Departure from Fourier's Law for Fluidized Granular Media

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Molecular dynamics simulations of the inelastic hard sphere model for granular media have been done to study the heat conduction between two parallel plates. The results show that Fourier's law is not valid and a new term proportional to the density gradient must be added to compute the heat flux. The new transport coefficient associated with the density gradient dependence has been measured vanishing in the case of elastic collisions.

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Much interest has been devoted to the study of granular media in recent years. The understanding of static and dynamic properties in this form of matter is crucial in many aspects of industrial processes ranging from pharmaceuticals to civil engineering, as well as in some basic physical phenomena such as those studied in geophysics [1,2].

In the last decade, many groups have developed new experimental and theoretical techniques to approach grain piles and flows from a fundamental perspective [2–7]. The observed flow properties, for instance, are often similar to those of fluids (convective instabilities, pattern formation, or time periodicity) but evidence of differences with fluids is also compelling: strain-stress localization, unexpected patterns, long range correlations, large inhomogeneities, or absence of spatial scale separation [8,9] call for a more specific description.

In addition to continuum theories, new approaches coming from statistical mechanics have also been proposed. Granular flow peculiarities have been reproduced using molecular dynamics techniques and simplified grain models [10,11]. The aim of such approaches is to define the simplest possible model for grains able to reproduce, at least qualitatively, the observed behavior and then to use the techniques of statistical mechanics to deduce macroscopic or continuum equations. This is precisely the rationale of the work that we present here: we will show evidence, obtained from molecular dynamics simulations of inelastic hard spheres (IHS), that Fourier's law relating heat flux and temperature gradient in fluids or solid materials has to be modified in the case of fluidized granular matter. Note that the concepts of temperature and heat flux have been generalized to granular systems using the kinetic theory definitions, neglecting the internal degrees of freedom of the grains.

The inelastic hard sphere model does simplify very much the interactions of grains. In this model, grains are described by smooth spheres of equal diameter, σ, that have only translational degrees of freedom. The collisions are instantaneous events and the energy dissipation in collisions is simplified to a description with only one parameter, the restitution coefficient, r, which is introduced in the following collision rules:

$$\mathbf{v}_1' = \mathbf{v}_1 + \frac{1}{2}(1 + r)[\hat{\mathbf{n}} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]\hat{\mathbf{n}}, \qquad (1)$$

$$\mathbf{v}_2' = \mathbf{v}_2 - \frac{1}{2}(1 + r)[\hat{\mathbf{n}} \cdot (\mathbf{v}_2 - \mathbf{v}_1)]\hat{\mathbf{n}}, \qquad (2)$$

where the primes indicate velocities after collision and $\hat{\mathbf{n}}$ is the unit vector pointing from the center of particle 1 towards the center of particle 2. It is convenient to define the dissipation coefficient $q = (1 - r)/2$ which vanishes when collisions are elastic.

This model is not sufficient for a quantitative description of real granular flows where roughness, rotational energy, static friction, or polydispersity are needed to be introduced to predict flow properties. But it has proved sufficient to reproduce clustering phenomena, shearing instabilities, vibrated bed convection, pipe flow, and so on [12–17]. And the simplicity of the model allows one to address the question of how the hydrodynamic equations for fluids are modified when dissipativity is introduced in the collision rules.

Hydrodynamic equations, modified by the addition of a sink term in the energy equation, have been proposed in order to describe the long-wavelength long-time behavior of granular fluids with a dissipativity coefficient of only a few percent [18–20]. In those approaches, phenomenological relations (Navier-Stokes and Fourier's laws) between thermodynamic forces (gradients of density, velocity, and temperature) and fluxes as well as equations of states are introduced, extending then the properties of fluids made of elastic hard spheres to dissipative systems. Theoretical results compare generally well with those obtained from simulations done on computers.

Despite the dissipative nature of collisions, if the macroscopic field gradients are not so large, it seems natural

to postulate linear relations between fluxes and thermodynamic forces. Then, in general, the heat flux can be expressed as [21]

$$\mathbf{J} = -k\nabla T - \mu\nabla n\,, \tag{3}$$

where k is the thermal conductivity and μ is a new transport coefficient. There is no dependence on the velocity gradient because of tensorial arguments (Curie's theorem).

If the system obeyed the second law of thermodynamics μ would vanish and k would be positive in order that heat flows from hot to cold. On the other hand, in granular systems—when one neglects the internal heating of the grains on collisions—entropy production is not expected to be positive and there is no *a priori* reason for discarding the dependence of J on the density gradient, but the new transport coefficient μ must go to zero with the dissipation coefficient q. Conservative systems put in far from equilibrium regimes also show deviations from Fourier's law and the linear corrections analog to (3) must be added [22–24].

The constitutive equation (3) has been proposed using a Chapman-Enskog type of expansion for the solution of Boltzmann and Enskog equations generalized to the case of dissipative systems [25–28]. The coefficient μ has been computed for some models, but in those approaches the macroscopic equations are not derived but, in fact, postulated. We will show that simulation results support Eq. (3) and compute the coefficients k and μ, the latter being different from zero.

In this Letter we start from a more fundamental level of description, i.e., molecular dynamics simulations of IHS, to study the macroscopic behavior of the heat flux. In particular, we examine the relation between the heat flux $\mathbf{J}$ and temperature and density gradients. That is, we examine whether Fourier's law is valid in this granular model or if it must be modified according to (3).

We have done molecular dynamics simulations of dilute two-dimensional systems composed of IHS under the influence of gravity. A total number of $N = 1000$ spheres are placed in a square box with horizontal periodic boundary conditions. Energy is injected in the system through thermal stochastic walls at the top and at the bottom. Each time a particle hits them a new random velocity is sampled out of a Maxwellian distribution at the same temperature T_0 for both walls.

Units are chosen such that the disk diameter σ and the disk mass m are equal to one. Also, since in the IHS model there is no intrinsic energy scale, the wall temperature T_0 is set to one. Finally, we define the granular temperature as the average kinetic energy per particle; that is, Boltzmann's constant is set to one.

Three series of simulations were done for different values of gravity acceleration, $g = 0.005$, $g = 0.01$, and $g = 0.02$. Global number density (defined as N/L^2, where L is the length of the box) was always set to $n_0 = 0.01$ and the dissipation coefficient took the values $q = 0.01$, $q = 0.02$, $q = 0.03$, $q = 0.04$, $q = 0.05$, $q = 0.07$, and $q = 0.10$.

Given a particular value of the global density n_0, gravity acceleration g, and dissipation coefficient q, the system is simulated until it reaches a stationary state characterized by time independent macroscopic fields and a vanishing velocity field. In these conditions the system is simulated for a long time (2.5×10^5 collisions per particle) where macroscopic fields are measured using carefully devised measurement routines described in [29]. In particular, the following fields were computed: number density $n(\mathbf{r})$, temperature $T(\mathbf{r})$, and heat flux $\mathbf{J}(\mathbf{r})$ (including both the kinetic and potential contribution). From these fields, once horizontally averaged, one obtains the density and temperature gradients. Under the above described simulation conditions (low density and dissipativity) the system does not show clustering, then all the system inhomogeneities are of hydrodynamic character.

Because of the dissipative character of the IHS, even if the top and bottom walls are at the same temperature, the temperature profile is not uniform and has a minimum at some height, y^*, in the interior of the system. The energy that is dissipated in the bulk comes from the walls producing a net heat flux that goes from the walls to the bulk.

Gravity produces a nonuniform pressure, monotonically decreasing with height, obeying, in fact, the barometric law

$$\nabla p(\mathbf{r}) = -gn(\mathbf{r})\,. \tag{4}$$

Assuming a local equation of state, $p(\mathbf{r}) = p[n(\mathbf{r}), T(\mathbf{r})]$ [30], the temperature gradient and the density gradient are related by

$$\frac{\partial p}{\partial n}\nabla n + \frac{\partial p}{\partial T}\nabla T = -gn\,. \tag{5}$$

Then, according to (3) and (5) a nonvanishing heat flux can be measured at y^* only if gravity is different from zero.

Figure 1 shows the density profile, the temperature profile, and the heat flux obtained in a simulation with $g = 0.01$ and $q = 0.05$. It is clear that the heat flux is not zero at the minimum of T, thus contradicting Fourier's law. Also, in the complete region between y^* and the point where the heat flux vanishes, Fourier's law is violated. In effect, in this region the heat flux is parallel to the temperature gradient, that is, heat is flowing from cold to hot, contradicting the second law of thermodynamics. Similar results are obtained in all the other simulations.

These results show that the modified heat law (3) must be used. The value of the new transport coefficient μ can be obtained directly by computing the heat flux and the density gradient at y^*. We define first the nondimensional coefficient $\hat{\mu} = n\mu/T^{3/2}$. This nondimensional coefficient could depend on density and dissipation but not on temperature since for the IHS there is no nondimensional number that can be built that depends on temperature (the

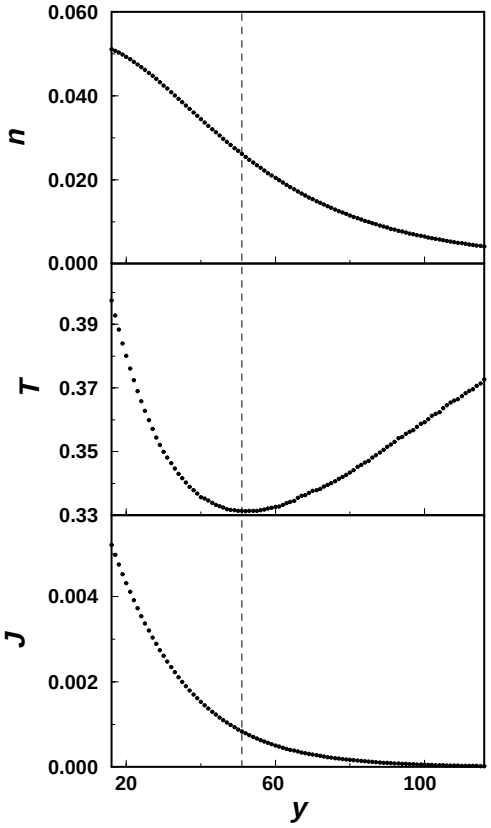

FIG. 1. Density (up), temperature (middle), and heat flux (bottom) profiles as a function of height for a simulation with $g = 0.01$ and $q = 0.05$. The total height of the system is $L = 316$, but only a section is shown. The minimum of T is located at $y^* = 51$ (indicated by the vertical dashed line), whereas the heat flux vanishes at $y = 149$ (outside the plot range).

number $mg\sigma/T$ should not be taken into account due to Galilean invariance).

For every simulation we located the position of y^* using a polynomial fit to the temperature profile and then computed $\hat{\mu}$ as

$$\hat{\mu} = -\frac{nJ}{T^{3/2}\nabla n}\bigg|_{y=y^*}. \tag{6}$$

Figure 2 shows the measured values of $\hat{\mu}$ as a function of q for the three series of simulations. The different values of the gravity acceleration g produce a change in the density at y^*, and thus different values for $\hat{\mu}$ are obtained. The error bars are computed from the uncertainty on the position of the minimum of T. In the simulations with $g = 0.005$ and q from 0.01 to 0.03 it was not possible to obtain with enough accuracy the position y^* because the effective dissipation was so small that the temperature profile was extremely flat.

It is clear that $\hat{\mu}$ vanishes with q. In all cases the density at y^* is small but not negligible so density corrections to the ideal gas expression should be expected. A fit to the

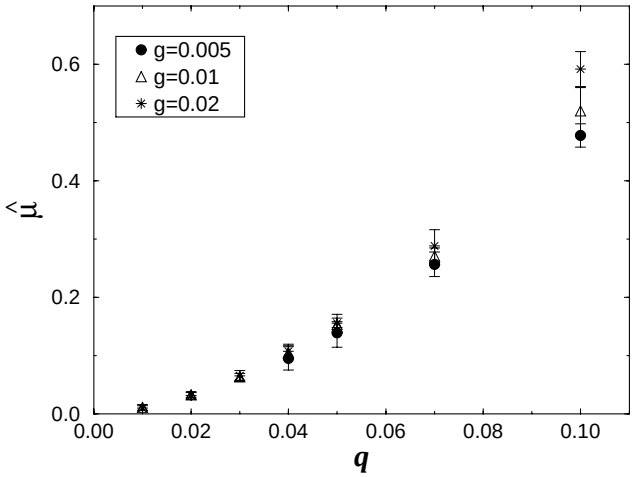

FIG. 2. Nondimensional transport coefficient $\hat{\mu}$ as a function of dissipation q. The three series of values correspond to different values of gravity acceleration g. Note that the value of density at y^*, minimum of temperature, depends on g.

obtained values of $\hat{\mu}$ was done including linear density and quadratic dissipation dependence, giving

$$\hat{\mu} = 0.7q[(1 + 13.3n) + 55.0q(1 + 0.77n)], \tag{7}$$

where the fact that $\hat{\mu}$ must vanish when q goes to zero was imposed in the fit.

The lack of independent computations of the thermal conductivity k does not allow one to test (3) and (7) outside y^*. To make a consistent analysis, q corrections to the thermal conductivity are needed as μ is proportional to q. This, however, does not restrict the general validity of (7) since its spatial dependence is given implicitly in terms of the density, temperature, and dissipativity.

The simulation methodology used to compute μ can be applied only to a limited range of values for the simulation parameters (global density, dissipation, gravity) since different unwanted phenomena start to happen outside that restricted range. If dissipation or density take larger values, the density at the center of the box increases near to solid values making the approach unsuitable. Also, when gravity is increased a spontaneous convective motion develops [31] which makes the field depend on the x coordinate. In the other extreme, low values of gravity or dissipation produce poor statistics, and a further decrease of density would make the mean free path comparable to the size of the box, not allowing to work with local transport laws.

In conclusion, molecular dynamics simulations for a simple granular model show that the standard Fourier's law of thermal conductivity should be modified, adding a dependence on the density gradient to the usual temperature gradient dependence. Using stationary nonequilibrium techniques we have computed the value of the new transport coefficient μ. This coefficient, that vanishes for elastic collisions, has a large dependence on the dissipation coefficient q and on density. It is expected that this

departure from Fourier's law is generic for granular media and not restricted to the IHS model.

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