (dotted line; ○) or $\alpha = 0.9$ (solid line; □). The inset shows $\mathcal{N}_r$ as a function of α for constant $\beta = 0$. Symbols stand for DSMC data.

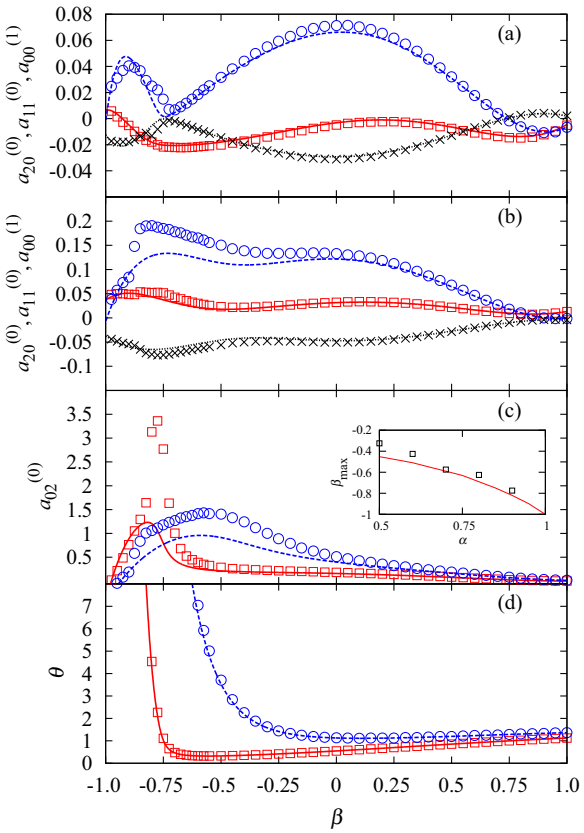

FIG. 3. (Color online) Stationary values of the cumulants and of the temperature ratio as functions of β. (a) ($\alpha = 0.9$) and (b) ($\alpha = 0.7$) show $a_{20}^{(0)}$ (solid lines; □), $a_{11}^{(0)}$ (dashed lines; ○), and $a_{00}^{(1)}$ (dotted lines, ×). (c) and (d) correspond to $a_{02}^{(0)}$ and θ, respectively, for $\alpha = 0.9$ (solid lines; □) and $\alpha = 0.7$ (dashed lines; ○). The inset in (c) shows the value $\beta_{\max}(\alpha)$ at which $a_{02}^{(0)}$ reaches its maximum value. Symbols stand for DSMC data.

see that the α dependence is not as critical as the β dependence, with $\mathcal{N}_r$ increasing dramatically as β approaches the smooth limit $\beta \to -1$. This agrees with the observed behavior of the theoretical quantity $-1/\mathrm{Re}(s)$ [25]. Interestingly, the inset of Fig. 2 (where the intermediate roughness $\beta = 0$ is chosen as a representative example) shows that the relaxation time ($\mathcal{N}_r \approx 10$) to the hydrodynamic state is not significantly different in the extreme limiting cases of complete inelasticity ($\alpha = 0$) and complete elasticity ($\alpha = 1$). We have checked by DSMC simulations that sixth- and eighth-degree moments relax over essentially the same time scale as the fourth-degree ones.

Let us now focus on the hydrodynamic ("steady") states. In Fig. 3 we plot the cumulants and the temperature ratio as functions of β for $\alpha = 0.7$ and 0.9. The agreement between theory and simulation for the translational velocity kurtosis $a_{20}^{(0)}$, the (orientational) translational-rotational correlation parameter $a_{00}^{(1)}$, and the temperature ratio θ is excellent for all values of β, especially at $\alpha = 0.9$. The agreement for $a_{11}^{(0)}$ is still very good, except in the ranges where $a_{02}^{(0)}$ reaches high values ($a_{02}^{(0)} \gtrsim 0.3$). Note that, according to our simulations, the angular velocity kurtosis at $\alpha = 0.9$ reaches values as high as $a_{02}^{(0)} \approx 3$ if the roughness is tuned to $\beta = \beta_{\max} \simeq -0.78$.

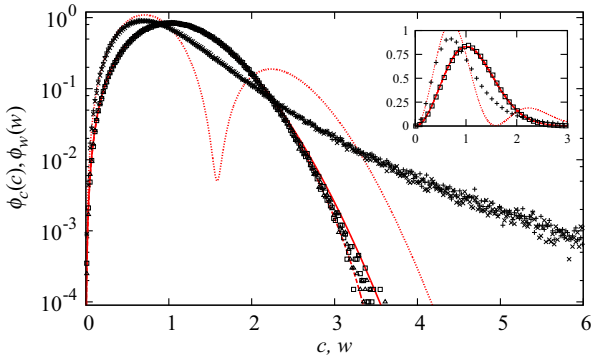

FIG. 4. (Color online) Marginal distribution functions $\phi_c(c)$ (dashed line; DSMC: □; MD: △) and $\phi_w(w)$ (dotted line; DSMC: +; MD: ×) at $\alpha = 0.9$, $\beta = -0.75$. The solid line stands for the (common) Maxwellian distribution function.

As the inelasticity increases to $\alpha = 0.7$, the maximum of $a_{02}^{(0)}$ decreases to $a_{02}^{(0)} \approx 1.5$ and occurs at a larger roughness ($\beta_{\max} \simeq -0.58$). The latter is precisely the case analyzed in Fig. 1. As seen from the inset in Fig. 3(c), the GS approximation captures qualitatively well the α dependence of $\beta_{\max}$. The existence of very large values of $a_{02}^{(0)}$ at $(\alpha, \beta_{\max})$ does not have a straightforward intuitive explanation but shows a subtle interplay between the translational and rotational degrees of freedom in the granular gas.

The results of Fig. 3 show that the hydrodynamic HCS distribution function can be highly non-Maxwellian, especially with respect to the angular velocities, if at a given α the roughness parameter β is close to $\beta_{\max}(\alpha)$. In those cases, truncation of the perturbative expansion (6) is not the adequate tool to accurately describe the distribution function, regardless of the truncation order, and an alternative approach is needed. This is illustrated by Fig. 4, where the marginal distribution functions $\phi_c(c) = 4\pi c^2 \int d\mathbf{w} \phi(\mathbf{c}, \mathbf{w})$ and $\phi_w(w) = 4\pi w^2 \int d\mathbf{c} \phi(\mathbf{c}, \mathbf{w})$ are plotted for the extreme case (see Fig. 3) $\alpha = 0.9$, $\beta \gtrsim \beta_{\max} = -0.75$. While $\phi_c(c)$ is close to the Maxwellian and is well represented by the GS truncated expansion, a large discrepancy is observed between the actual distribution $\phi_w(w)$ and the corresponding GS distribution, even if the latter is parametrized with the empirical kurtosis $a_{02}^{(0)}$. The GS distribution $\phi_w(w)$ is bimodal (with an almost zero local minimum) whereas simulation data do not exhibit this feature. More interestingly, both DSMC and MD simulation data for $\phi_w(w)$ show extremely large high-energy tails (perhaps the largest ones reported for granular gases of hard spheres so far [19]) consistent with $\phi_w(w) \sim \exp(-Aw)$.

In summary, we have studied the temporal evolution of the HCS for a granular gas of rough hard spheres by a GS truncated expansion and by DSMC and MD simulations. The three methods confirm that, after a kinetic stage, a hydrodynamic regime is reached where the whole time dependence of the velocity distribution function is enslaved by the temperature. The GS theory provides an excellent description of the evolution of the temperature ratio and the four velocity cumulants, except when the angular velocity kurtosis becomes so large ($a_{02}^{(0)} \gtrsim 0.3$) that it compromises the assumptions behind the truncation and linearization scheme. Even in those cases, the GS theory predicts well the relaxation time (see Fig. 2) and describes qualitatively the roughness dependence of the stationary cumulants (see Fig. 3). Quite surprisingly, and in contrast to what was generally believed, the relaxation to the hydrodynamic state is practically independent of the inelasticity coefficient α and is rather fast (no more than about ten collisions per particle, even in the most inelastic case, $\alpha = 0$) if the spheres are sufficiently rough ($\beta \gtrsim 0$). Therefore, we may conclude that high inelasticity does not preclude by itself the applicability of hydrodynamics. On the other hand, paradoxically, if the spheres are weakly rough ($\beta \gtrsim -1$), the relaxation time increases dramatically to values on the order of at least 10^3 collisions per particle. This is because, as roughness decreases, more and more collisions are needed to activate the rotational degrees of freedom, which are absolutely quenched in the smooth-sphere model. Interestingly, the duration of the relaxation stage and the departure from the (two-temperature) Maxwellian are not fully correlated, as comparison between Figs. 2 and 3 shows. In particular, at a given α, the maximum distortion from the Maxwellian (as monitored by the kurtosis $a_{02}^{(0)}$) does not take place in the limit $\beta \to -1$ but at a certain value $\beta_{\max}(\alpha) < 0$ [see the inset in Fig. 3(c)].

Given that the HCS is the base state for a granular gas and for the application of the Chapman-Enskog method [2], we expect these results to be of help in further developments of hydrodynamic transport theories of inhomogeneous granular gases. In this respect, it is interesting to note that most of the materials are characterized by positive values of the roughness parameter (typically, $\beta \sim 0.5$) [33], where the GS theory developed here is highly accurate.

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