Thermal conductivity at the high-density limit and the levitating granular cluster

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(Received 21 March 2018; published 16 July 2018)

The granular Leidenfrost state consists of a dense granular cluster levitating above a hot granular gas. The density of particles inside the cluster can be very high and even close to the density of crystalline packing. To describe this state theoretically, one needs to know the density dependence of constitutive relations (pressure, heat losses, thermal conductivity) at these very high densities. However, the accurate expression for the coefficient of thermal conductivity is lacking. In this work, the constitutive relations were measured at high densities in molecular dynamics simulations in three different settings: a uniform freely cooling dense granulate (to measure heat losses), a uniform ensemble of elastically colliding particles (to measure pressure), and a dense granular medium between two thermal walls under gravity (to measure thermal conductivity). Next, the hydrodynamic equations with the resulting expressions were solved to describe the levitating cluster state in various parameter regimes. Separate molecular dynamics simulations were performed to test the theoretical predictions and measure the density and temperature profiles of the granular Leidenfrost state, and a good agreement with theoretical results was observed.

DOI: 10.1103/PhysRevE.98.012903

I. INTRODUCTION

The validity of the hydrodynamics approach to granular media (a matter consisting of a large number of inelastically colliding particles) was questioned [1] soon after the granular hydrodynamics equations were formulated [2]. A practical way of testing the validity of this approach is to solve specific problems and compare theoretical predictions with the results of molecular dynamics (MD) simulations [3]. However, there is a major difficulty: hydrodynamics equations should be accompanied by constitutive relations (equation of state, transport coefficients, heat loss term), but these expressions were not known at high densities, see Ref. [4] for review. How can we theoretically describe granular systems, which often exhibit a high-density contrast as the granular Leidenforst state [5,6], where a dense cluster is levitating over a hot gas?

The first attempt in this direction was done in the pioneering paper by Grossman, Zhou, and Ben-Naim [7], who came up with simple arguments for the high-density behavior of pressure $P(n,T)$, heat losses $I(n,T)$, and the coefficient of thermal conductivity $\kappa(n,T)$ and proposed interpolation functions for P, I, and κ between low density and the density of close packing. These expressions (which included a few fitting parameters) were adapted in subsequent works [5,8]; however, they have never been tested in MD simulations. Another approach was pioneered by Luding [9], who performed MD simulations, measured the equation of state of an ensemble of hard disks up to high densities, and suggested a theoretical expression for the pressure that matched the observations. This approach was expanded to measure the density dependence of inelastic heat losses and shear viscosity [10], and the resulting expressions were used to describe fluid-solid coexistence in granular shear flows [11].

Granular clusters can present a crystalline order; this was observed both for a levitating cluster in a system driven by a thermal wall [5,12] and for a solid cluster in a plug flow in a dense sheared system [11]. Without knowing constitutive relations at such high densities (in particular, in the vicinity of the dense close packing), one cannot accurately theoretically describe such systems. However, measuring the coefficient of thermal conductivity is challenging (it was measured only for small and moderate densities [13]): it is difficult to come up with a system exhibiting a nonzero temperature gradient but nevertheless with a uniform density across the system, so that the measured $\kappa(n,T)$ would correspond to a specific density. In this work, we overcame this challenge and measured the coefficient of thermal conductivity in a dense granular medium between two thermal walls under gravity—a system that can have a uniform density in some parameter regime (see Sec. II). The same section also presents measurements of heat losses (in a homogeneous freely cooling dense granulate) and pressure (in a homogeneous ensemble of elastically colliding particles) to check the previously obtained results. We also proposed a theoretical expression for $\kappa(n,T)$ that matched the results of MD simulations. In Sec. III, the hydrodynamic equations with the resulting expressions for P, I, and κ were solved to describe the levitating cluster state in various parameter regimes; these theoretical predictions were tested in a separate set of MD simulations. Section IV presents the summary and discussion of our results.

II. MEASURING CONSTITUTIVE RELATIONS AT HIGH DENSITIES

In this section, we perform molecular dynamics simulations in three different settings to measure the density dependence of pressure $P(\nu)$, inelastic heat losses $I(\nu)$, and the coefficient of thermal conductivity $\kappa(\nu)$ at high densities close to $\nu_c = \pi/(2\sqrt{3})$, the area fraction of crystalline close packing. Here, $\nu = n(\pi d^2/4)$ is the area fraction, n is the number density, and d is the particle diameter. Next, we propose the expressions

that fit the data and suggest interpolation functions between low and high densities. Our goal is to accurately measure $\kappa(\nu)$, but we start with testing the known results for $P(\nu)$ and $I(\nu)$.

A. Equation of state

We considered an ensemble of elastically colliding hard disks without gravity. Periodic boundary conditions in the y direction ($-L/2 \leqslant y \leqslant L/2$) were implemented; in the x direction there were two elastic walls at $x = -H/2$ and $x = H/2$. The total momentum transferred by particles to the walls was measured as a function of time. The resulting curve is indistinguishable from a straight line, and the pressure was computed as the slope of this straight line divided by L. We checked that in all of the simulations the system remained uniform and that the same pressure was measured at the two opposite walls. The simulations were performed for various area fractions ν relatively close to the maximal crystalline close packing area fraction ν_c. The results of the simulations were compared to the two theoretical expressions existing in the literature. Grossman and coauthors [7] suggested $P = nT\,(n_c + n)/(n_c - n)$, while Luding [9] proposed the following expression close the the density of close packing: $P_{\text{dense}} = nT[2\nu_c/(\nu_c - \nu)]$. The interpolation function between the low- and high-density limits has been also proposed, and the resulting equation of state can be written as

$$P = nT\,(1 + 2\nu\, g_l), \tag{1}$$

with

$$g_l = g + m\left[\frac{\nu_c + \nu}{2\nu\,(\nu_c - \nu)} - g\right], \tag{2}$$

where m is an interpolation function, given by $m = \{1 + \exp[(\bar{\nu} - \nu)/m_0]\}^{-1}$, with $\bar{\nu} = 0.70$ and $m_0 = 0.0111$ [9], and $g = (1 - 7\nu/16)/(1 - \nu)^2$ is the equilibrium pair correlation function [14]. Both the theoretical and simulations results are shown in Fig. 1. Since the pressure diverges as $(\nu_c - \nu)^{-1}$, we show $P(\nu_c - \nu)$ on the vertical axis; the horizontal axis shows $\ln(\nu_c - \nu)$ to make the high-density region more visible. The squares show the results of MD simulations, the black dash-dotted curve presents the expression proposed in Ref. [7], and the blue solid curve corresponds to the expression given in Eqs. (1) and (2) and is in an excellent agreement with the measured pressure.

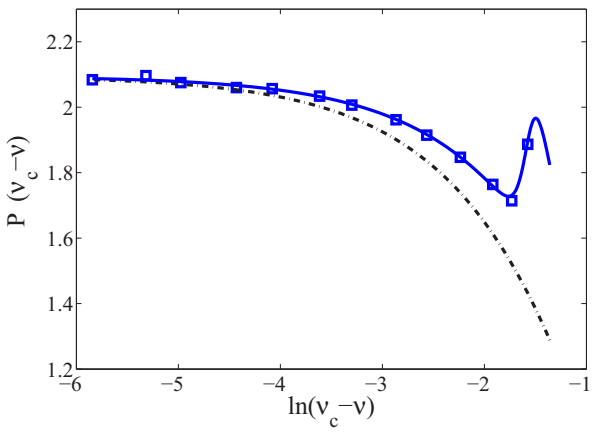

FIG. 1. Equation of state for an ensemble of elastically colliding hard disks at high densities: the rescaled pressure as a function of the area fraction for unit temperature. The blue solid curve given by Eqs. (1) and (2) is in excellent agreement with the results of MD simulations (squares); the black dash-dotted black curve presents the expression proposed in Ref. [7] (see text).

B. Inelastic heat losses

To measure inelastic heat losses in the MD simulations, we considered a system of inelastically colliding hard disks. The collisions were assumed to be binary and instantaneous; the inelasticity of collisions was modeled by the coefficient of normal restitution, $r < 1$. Particles' velocities after a collision are related to their velocities before the collision; their tangential velocities remain unchanged, while the normal velocities after a collision are given by

$$\begin{pmatrix} v'_{i\parallel} \\ v'_{j\parallel} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1-r & 1+r \\ 1+r & 1-r \end{pmatrix}\begin{pmatrix} v_{i\parallel} \\ v_{j\parallel} \end{pmatrix}, \tag{3}$$

where the final velocities of two colliding particles i and j are indicated by primes. Without an external energy input, the temperature of the granulate decreases with time. If the inelasticity of particle collisions is small enough, the system remains homogeneous, and the temperature obeys Haff's law [2]: $T = T_0\,(1 + t/t_0)^{-2}$, where the characteristic cooling time t_0 depends on the form of inelastic heat losses $I(n, T)$. Therefore, measuring t_0 in simulations for various densities provides information about I. This procedure was performed in Ref. [10] for moderately high densities, and the following interpolation between low and high densities for I was suggested:

$$I(n, T) = \frac{8(1 - r)n\,T^{3/2}\,\nu\,g_l}{\pi^{1/2}\,d}, \tag{4}$$

where g_l is given by Eq. (2). Notice that a change of g to g_l is the only difference between the usual Enskog-type form of pressure and heat losses [2] and the formulas given by Eqs. (1) and (4). Equation (4) also assumes the limit of nearly elastic collisions: $1 - r \ll 1$. The inelastic heat losses term is proportional to $1 - r^2$, but in this limit $1 - r^2 \simeq 2(1 - r)$.

Figure 2 shows the results for inelastic heat losses close to the maximal crystalline close packing. Similar to pressure, $I(\nu)$ diverges as $(\nu_c - \nu)^{-1}$; therefore we show $I(\nu_c - \nu)$ on the vertical axis. The results of MD simulations (squares) nicely agree with the theoretical (rescaled) density-dependent part of Eq. (4), $I = (32/\pi^{3/2})\,(1 - r)\,\nu^2\,g_l$ [10] shown by a black solid curve. Figure 2 also shows the expression for inelastic heat losses proposed in Ref. [7] (and still widely used [5,8]). This expression shown by the blue dashed curve (see the Appendix) is clearly much less accurate at moderate and high densities.

C. The coefficient of thermal conductivity

For low and moderate densities, the coefficient of thermal conductivity is given by the standard Enskog-type formula

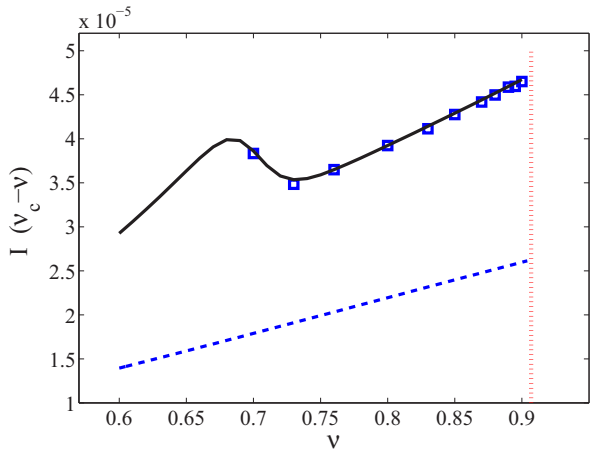

FIG. 2. Inelastic heat losses at high densities: rescaled I as a function of the area fraction (see text). The solid line [Eq. (4), black solid curve] shows an excellent agreement with the results of MD simulations (squares). The vertical red dotted line marks $\nu = \nu_c$, while the blue dashed curve presents the expression proposed in Ref. [7] (see Appendix for details). The simulations were performed for $r = 0.999\,99$.

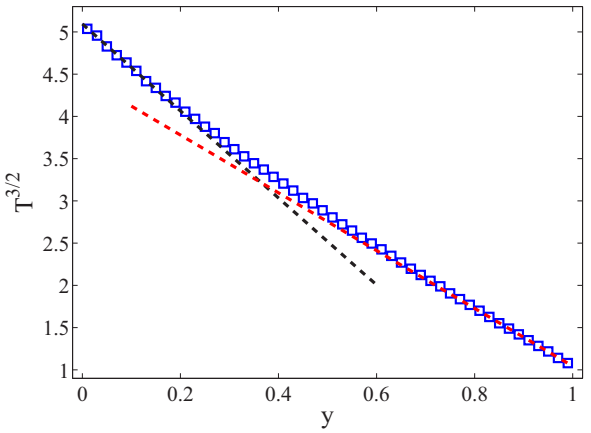

FIG. 3. Temperature profile: $T^{3/2}$ as a function of the rescaled height y. Squares denote the results of MD simulations, and the two dashed lines are linear fits at $y = 0$ and at $y = 1$. These simulations were performed for area fraction $\nu = 0.87$, gravity $g = 0.5$, restitution coefficient $r = 0.999\,99$, and total number of particles $N = 40\,000$.

$\kappa_E(\nu)T^{1/2}/d$ [2,15], with

$$\kappa_E = \frac{8\nu^2 g}{\pi^{3/2}}\left[1 + \frac{9\pi}{16}\left(1 + \frac{2}{3\,\nu\, g}\right)^2\right]$$

and $g = (1 - 7\nu/16)/(1 - \nu)^2$ [14]. Here we aim at finding the expression that works up to the density of close packing. To measure $\kappa(\nu)$, one has to consider a system with a nonuniform temperature profile (so that heat conduction does take place), but nevertheless a uniform density profile. This major difficulty has prevented accurate measurements of $\kappa(\nu)$; a few attempts have been made for low and moderate densities [13,16]. To overcome this challenge, we considered a system of inelastically colliding hard disks between two thermal walls under gravity. Choosing different values for the gravitational acceleration g and for the inelasticity of collisions r in our molecular dynamics simulations allowed us to satisfy the hydrodynamic equations [Eqs. (8), see the next section] with the density that remained almost uniform across the system. The key idea was to choose the hydrodynamic parameter F for each average density in such a way that the hydrostatic equation [the first equation in Eqs. (8)] may be satisfied, had the temperature profile been linear and the density been equal to the average density everywhere. Periodic boundary conditions were implemented in the x direction, and the two walls at $y = 0$ and $y = H$ were thermal with temperatures T_1 and T_2, respectively, with $T_1 < T_2$. In molecular dynamics simulations, particles colliding with the thermal wall forgot their previous normal velocities; the new normal velocities were taken from the Maxwell-Boltzmann distribution with the wall temperature. Gravity pointed in the negative y direction. The heat flux was measured at each of the two thermal walls by computing the energy gained (or lost) by particles colliding with the wall as a function of time. The resulting curve is indistinguishable from a straight line, and the heat flux was computed as the slope of this straight line divided by L, the length of the wall. The magnitude of the heat flux can be written as $(2/3)\,\kappa(\nu)\,(d/dy)T^{3/2}$. To proceed, the temperature profile was measured in the simulations, and then $T^{3/2}$ was plotted as a function of height; two linear fits were made in the vicinity of the two walls (see Fig. 3).

Based on these measurements, $\kappa(\nu)$ was computed. We checked that the system remained almost uniform (the largest density contrast was about 2%, not too close to ν_c and vanishingly small close to ν_c, as for parameters of Fig. 3). We also checked that the values of $\kappa(\nu)$ measured at the two walls were approximately the same. The simulation results can be fitted by the following expression of the form $\kappa(\nu)T^{1/2}/d$ that also interpolates between low and high densities:

$$\kappa = \kappa_E + m\left[\frac{3\nu_c}{2}\frac{(\nu_c + 2\nu)}{\nu_c - \nu} - \kappa_E\right], \tag{5}$$

where the function m is the same as the one used in expressions for pressure and heat losses [see text after Eq. (2)]. Figure 4 shows the measured coefficient of thermal conductivity (black squares) together with the various expressions used in the literature (the details are given in the Appendix). Again, as $\kappa(\nu)$ diverges as $(\nu_c - \nu)^{-1}$, we show $\kappa\,(\nu_c - \nu)$ on the vertical axis. The inset shows that the expression given by Eq. (5) provides an excellent fit to the data, while some of the other expressions for thermal conductivity can be wrong by a factor of 4. Deriving the dense part of Eq. (5) analytically $\kappa_{\text{dense}} = (3\nu_c/2)\,(\nu_c + 2\nu)/(\nu_c - \nu)$ looks tempting due to the relative simplicity of this formula, but it still presents a challenge for the theory.

Once the expressions for the constitutive relations are obtained, one can employ them to analyze a variety of systems by using the hydrodynamic approach. The next section considers as an example the granular Leidenfrost state, where a very dense cluster is levitating over a hot granular gas.

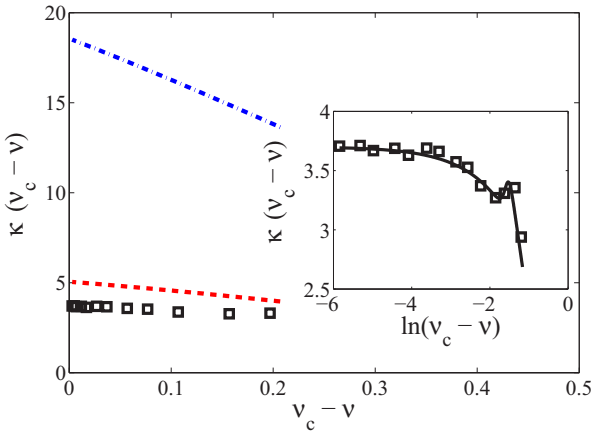

FIG. 4. The coefficient of thermal conductivity at high densities: rescaled $\kappa(\nu)$ as a function of the area fraction. Shown is the comparison between the results of MD simulations (squares) and the expressions used in the literature (the red dashed line is from Ref. [7] and the blue dash-dotted line is from Refs. [5,8], see the Appendix for details). The inset zooms in on the results of MD simulations (squares) and the proposed expression for κ [Eq. (5), black solid line]. Since κ diverges as $(\nu_c - \nu)^{-1}$, the vertical axis shows the product $\kappa\,(\nu_c - \nu)$; the horizontal axis presents $\ln(\nu_c - \nu)$ to make the high-density behavior visible. Each symbol from MD simulations corresponds to a different set of parameters; the gravity g ranged from 0.115 for $\nu = 0.75$ to 6.88 for $\nu = 0.904$ to ensure that the density remained almost uniform across the system. The total number of particles was $N = 40\,000$, and in most of the simulations the restitution coefficient was $r = 0.999\,99$.

III. GRANULAR LEIDENFROST STATE: THEORY AND SIMULATIONS

Consider an ensemble of moving hard disks that collide inelastically; particles of mass $m = 1$ and diameter $d = 1$ are placed into a two-dimensional system of width L and height H. The bottom wall is thermal and is maintained at temperature T_b; gravity points in the negative y direction. As before, we employ periodic boundary conditions in the horizontal x direction. Granular temperature decreases with height due to inelastic collisions between the particles; as a result, in some parameter regimes, one can observe denser granulate above a more dilute gas [6]. In the extreme case, one can observe a solid cluster, which is levitating above hot granular gas. It is known that this state can become unstable, leading to convection [8,17]; the cluster can also break due to a large fluctuation [12]. In this work, we consider the regime of parameters where the cluster is stable.

Equations of granular hydrodynamics are written for the number density of grains $n(\mathbf{r}, t)$, the granular temperature $T(\mathbf{r}, t)$, and the mean flow velocity [2]:

$$\begin{aligned} dn/dt + n\nabla\cdot\mathbf{v} &= 0,\\ (d\mathbf{v}/dt) &= \nabla\cdot\mathbf{P},\\ n\,(dT/dt) &= -\nabla\cdot\mathbf{Q} + \mathbf{P}\,:\nabla\mathbf{v} - \Gamma. \end{aligned} \tag{6}$$

Here $\mathbf{P}$ is the stress tensor, $\mathbf{Q}$ is the heat flux, and Γ is the new term representing energy losses due to the inelasticity of particle collisions. The stress tensor $\mathbf{P}$ is given by $\mathbf{P} = [-P(n,T) + \mu(n,T)\mathrm{tr}(\mathbf{D})]\mathbf{I}_0 + 2\eta(n,T)\,\hat{\mathbf{D}}$, where $\mathbf{D} = (1/2)[\nabla v + (\nabla v)^T]$ is the rate of deformation tensor, $\hat{\mathbf{D}} = \mathbf{D} - \frac{1}{2}\,\mathrm{tr}\,(\mathbf{D})\,\mathbf{I}_0$ is the deviatoric part of $\mathbf{D}$, $\mathbf{I}_0$ is the identity tensor, and $\eta(n,T)$ and $\mu(n,T)$ are the shear (first) and bulk (second) viscosities, respectively. Although the behavior of shear viscosity at high densities is highly nontrivial [10,18], no shear is present in the case of the granular Leidenfrost state. In systems of inelastically colliding particles, the heat flux depends not only on the temperature gradient but also on the density gradient [19]. In the limit of nearly elastic collisions, however, the density gradient term vanishes, and the heat flux $\mathbf{Q}$ is given by $\mathbf{Q} = -\kappa(n,T)\nabla T$, where $\kappa(n,T)$ is the coefficient of thermal conductivity.

In the static case (zero mean flow velocity) and when the density and the temperature depend on the vertical coordinate y only, the equations are reduced to

$$\begin{aligned} \frac{dP}{dy} + mng &= 0,\\ \frac{d}{dy}\left(\kappa(n,T)\frac{dT}{dy}\right) - I(n,T) &= 0. \end{aligned} \tag{7}$$

The hydrodynamic equations are accompanied by the constitutive relations obtained in Sec. II. Measuring y in units of the system height H, T in units of the bottom wall temperature T_b, n in units of n_c, and P in the units of $n_c T_b$, we get the following dimensionless equations:

$$\begin{aligned} \frac{dP}{dy} + Fn &= 0,\\ \frac{d}{dy}\left(\kappa(n,T)\frac{dT}{dy}\right) - RI(n,T) &= 0, \end{aligned} \tag{8}$$

where the parameter $F = mgH/T_b$ is an analog of the Richardson number, the ratio of potential to thermal energies of a particle, and $R = (1-r)H^2/d^2$ is the heat loss parameter. The final dimensionless parameter is the average area fraction, $f = \bar{\nu}/\nu_c = \int_0^1 n(y)dy$. Below we consider the granular Leidenfrost state for two completely different sets of these dimensionless parameters (F, R, f); one set was used in Ref. [5], another one in Ref. [12], but with a different aspect ratio (see Fig. 6). In addition to numerically solving Eqs. (8) in MATLAB, we performed MD simulations that correspond to these hydrodynamic parameters and compared the measured temperature and density profiles with the theoretical predictions. A substantial temperature jump [16] was observed in simulations at the bottom thermal wall, so we used the measured gas temperature near the wall as the wall temperature in the boundary conditions for the hydrodynamic equations.

Figures 5 and 7 present the temperature and density profiles obtained by employing hydrodynamic theory, which incorporated the expression for pressure [Eqs. (1)–(2)], heat losses [Eq. (4)], and the revised expression for thermal conductivity [Eq. (5)]. The symbols show the results of MD simulations, a very good agreement between simulations and theory was obtained. It is worth emphasizing that although one can obtain a good agreement with the simulation results even for a very nonaccurate set of constitutive relations (using fitting parameters, see the Appendix), this might work only for one specific set of hydrodynamic parameters (R, F, f). Correct

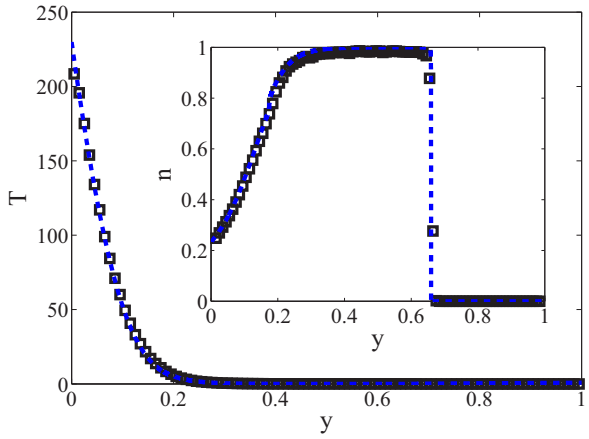

FIG. 5. Granular Leidenfrost state: dense levitating cluster over hot granular gas. Shown is the comparison between the results of MD simulations (squares) and the theoretical predictions for both the temperature profile (not rescaled, dashed line) and the density profile (inset, dashed line). The parameters for the simulations are as in Ref. [5]: $g = 1$, $r = 0.988\,15$, $N = 10\,000$, the aspect ratio is $H/L = 1.5625$; this corresponds to the hydrodynamic parameters $R = 289.3066$, $F = 0.6793$, and $f = 0.5543$.

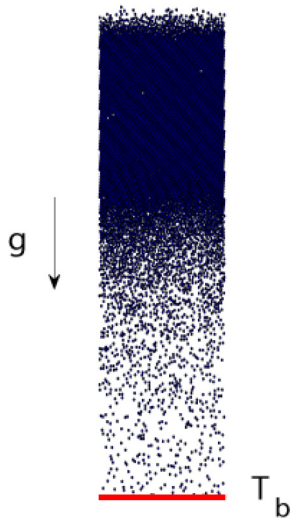

FIG. 6. Snapshot of the system corresponding to Fig. 7. The red line represents a thermal wall, and gravity is in the negative y direction. The snapshot is a narrow vertical column, a slice of the system considered in Ref. [12]. The parameters for the simulations are as follows: $g = 0.000\,67$, $r = 0.992$, $N = 7500$, and the aspect ratio is $H/L = 3$.

constitutive relations, however, should provide good agreement with simulations for any set of hydrodynamic parameters.

IV. SUMMARY AND DISCUSSION

In this work, we performed measurements of pressure $P(n)$, heat losses $I(n)$, and the coefficient of thermal conductivity $\kappa(n)$ at high densities in molecular dynamics simulations. We confirmed that all the constitutive relations diverge at ν_c as $(\nu_c - \nu)^{-1}$. We tested the expressions for P and I and proposed an accurate expression for κ for a wide range of densities from the dilute limit to the density of close packing. Interestingly, to measure thermal conductivity of a hard disk's fluid, an ensemble of inelastically colliding particles was considered. Once constitutive relations were obtained, these expressions were employed to obtain hydrodynamic profiles of density and temperature in a completely different setting: an ensemble of inelastically colliding particles driven by a thermal wall from below in the presence of gravity. Such a system presents a fascinating phenomenon: a dense and cold solid cluster levitating over a hot gas (Fig. 6). Overall, the theoretical density and temperature profiles agree very well with the results of the separately performed MD simulations for two completely different sets of hydrodynamic parameters.

A small discrepancy, however, can still be observed in the density profile: the theoretical curve shows a very sharp decrease (the top of the cluster), while in MD simulations the decrease is slightly smoother (see Fig. 7). This occurs since the theory assumes a static solution, while in simulations, the center mass of the system exhibits small amplitude oscillations; these oscillations have already been observed in Ref. [5] and were recently investigated in a separate work [20]. Accurate constitutive relations obtained in this paper will allow for a better theoretical analysis of such oscillations, helping to clarify if this is an instability (analogous to one observed without gravity between two thermal walls [21]) or if the cluster is stable, but the decaying oscillatory mode gets a continuous energy input due to the stochastic nature of the system [20].

The focus of the paper was on very dense systems, and determining constitutive relations at the high-density limit remained a challenge (even) for elastically colliding particles. Therefore, in this paper we considered the quasielastic limit, $1 - r \ll 1$. Theoretically, the dependence of pressure and transport coefficients on the restitution coefficient r has been derived for low and moderate densities [22], and testing this dependence in simulations would be an interesting avenue of future research. In order to see the effect clearly (for example,

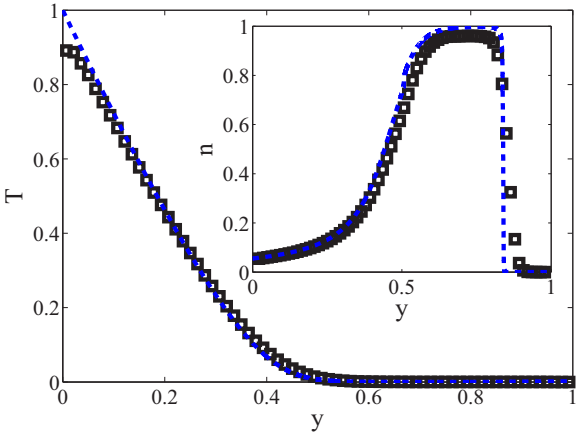

FIG. 7. Granular Leidenfrost state: dense levitating cluster over hot granular gas; the snapshot is presented in Fig. 6. Shown is the comparison between the results of MD simulations (squares) and the theoretical predictions for both the temperature profile (not rescaled, dashed line) and the density profile (inset, dashed line). The hydrodynamic parameters are as follows: $R = 360$, $F = 0.1414$, and $f = 0.433$.

beyond 10% difference), the inelasticity of collisions needs to be large enough. The difficulty that might arise in this case in event-driven molecular dynamics simulations is related to the phenomenon of inelastic collapse, which can occur even in driven systems [23].

Trying the expand this approach to three-dimensional systems can be challenging. For low densities, the pressure and the transport coefficients for granular gases in three dimensions are known. Simulating the three-dimensional system at high densities is significantly harder, as there are two possible packings that reach the largest density: face-centered cubic (fcc) and hexagonal close-packing (hcp). In simulations, mixtures of hcp and fcc clusters may coexist for a long time [24]. It is likely that the expressions for pressure and transport coefficients depend on the specific ordering regime. Therefore, measuring the constitutive relations for a specific phase might be a nontrivial task.

APPENDIX

As we discussed in the main text, a set of constitutive relations was proposed in Ref. [7] to interpolate between the low-density and high-density limits. It was a pioneering work and the first attempt to apply a hydrodynamic approach to dense systems. However, these relations were not tested in MD simulations, and a careful analysis shows that they are not accurate (see below). We discussed the equation of state in detail in Sec. II A; now we present the expressions for the heat losses and the coefficient of thermal conductivity from Ref. [7] to explain the corresponding curves plotted in Figs. 2 and 4. The heat losses for nearly elastic collisions ($1-r \ll 1$) can be written as

$$I(n,T) = c_I \frac{(1-r)n\,T^{3/2}}{L}, \tag{A1}$$

where c_I is an unknown constant and L is the mean free path, given by

$$L = \frac{1}{\sqrt{8}nd}\frac{n_c - n}{n_c - (1-\sqrt{3/8})\,n}. \tag{A2}$$

Notice that in the limit of low densities the expression for the mean free path tends to the correct formula. The dilute limit of the heat losses was not discussed in Ref. [7], but it is not hard to find the constant c_I demanding that at low densities we get the known expression

$$I(n,T) = \frac{8(1-r)nT^{3/2}\nu g_l}{\pi^{1/2}d}.$$

This leads to $c_I = (\pi/8)^{1/2}$. The formula given by Eq. (A1) with this value for c_I is plotted in Fig. 2 (dashed blue line), and it is off approximately by a factor of 2 at high densities.

The expression for the coefficient of thermal conductivity, suggested in Ref. [7], is

$$\kappa = c_\kappa \sqrt{T}\frac{n(\alpha L + d)^2}{L}, \tag{A3}$$

where c_κ is an unknown constant, L is the mean free path, d is the particle's diameter, and $\alpha = 1.15$ is a fitting parameter. Again, c_κ was not discussed in Ref. [7], but demanding that in the dilute limit we get the standard expression $\kappa = 2\,T^{1/2}/(\pi^{1/2}d)$, one gets $c_\kappa = (32/\pi)^{1/2}/\alpha^2$. In subsequent works, a different value for the fitting parameter α was adopted (see, for example, Refs. [5,8]): $\alpha = 0.6$. Figure 4 presents the expression given by Eq. (A3) with the proper c_κ for both values of the fitting parameter α: the red dashed curve corresponds to $\alpha = 1.15$ (off by 25%) and the blue dash-dotted curve corresponds to $\alpha = 0.6$ (off by a factor of 5 at high densities).

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