Understanding the breakdown of Fourier's law in granular fluids

D. Candela
Physics Department, University of Massachusetts, Amherst, Massachusetts 01003

R. L. Walsworth
Harvard-Smithsonian Center for Astrophysics, Cambridge, Massachusetts 02138

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In fluidized granular matter (such as rapidly flowing sand) heat can flow from colder to hotter granular temperatures, violating Fourier's law. A simple heuristic explanation for this anomalous heat current is presented, based on the non-equilibrium nature of granular fluids. The heuristic explanation leads to a straightforward calculation of the heat current which is in good agreement with existing, more detailed calculations and with recent experiments.

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To understand the physics of granular fluids (such as rapidly flowing sand), a *granular temperature* is defined that is proportional to the mean fluctuating kinetic energy of the grains (that part of the kinetic energy that does not include the grain flow velocity). Granular temperature gradients drive the flow of grain-scale kinetic energy (granular heat), just as ordinary temperature gradients drive the flow of molecular-scale kinetic energy.[1] For matter close to equilibrium, a heat current, $\mathbf{q}$, always flows from hot to cold and is proportional to the temperature gradient ∇T (following Fourier's law, $\mathbf{q}=-\kappa\nabla T$, where κ is the thermal conductivity).[2] In contrast, in granular fluids there is an additional "anomalous heat current" proportional to the density gradient ∇n—anomalous because it permits a flow of heat from cold to hot, which would violate the second law of thermodynamics for a system close to equilibrium.

The anomalous heat current was clearly observed in a recent NMR experiment,[3] has been calculated using sophisticated statistical physics methods,[1,4–7] and found in numerical simulations.[8–10] However, a simple heuristic explanation for the anomalous heat current has been lacking. Here we present such an explanation to complement the more theoretical calculations. In particular, we show how the anomalous current is tied directly to the out-of-equilibrium nature of granular fluids, which lose energy continuously due to inelastic grain collisions.

In a granular fluid with a free upper surface (confined by gravity and excited from below), the anomalous heat current leads to a temperature inversion: the temperature first falls as a function of height and then rises again in the vicinity of the upper surface.[10] This granular temperature inversion resembles the atmospheric phenomenon of the same name, in which the temperature first falls as a function of altitude above the Earth's surface, and then rises again at higher altitudes. Unlike an atmospheric temperature inversion, which typically is caused by the movement of a warm air mass over a cooler one, a granular temperature inversion can exist in a steady state with no convection—a consequence of the anomalous heat current.[10]

Such a temperature inversion was observed in our recent experiment[3] using NMR to probe vibrofluidized mustard seeds. As can be seen in Fig. 1, the anomalous heat current is not a small correction; rather it leads to large qualitative changes in the temperature profile for a fairly ordinary granular system. Similar temperature inversions may be visible in data from several earlier experiments on quasi-2D granular systems.[11–13]

The heat current including the anomalous term is

$$\mathbf{q}=-\kappa\nabla T-\mu\nabla n, \tag{1}$$

where T is the granular temperature (proportional to the mean fluctuating kinetic energy of the grains), and n is the number density. Here μ is a new transport coefficient that is nonzero only for inelastic systems. Existing theories calculate μ by using the Chapman–Enskog[4–7] or Grad[7] expansions to solve the Boltzmann equation for the full particle distribution function $f(\mathbf{v},\mathbf{r})$. These treatments provide detailed calculations of the anomalous term $\mu\nabla n$, but lack intuitive explanations appropriate for the non-specialist and beg the fundamental physical question: why is there a flow of heat proportional to the density gradient?

Rather than work with the full Boltzmann equation, we use the much simpler relaxation-time model for the evolution of the heat current,

$$\frac{\partial\mathbf{q}}{\partial t}=-A\nabla T-\nu\mathbf{q}. \tag{2}$$

The ∇T term describes the build-up of the heat current due to the free streaming of grains, and the second term expresses the relaxation of $\mathbf{q}$ toward zero due to grain collisions. The relaxation rate, ν, is roughly equal to the frequency at which a grain collides. (See the Appendix for explicit expressions for ν and the prefactor A.) In an elastic system perturbed by weak, long-wavelength temperature and density gradients, the temperature varies slowly in time. Hence, a near-equilibrium steady state is reached with $\partial\mathbf{q}/\partial t\approx 0$, immediately giving Fourier's law: $\mathbf{q}=-\kappa_0\nabla T$ with $\kappa_0=A/\nu$. Although the thermal conductivity of a fluid is not typically calculated in introductory physics courses, this derivation closely parallels the familiar Drude model of the electrical conductivity.[14] In that model the electric force on the carriers substitutes for the $A\nabla T$ term in Eq. (2), but the relaxation term $\nu\mathbf{q}\approx\mathbf{q}/$ (collision time) is the same.

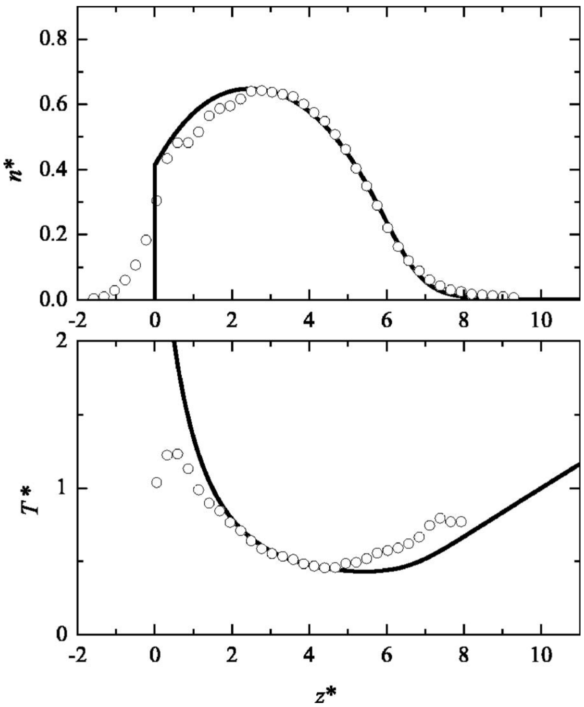

Fig. 1. Granular density (top) and temperature (bottom) as functions of height for a granular fluid vibrofluidized from below (Ref. 3). The symbols show NMR measurements for mustard seeds vibrated vertically at 15 g and 50 Hz; the curves show a fit to the hydrodynamic theory of Ref. 6. Dimensionless units $z^*=z/\sigma$, $n^*=n\sigma^3$, $T^*=T/mg\sigma$ are used (σ,m are the grain diameter and mass; g is gravity). The sample was confined by gravity to the bottom region of the sample chamber with a free upper surface. The experimental data show a clear minimum in the granular temperature T^* as a function of height z^*. At heights above the temperature minimum, the heat current (always upward) flows from cold to hot.

This derivation of Fourier's law breaks down for a granular fluid with inelastic collisions because the system continually loses energy, which causes temperature changes at rates comparable to ν. If energy is supplied at the boundary of the system to maintain a steady state, there are density and temperature variations on length scales comparable to λ, the mean free path between collisions. Thus, the system is inherently not in equilibrium due to inelasticity,[15] and the nonlocality of the grain collision process must be taken into account.[6,7]

Our heuristic argument leads to essentially the same result as the theoretical calculations in Refs. 6 and 7 and is as follows: Grains that collide at the point, $\mathbf{r}$, and time, t, suffered their last collisions at locations typically a mean free path λ distant from $\mathbf{r}$ and a mean collision time $1/\nu$ earlier than t. Therefore, the temperature gradient ∇T in Eq. (1) may be replaced by its nonlocal average $\langle\nabla T\rangle$ over an extended spacetime region $(\lambda,1/\nu)$ around the point $(\mathbf{r},t)$ [see Eq. (A2) in the Appendix].

We now show that replacing the temperature gradient in Fourier's law by the nonlocal temperature gradient (that is, $\mathbf{q}=-\kappa_0\langle\nabla T\rangle$) leads directly to the anomalous heat current, in good agreement with more theoretical treatments. In this picture, the heat current is driven only by the (nonlocal) temperature gradient. The appearance of an anomalous (density-driven) heat current is in a sense an artifact of expressing the nonlocal temperature gradient in terms of local quantities.

This argument is easiest to understand for a freely-cooling granular fluid (that is, no external energy input) with small spatial gradients in T and n.[16] In the Earth's gravity a freely cooling granular fluid quickly collapses, but this system has been a popular and useful system for computer simulations.[17] In such a state $\partial T/\partial t=-\zeta T$, with the cooling rate, ζ, an increasing function of n. In this case the effective temperature gradient $\langle\nabla T\rangle$ is approximately equal to the actual temperature gradient ∇T one collision time $1/\nu$ earlier. This time lag, coupled with the density-dependent cooling rate, leads immediately to the anomalous (density-dependent) heat current. For example, if at time $t=0$ there is a density gradient but no temperature gradient, then the denser regions cool faster so they must have been hotter at earlier times. Therefore, averaging ∇T over times $t<0$ yields a nonzero heat current in the absence of a temperature gradient at $t=0$. As this example shows, the existence of the anomalous heat current depends crucially on the variation of the cooling rate with density.

A simple calculation based on this argument (see the Appendix) yields the anomalous heat transport coefficient $\mu=\kappa_0\zeta T/\nu n$, which is close to the results of theoretical calculations.[4–7] Note that μ is proportional to the parameter ζ/ν (cooling rate/grain collision rate), a dimensionless measure of the degree to which a granular fluid is out of equilibrium.[7]

As a second example, we consider a boundary-driven steady-state, for example, a vertically-vibrated granular medium such as that represented in the experimental data of Fig. 1 and described in Ref. 3. Due to inelastic energy losses, a boundary-driven steady-state necessarily has the strong spatial variations of T. For example, the system would typically be hotter at the boundary (where energy is supplied), and cooler in the interior.

In this case it is the spatial (rather than the time) average of ∇T that is relevant, along with the density dependence of the inelastic power loss. By energy conservation, the inelastic loss in a steady state must be balanced by a divergence of the heat current. Where there is a density gradient, this divergence must have a gradient, which forces the heat current and, hence, the temperature gradient to have a large, nonzero second spatial derivative (curvature). The curvature of the temperature gradient over distances comparable to the mean free path in turn implies that the effective (nonlocal) temperature gradient $\langle\nabla T\rangle$ is different than the local gradient, leading to an extra term in the heat current that is proportional to the density gradient (see Fig. 2). This argument leads to a simple calculation (see the Appendix), which (up to a factor of order unity) yields the same value for the anomalous heat current as that derived for the freely cooling state.

We emphasize that the physical mechanism we have identified for the anomalous heat current is fundamentally the same in the cooling and steady states: the effective averaging of the temperature gradient over the spacetime extent of the collision process [Eq. (A2)]. Although the steady-state mechanism may appear to depend on higher derivatives of the temperature, these higher derivatives are a direct conse-

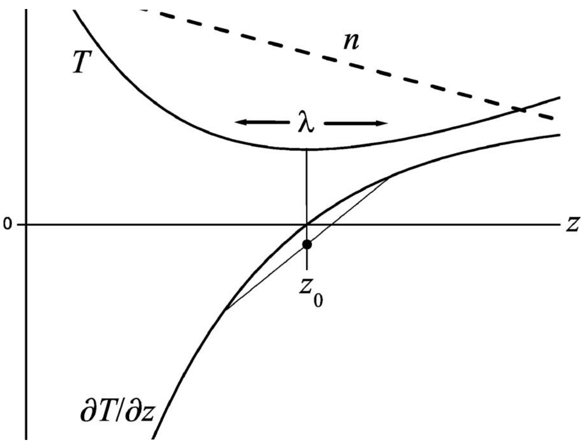

Fig. 2. Schematic of the mechanism for anomalous heat currents in a steady-state situation similar to that shown in Fig. 1. At the height, z_0, of the temperature minimum, the gradient $\partial T/\partial z$ has nonzero curvature due to the density gradient and the density dependence of the inelastic power loss. As a result, the average of the temperature gradient over the mean free path, λ, is nonzero (filled dot on graph). This nonzero effective gradient in turn drives a heat current even though $\partial T/\partial z$ is zero at this height.

quence of energy conservation coupled with ordinary (linear) thermal conductivity. Hence, consistent with a hydrodynamic picture, the anomalous transport coefficient, μ, is the same in the cooling and steady states.

We also emphasize that it is the large space or time derivative of the temperature, rather than the inelasticity *per se*, that is the source of the anomalous heat current. From this point of view, the role of inelasticity in a granular fluid is primarily to create a highly non-equilibrium state. Some novel physical properties of granular fluids (like the anomalous heat current) are due fundamentally to the large deviation from equilibrium rather than the inelastic energy loss.

The general problem of non-equilibrium temperature and heat flow is a large and interesting field, beyond the scope of the present article.[18] We mention only that deviations from Fourier's law are predicted for elastic systems like molecular gases in highly non-equilibrium states.[18–20] In general, the additional heat-current terms are not driven by density gradients, which have a special role in granular systems due to the density-dependent energy loss rate. For example, in the highly non-equilibrium Poiseuille (channel) flow of an elastic gas, there is a heat current driven by gradients in the shear rate.[19,20]

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APPENDIX: CALCULATION OF THE ANOMALOUS HEAT CURRENT

To avoid masking the essential simplicity of the argument, we have collected detailed calculations including prefactors in this Appendix. We consider a system of hard, inelastic spheres of mass, m, and diameter, σ, in d space dimensions. The granular temperature is $T=m\langle v^2\rangle/d$, where $\langle v^2\rangle$ is the mean-square grain velocity. The inelasticity is measured by the coefficient of normal restitution $\alpha\in[0,1]$, equal to the ratio of post-collision to pre-collision grain speeds in the center-of-mass frame. For simplicity we assume a dilute, weakly inelastic system ($n\sigma^3 \ll 1$, $(1-\alpha)\ll 1$), although the mechanism we identify for the anomalous heat current is not limited to this regime.

Table I. Values of the dimensionless prefactors that occur in expressions for temperature- and density-dependent quantities. The b_q values are calculated for a Maxwell–Boltzmann velocity distribution, and b_ν and b_ζ are computed from Appendix A of Ref. 9. The b_λ values are those required for the anomalous transport coefficient, μ, to be the same for cooling states and steady states according to the approximate calculation presented in this paper.

Prefactor	quantity	$d=2$	$d=3$
b_q	Heat current	$4/3$	$5/2$
b_ν	Relaxation rate	$2\sqrt{\pi}/3$	$32\sqrt{\pi}/15$
b_ζ	Cooling rate	$2\sqrt{\pi}$	$8\sqrt{\pi}/3$
b_λ	Mean free path	$\sqrt{4/3}$	$\sqrt{5/3}$

The relaxation-time model for the heat current [Eq. (2)] is

$$\frac{\partial \mathbf{q}}{\partial t} = -\frac{b_q n T}{m}\nabla T - \nu \mathbf{q}, \tag{A1}$$

where the relaxation rate $\nu=b_\nu n\sigma^{d-1}(T/m)^{1/2}$. Here $b_q, b_\nu, \ldots$ are dimensionless prefactors (Table I).

The central idea is that the temperature gradient, ∇T, should be replaced by its nonlocal average over the mean-free-path, λ, in space and over the collision time, $1/\nu$, in time,

$$\langle \nabla T\rangle(\mathbf{r},t) = \int\int_{-\infty}^{t} \nabla T(\mathbf{r}',t')K(\mathbf{r}'-\mathbf{r},t'-t)d\mathbf{r}'dt'. \tag{A2}$$

The averaging kernel, K, should be normalized and extend over $\sim\lambda$ in space and $\sim 1/\nu$ back in time, but otherwise its form is irrelevant. For calculational simplicity we choose K to be gaussian in space and exponential in time, $K(\mathbf{r},t) = (2\pi)^{-d/2}\nu\lambda^{-d}e^{-r^2/2\lambda^2}e^{\nu t}$. The mean free path is $\lambda = b_\lambda (T/m)^{1/2}/\nu$, where b_λ is another dimensionless prefactor of order unity.

By making the substitution $\nabla T\to\langle\nabla T\rangle$ directly in Fourier's law rather than in Eq. (A1), we account both for time dependent situations ($\mathbf{q}$ changes significantly during a collision time $1/\nu$) and steady-state situations ($\partial\mathbf{q}/\partial t=0$, but ∇T varies significantly over a mean-free-path distance λ).

In the freely cooling state with weak temperature and density gradients, the cooling rate is[5]

$$\zeta = b_\zeta n\sigma^{d-1}(T/m)^{1/2}(1-\alpha) \tag{A3}$$

to leading order in the inelasticity $(1-\alpha)$, with b_ζ another dimensionless prefactor. In this state only the time average in Eq. (A2) is relevant, giving

$$\langle \nabla T \rangle \approx \nabla T - (1/\nu)\, \partial(\nabla T)/\partial t. \tag{A4}$$

That is, the effective temperature gradient $\langle \nabla T \rangle$ is approximately equal to the local gradient ∇T one collision time $1/\nu$ earlier in time.

The second term in Eq. (A4) is readily calculated:

$$\partial(\nabla T)/\partial t = \nabla(-\zeta T) \tag{A5a}$$

$$= -\zeta \nabla T - T\left[\frac{\partial \zeta}{\partial T}\nabla T + \frac{\partial \zeta}{\partial n}\nabla n\right] \tag{A5b}$$

$$= -\frac{3\zeta}{2}\nabla T - \frac{T\zeta}{n}\nabla n, \tag{A5c}$$

where $\zeta \propto nT^{1/2}$ has been used. Therefore,

$$\mathbf{q} \approx -\kappa_0 \langle \nabla T \rangle \tag{A6a}$$

$$\approx -\left(1 + \frac{3\zeta}{2\nu}\right)\kappa_0 \nabla T - \frac{\kappa_0 \zeta T}{\nu n}\nabla n. \tag{A6b}$$

From Eq. (A6) we can read off the anomalous transport coefficient, $\mu = \kappa_0 \zeta T/\nu n$, which is proportional to the small but non-negligible parameter ζ/ν (for example, $\zeta/\nu \approx 0.1$ for $\alpha = 0.9$ in 3D). This value for μ is consistent with the theoretical calculations. For example, it is 5/4 times the value calculated in Ref. 5. The ordinary thermal conductivity also acquires a correction proportional to ζ/ν.

To simplify the discussion of a boundary-driven steady state, we assume that T and n depend only on the vertical coordinate z. In analogy to Eq. (A4), we have

$$\langle \partial T/\partial z \rangle \approx \partial T/\partial z + (\lambda^2/2)\partial^3 T/\partial z^3. \tag{A7}$$

To lowest order in ζ/ν we have $\partial T/\partial z = -q_z/\kappa_0$, where q_z is the z-component of the heat current $\mathbf{q}$. Hence,

$$\partial T^3/\partial z^3 \approx -\kappa_0^{-1}\partial^2 q_z/\partial z^2. \tag{A8}$$

Equation (A8) omits corrections proportional to derivatives of κ_0, which complicate the calculation but do not affect the leading-order estimate for μ.

In a steady state the energy loss rate per unit volume due to inelastic collisions, P_c, must be balanced by the divergence of the heat current: $P_c = -\partial q_z/\partial z$. The energy loss rate is proportional to the cooling rate ζ: $P_c = c\zeta T = dn\zeta T/2$, where $c = dn/2$ is the specific heat (ignoring grain rotations). Using Eqs. (A7) and (A8) we have

$$\langle \partial T/\partial z \rangle - \partial T/\partial z \approx -(\lambda^2/2\kappa_0)\partial^2 q_z/\partial z^2 \tag{A9a}$$

$$= (\lambda^2 d/4\kappa_0)\, \partial(n\zeta T)/\partial z \tag{A9b}$$

$$= \frac{\lambda^2 d\zeta n}{2\kappa_0}\left[\frac{3}{4}\frac{\partial T}{\partial z} + \frac{T}{n}\frac{\partial n}{\partial z}\right], \tag{A9c}$$

where $\zeta \propto nT^{1/2}$ has again been used. Thus, we find for the steady-state heat current:

$$q_z \approx -\kappa_0 \langle \partial T/\partial z \rangle \tag{A10a}$$

$$\approx -\kappa_0\left(1 + \frac{3b_\lambda^2 d\zeta}{8b_q \nu}\right)\frac{\partial T}{\partial z} - \frac{b_\lambda^2 d\kappa_0 \zeta T}{2b_q \nu n}\frac{\partial n}{\partial z}, \tag{A10b}$$

giving $\mu = b_\lambda^2 d\kappa_0 \zeta T/2b_q \nu n$ for the anomalous heat transport coefficient in a boundary-driven steady-state. This value of μ for a steady state agrees with the cooling-state value of μ and, hence, also with the theoretical calculations,[5] up to the dimensionless factor $b_\lambda^2 d/2b_q$. Reasonable values for b_λ (Table I) make the two estimates equal.

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