Steady state velocity distributions of an oscillated granular gas

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We use a three-dimensional molecular dynamics simulation to study the single particle distribution function of a dilute granular gas driven by a vertically oscillating plate at high accelerations (15g – 90g). We find that the density and the temperature fields are essentially time-invariant above a height of about 35 particle diameters, where typically 20% of the grains are contained. These grains form the nonequilibrium steady state granular gas with a Knudsen number unity or greater. In the steady state region, the distribution function of horizontal velocities (scaled by the local horizontal temperature) is found to be nearly independent of height, even though the hydrodynamic fields vary with height. The high energy tails of the distribution functions are described by a stretched exponential $\sim \exp(-B\varepsilon^\alpha)$, where $\alpha$ depends on the normal coefficient of restitution $\varepsilon$ ($1.2 < \alpha < 1.6$), but $\alpha$ does not vary for a wide range of the friction parameter. We find that the distribution function of a frictionless inelastic hard sphere model can be made similar to that of a frictional model by adjusting $\varepsilon$. However, there is no single value of $\varepsilon$ that mimics the frictional model over a range of heights.

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I. INTRODUCTION

A dilute gas in thermal equilibrium is sufficiently characterized by the pressure and temperature and is described by a simple relation, the equation of state. However, when a gas is far from equilibrium, there is no general, finite set of variables specifying the state. The single particle distribution function $f(r, v, t)$ is often sufficient to characterize the statistical properties of a dilute nonequilibrium gas when correlations are negligible. Given this function, other quantities, such as moments of the distribution and transport coefficients, can be evaluated. Dilute granular materials subject to an external forcing exhibit gaseous behaviors that share many analogies with a molecular gas, and they are often called granular gases. Such a granular gas is always far from equilibrium due to the dissipative collisions, and the deviation of $f(r, v, t)$ from the Maxwell-Boltzmann (MB) distribution has been of great interest in recent years [1–8].

The velocity distributions of a vibro-fluidized granular gas were first measured by Warr et al. [1]; they studied the distribution functions of grains confined between two transparent plates and concluded that the distribution was consistent with the MB distribution function. Recently, the same system has been studied by Rouyer et al. [2], who found a universal distribution function of the form $\sim \exp(-B|v|^{1.5})$ for the entire range of velocities studied, where $B$ was a parameter. The authors reported that this functional form fit their measurements for a wide range of oscillation parameters for various materials; thus the granular temperature, the second moment of the distribution, was the only parameter of the distribution function.

There have been numerical studies of vibrated inelastic hard disks, subject to a saw-tooth type oscillation, in the presence of gravity [2] and in the absence of gravity [3]. Such forcing is often used in theoretical studies as a simplification of the sinusoidal oscillation used in experiments, assuming that the asymptotic behavior of the hydrodynamic fields far from the plate is the same; however, it is not known a priori how far from the oscillating plate one must be in order for this assumption to be valid.

In this paper, we perform a simulation that is as close as possible to three-dimensional experiments on vertically oscillated granular gases. We use a previously validated molecular dynamics (MD) simulation [3, 4]. The hydrodynamic fields are oscillatory near the plate, and their oscillatory behavior decays with height. Above some height, the fields are not correlated with the oscillation of the plate and are essentially time-invariant. We study the distribution functions in this nonequilibrium steady state region. To focus on the distributions due to the intrinsic dynamics of the granular gas, we do not impose sidewalls or include air. We also study how the distribution changes with the friction. In many theoretical or numerical studies of granular fluids, granular materials are modeled as frictionless inelastic hard disks or spheres; however, no granular materials are frictionless, in the same way that none of them are elastic. We check if the role of friction can be incorporated into the inelasticity by adjusting the value of the normal coefficient of restitution. In this paper we discuss the distributions only in the steady state region; those in the oscillatory region near the plate will be discussed in a separate paper [10].

The rest of the paper is organized as follows. In Section II, the system under consideration, the data analysis method, and the collision model are described. Results
are presented in Section III and discussed in Section IV.

II. METHOD

A. System and data analysis

We use both a frictional and frictionless, inelastic hard sphere MD simulation. We consider 133 328 monodisperse spheres of unit mass and of diameter $\sigma = 165 \mu m$ in a container with square bottom of area $200\sigma \times 200\sigma$ (the average depth of the layer at rest is approximately $3\sigma$), where periodic boundary conditions are imposed in both horizontal directions. We choose the same particle size as in Ref. [8], as the patterns were quantitatively reproduced for a wide range of oscillation parameters with this particle size; however, as long as the collision model is valid, all the length scales can be normalized by $\sigma$. We assume the bottom plate of the container is made of the same material as grains; we use the same material coefficients for the inelasticity and the friction as grains. The bottom plate is subject to a vertical sinusoidal oscillation with an amplitude $A$ and a frequency $f$. We vary the oscillation parameters in the range of $3\sigma < A < 10\sigma$ and $40 \text{ Hz} < f < 170 \text{ Hz}$, which approximately corresponds to $0.35 \text{ m/s} < V_{\text{max}} = 2\pi f A < 0.75 \text{ m/s}$ and $15g < a_{\text{max}} = |A(2\pi f)^2| < 90g$, where $g$ is the acceleration due to gravity. We check that with our parameters no mean flow develops and that grains rarely reach to the top, which is fixed at $300\sigma$.

Hydrodynamic fields and the distribution functions are analyzed by binning the box into horizontal slabs of height $\sigma$, as the system is invariant under the translation in both horizontal directions, in the absence of any mean flow. We use the granular volume fraction $\nu$ for the density, which is the ratio of the volume occupied by grains to the volume of each horizontal slab. We consider the following three granular temperatures separately:

$$T_x = \frac{1}{2} \langle (v_x - \langle v_x \rangle)^2 + (v_y - \langle v_y \rangle)^2 \rangle,$$

$$T_z = \langle (v_z - \langle v_z \rangle)^2 \rangle,$$

$$T = \frac{1}{3} \langle |v - \langle v \rangle|^2 \rangle = \frac{1}{3} (2T_x + T_z),$$

where $x$ and $y$ are horizontal directions that are indistinguishable, $z$ is the vertical direction, $v$ is a velocity vector for each grain, and the ensemble average $\langle \rangle$ is taken over the particles in the same bin at the same phase angle during 40 cycles, after initial transients have decayed. We define the scaled horizontal velocity to be

$$c_x = (v_x - \langle v_x \rangle)/\sqrt{2T_x}.$$

B. collision model

We implement the collision model that was originally proposed by Mav et al. [11], simplified by Walton [12], and then experimentally tested by Foerster et al. [13]. This model updates the velocity after a collision according to the three parameters, the normal coefficient of restitution $e \in [0, 1]$, the coefficient of friction $\mu$, which relates the tangential force to the normal force at collision using Coulomb's law and then determines the tangential coefficient of restitution $\beta \in [-1, 1]$, and the maximum tangential coefficient of restitution $\beta_0$, which represents the tangential restitution of the surface velocity when the colliding particles slide discontinuously at the contact point.

At collision, it is convenient to decompose the relative colliding velocities into the components normal ($v_n$) and tangential ($v_t$) to the normalized relative displacement vector $r_{12} = (r_1 - r_2)/|r_1 - r_2|$, where $r_1$ and $r_2$ are displacement vectors of grains 1 and 2, and the same notation is used for $v$:

$$v_n = (v_{1n} \cdot r_{12})r_{12} \equiv v_n \hat{r}_{12},$$

$$v_t = r_{12} \times (v_{12} \times r_{12}) = v_{12} - v_n.$$

The relative surface velocity at collision, $v_s$, for monodisperse spheres of diameter $\sigma$ is

$$v_s = v_t + \frac{\sigma}{2} r_{12} \times (w_1 + w_2) \equiv v_s \tilde{v}_s,$$

where $w_1$ and $w_2$ are the angular velocities of grains 1 and 2, respectively.

For monodisperse spheres of diameter $\sigma$ and unit mass, the linear and angular momenta conservations and the definitions of the normal coefficient of restitution $e = -v_n^s/v_n$ and the tangential coefficient of restitution $\beta = -v_t^s/v_s$ (post-collisional velocities are indicated by superscript $\ast$, and pre-collisional values have no superscript) give the changes in the velocities at the collision:

$$\Delta v_{1n} = -\Delta v_{2n} = \frac{1}{2} (1 + e) v_n,$$

$$\Delta v_{1t} = -\Delta v_{2t} = \frac{K (1 + \beta)}{2(K + 1)} v_s,$$

$$\Delta w_1 = -\Delta w_2 = \frac{(1 + \beta)}{\sigma (K + 1)} \tilde{r}_{12} \times \tilde{v}_s,$$

where $K = 4I/\sigma^2$ is a geometrical factor relating the momentum transfer from the translational degrees of freedom to rotational degrees of freedom, and $I$ is the moment of inertia about the center of the grain. For a uniform density sphere, $K$ is 2/5.

We use a velocity-dependent normal coefficient of restitution as in Ref. [8], to account for the viscoelasticity of the real grains:

$$e = \max \left[ e_0, 1 - (1 - e_0) \left( \frac{v_n}{\sqrt{g\sigma}} \right)^{3/4} \right].$$
where $\epsilon_0$ is a positive constant less than unity. Since we impose high forcing ($V_{\text{max}} > 0.35 \text{ m/s}$ while $\sqrt{\sigma} = 0.04 \text{ m/s}$) the collision probability for relative colliding velocities $v_n$ less than $\sqrt{\sigma}$ is small, and using a velocity-independent $\epsilon$ does not result in any noticeable difference, compared to using a velocity-independent one $\epsilon = \epsilon_0$; the same was true in Ref. [18]. We use the symbol $\epsilon$ for $\epsilon_0$ hereafter.

In collisions of real granular materials, not only is the relative surface velocity reduced, but also the stored tangential strain energy in the contact region can often reverse the direction of the relative surface velocity. To account for this effect, the tangential coefficient of restitution $\beta$ could be positive, leading to the range of $\beta$ as $[-1,1]$. There are two kinds of frictional interaction at collisions, sliding and rolling friction, which are accounted for by the following formula for $\beta$:

$$\beta = \min \left[ \beta_0, -1 + \mu \left( 1 + \frac{1}{K} \right) \frac{v_n}{v_s} \right], \quad (13)$$

where $\beta_0$ is the maximum tangential coefficient of restitution. For sliding friction, the tangential impulse is assumed to be the normal impulse multiplied by $\mu$. When $\beta$ is identically negative unity (or simply $\mu = 0$), this model reduces to the frictionless interaction. For the special case $v_s = 0$, the collision is treated as frictionless. This friction model is still a simplification of the real frictional interaction; there is no clear-cut distinction between the two types of frictions for real grains, and even a transfer of energy from the rotational to translational degrees of freedom, which results in $\epsilon$ larger than unity, has been observed [14]. However, this collision model is accurate enough to reproduce many phenomena, including standing wave pattern formation in vertically oscillated granular layers, when the parameters are properly chosen. In Refs. [8] and [9], $\epsilon = 0.7$, $\beta_0 = 0.35$, and $\mu = 0.5$ were used.

### III. RESULTS

#### A. Hydrodynamic fields and steady state

Due to the oscillatory boundary forcing, the hydrodynamic fields, the volume fraction $\nu$ and the granular temperatures ($T$, $T_x$, and $T_z$), depend on height $z$ and time $t$ (Fig. 1) near the oscillating plate; the temperatures exhibit stronger oscillatory behaviors than the density. Since the energy is injected mainly through the vertical velocities, the granular temperature is anisotropic, as illustrated in Fig. 1. $T_z$ is larger than its horizontal counterpart $T_x$, and the former is significantly larger near the bottom plate, where the hydrodynamic fields are oscillatory. The vertical temperature increases almost linearly with height for $z/\sigma > 35$; however, the temperature $T$ increases slower than linearly, as the slope of $T_z$ decreases with height and $T_x$ levels off for $z/\sigma > 120$ (Fig. 1). A similar increase of the temperature with height was observed in an open system of frictionless inelastic hard disks or spheres subject to a thermal bottom heating [10] and a saw-tooth type vibration [10]. We characterize the oscillation parameters only by $V_{\text{max}}$, as we observe for the parameters in our study that the hydrodynamic fields in

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Depending on the oscillation parameters, 20% of the grains are contained in this case; this fraction forms a nonequilibrium steady state (Fig. 2), where about a dynamical fields are invariant in time, and the granular gas propagating up through the entire granular media (which was detectable above some height (z/σ ≈ 35). As the shock propagates, it decays and becomes undetectable above some height (z/σ ≈ 35), rather than propagating up through the entire granular media (which was the case in Ref. [18]). Above this height, the hydraulic fields are invariant in time, and the granular gas forms a nonequilibrium steady state (Fig. 2), where about 20% of the grains are contained in this case; this fraction depends on the oscillation parameters.

With the parameters used in this paper the granular temperatures are nonzero throughout the cycle, as grains do not solidify after the shock passes through, in contrast to the case in Ref. [18]. As a result, when the bottom plate moves down, the granular gas expands, and an expansion wave propagates downward (see the temperature peaks near the plate for ft > 0.4 in Fig. 4).

We count the number of grain-grain collisions per grain during a cycle (Ncoll in Fig. 3), and find that Ncoll is less than unity in the steady state region; the granular gas in the steady state is nearly collisionless. We estimate the mean free path using the formula for a gas of hard spheres λ(z)/σ = (2√2πnσ^3)^{-1} = √π/(12√2ν) (where n is the number density) [19], which ranges between 5 and 280 for 40 < z/σ < 100 (Fig. 4). When we estimate the mean free path using the measured collision frequency and the thermal speed, we get a similar result.

We fit the density with piecewise exponential functions [~ exp(−(z − z0)/lν)] in the steady state region, and obtain a hydrodynamic length scale lν/σ between 12 and 15 for 40 < z/σ < 100. We obtain a similar length scale from piecewise linear fitting of the temperature T in the same region. We calculate the Knudsen number Kn, defined as the ratio of the mean free path to the length scale of the macroscopic gradients [20], using λ(z) and lν; Kn ranges from 0.5 to 20 in the region 40 < z/σ < 100 (Fig. 4).

B. Height-independence of the distribution

The distribution of scaled horizontal velocities should be symmetric as a consequence of the symmetry of the system. We calculate the skewness of the distribution, γ3 = M3/M2^{3/2}, where M_n is the n^{th} moment of the distribution

\[ M_n = \int c^n f(c) dc, \quad (14) \]
and check that $|\gamma_4|$ is less than 0.01 for all the distributions we study. The lowest order deviation from the MB distribution is characterized by the flatness of the distribution, which is called the fourth cumulant or the kurtosis. It was used to quantify the deviation from the MB distribution of the homogeneously cooling state, the homogeneously heated state, and granular gases subject to a boundary forcing. The kurtosis $\gamma_4 (\equiv M_4 / M_2^2 - 3)$ is defined so that it vanishes for the MB distribution, and we find that it also does not change in time above some height (Fig. 5). Further, in the steady state region, $\gamma_4$ is nearly independent of the height, even though both the density and the temperature change; the distributions at different heights in the steady state region are hardly distinguishable (Fig. 6). Also, the kurtosis in the steady state region does not vary much for a wide range of the oscillation parameters: for $0.35 \text{ m/s} < V_{\text{max}} < 0.75 \text{ m/s}$ (and other parameters fixed), $\gamma_4$ changes less than 10%. A similar absence of height dependence of the velocity distribution function was found in a recent experiment on a vertically oscillated quasi-2d granular gas.

### C. Velocity distributions

We first examine the dependence of the distribution on $e$; we measure $\gamma_4$ for three different values of $e$, while $\beta_0$ and $\mu$ are kept at 0.35 and 0.5, respectively. We find that $\gamma_4$ significantly decreases with increasing $e$ in the oscillatory state, however, it decreases only slightly in the steady state region (Fig. 7).

Now we compare our results with the MB distribution of variance $1/\sqrt{2}$,

$$f_{MB}(c_x) = \frac{1}{\sqrt{\pi}} \exp(-c_x^2).$$  \hfill (15)

The steady state distributions obtained for the parameters in Fig. 7 are overpopulated in the high energy tails and underpopulated at small velocities (Fig. 5), compared to $f_{MB}$. The differences of the distributions for various $e$'s are hardly noticeable both on linear and logarithmic scales (Fig. 5), but on a double logarithmic scale plot the tails of the distributions are described by different functions (Fig. 7). We investigate the functional form of the distributions by fitting them (after the normalization by the value at $c_x = 0$) with a stretched exponential function $\exp(-c_x^{\alpha})$. We find that the exponent $\alpha$ changes from 1.9 (indicated by dashed lines) to some smaller value (solid lines), depending on $e$, as the velocity increases. We have not investigated lower values of $e$ to avoid issues such as cluster formation.

We now keep $e$ and $\beta_0$ at 0.9 and 0.35, respectively, and change the value of $\mu$. The profile of $\gamma_4$ in the os-
FIG. 8: The distribution functions of scaled horizontal velocities $f(c_x)$ for the cases in Fig. 7, on linear (top panel) and logarithmic (bottom panel) scales. Although the kurtosis slightly decreases with $e$, the difference between the distributions is hardly distinguishable on both scales. The ranges for the averaging in height were between $30\sigma$ and $45\sigma$ for $e = 0.95$, $40\sigma$ and $55\sigma$ for $e = 0.9$, and $45\sigma$ and $60\sigma$ for $e = 0.85$; the averaging was done over relatively similar heights in the steady state regions (see Fig. 7). The solid line is the MB distribution.

D. Frictionless inelastic hard sphere model

In theoretical and numerical studies, granular materials are often modeled as smooth (frictionless) inelastic disks or spheres, assuming that the friction is a secondary effect that can be neglected or that both the inelasticity and the friction can be incorporated together into a so-called effective coefficient of restitution. In this Section, we discuss how the velocity distribution changes when the friction is not included, and we show that the frictionless model exhibits qualitative differences from the frictional model.

The rotational kinetic energy is two orders of magnitude smaller than its translational counterpart for the cases studied in this paper. However, the presence of the friction reduces the expansion of the granular gas significantly, because the friction reduces the mobility of the grains and increases the collision frequency [27]. The mean height of frictional inelastic hard spheres exhibits a different scaling behavior with the plate velocity from that of frictionless spheres. Only the frictional sphere model reproduces the experimental observations [27, 28].

The $\gamma_4$'s obtained from the simulations of frictionless
particles for the same forcings as in Fig. 7 are illustrated in Fig. 11. In the absence of friction, the layer expands much more, and the steady state occurs at greater height, \( z/\sigma > 100 \). In both the oscillatory and the steady state regions, values of \( \gamma_4 \) are smaller than those of frictional spheres (compare Fig. 11 with Figs. 7 and 10); the distribution deviates from \( f_{MB} \) only slightly. The kurtosis decreases with increasing \( e \), and the difference among the distributions for the three \( e \)'s are small. These distributions have four crossovers with \( f_{MB} \); they are overpopulated both at very small and high velocities and are underpopulated in between, compared to \( f_{MB} \). We fit them with a stretched exponential function, and find that \( \alpha \) is 2.0 for small velocities, and that it depends on \( e \) for the high energy tails (Fig. 12), as in frictional hard spheres.

Since the functional form of the distribution depends on \( e \), we can get a similar distribution function for the steady state by adjusting \( e \). For instance, for \( \mu = 0 \), \( e = 0.7 \), and \( V_{max} = 0.55 \text{ m/s} \) (the same forcing as in Fig. 7), we obtain \( \gamma_4 \approx 0.5 \) for the steady state region; the steady state distribution is similar to the one in Fig. 7 for \( e = 0.9 \) and \( \mu = 0.5 \). However, we find that no single value of \( e \) mimics the hydrodynamic fields or the distribution function of frictional hard spheres, both in the oscillatory and steady state regions; the effect of friction cannot be taken over by an adjusted normal coefficient of restitution. The difference between the results of the two models is illustrated in Fig. 13, where velocities are not rescaled for better comparison. The outermost contour lines in both models become similar when \( e \) in the frictionless model is adjusted as a free parameter [compare Figs. 13(a) and (c), or (b) and (d)]; however, the overall
shape of the density contours cannot be matched by adjusting only $e$. Note that the density changes rapidly with height and $\nu > 1.5 \times 10^{-3}$ at $z/\sigma \approx 10$ near $v_z \approx v_x \approx 0$ in the frictional model, whereas in the frictionless model, the particles spread more smoothly in height, and there is no region for $\nu > 1.2 \times 10^{-3}$.

IV. CONCLUSIONS

We have studied the horizontal velocity distribution function of vertically oscillated dilute granular gas, using a molecular dynamics simulation of frictional, inelastic hard spheres. The hydrodynamic fields are oscillatory in time near the oscillating bottom plate due to a shock wave and an expansion wave. However, the fields are nearly stationary above some height, thus constituting a granular gas in a nonequilibrium steady state. The steady state region forms a granular analog of a nearly collisionless Knudsen gas (Figs. 4 and 3). We find that the dependence of the distribution functions in this granular Knudsen gas regime on the forcing and material parameters is very weak, even though the distributions in the collisional bulk at lower heights depend strongly on the forcing and material parameters (Figs. 7 and 10). The behavior of an ordinary Knudsen gas is determined by boundary conditions [21]. Although we do not know whether boundary conditions or collisions are dominant in determining the behavior of our granular Knudsen gas, we note that this gas does not depend much on the properties of its only boundary, which is the oscillatory region close to the plate.

The functional form of the horizontal velocity distribution in the steady state region is nearly independent of height, when velocities are scaled by horizontal temperature (Fig. 9), even though the hydrodynamic fields continue to change. The distribution function is broader than the MB distribution, being underpopulated at small velocities and overpopulated in the high energy tails (Fig. 8). We do not observe a universal functional form for the distribution function (Fig. 9). The functional form of the high energy tail changes with the dissipation parameters ($e$ and $\mu$) and the oscillation parameter ($V_{\text{max}}$). The dependence on $\mu$ in the steady state region is very weak (Fig. 10).

Our conclusions regarding the absence of a universal distribution function differ from that of Ref. [2], because: (1) We studied the local distribution function, while in Ref. [2] the authors obtained the distribution by averaging over space and time; they assumed that the spatial and temporal variation was negligible near the center of the oscillating box, based on their observation of a weak dependence of the density. We find that the time dependence of the density is weak, but that of the temperature is strong in the oscillatory state region (Figs. 1 and 2). Note that if a distribution is averaged over different temperatures, even the MB distribution function leads to a different resultant distribution function. (2) Our system is different from that in Ref. [2]: we do not have either air or sidewalls, and our container is much taller, so that the bottom plate is the only energy source in our case. How air and sidewalls affect the dynamics of a granular gas is yet to be clarified.

We also studied the velocity distributions of frictionless inelastic hard spheres, and examined the possibility of including frictional effects using an effective normal coefficient of restitution. We found that no single effective restitution coefficient could describe the frictionless gas at different heights.

Velocities of a granular gas, even in the dilute limit, are strongly correlated, and the correlations depend on the density and the coefficient of restitution [24]. The dependence of the distribution on the density implies that the single particle distribution of a dilute granular gas cannot play a role equivalent to that in a dilute ordinary gas; it is not sufficient to specify statistical properties of the gas. However, the knowledge of the single particle distribution of this complex nonequilibrium gas is still of great importance for the purpose of the first approximation.

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