Coupled Normal Heat and Matter Transport in a Simple Model System

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We introduce the first simple mechanical system that shows fully realistic transport behavior while still being exactly solvable at the level of equilibrium statistical mechanics. The system is a Lorentz gas with fixed freely rotating circular scatterers which scatter point particles via perfectly rough collisions. Upon imposing either a temperature gradient and/or a chemical potential gradient, a stationary state is attained for which local thermal equilibrium holds. Transport in this system is normal in the sense that the transport coefficients which characterize the flow of heat and matter are finite in the thermodynamic limit. Moreover, the two flows are nontrivially coupled, satisfying Onsager's reciprocity relations.

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The phenomenological equations of irreversible thermodynamics, which describes diffusion, heat conduction, and viscosity among a host of other phenomena, are of great significance in many fields. To link these phenomena to the underlying microscopic dynamics is, however, highly nontrivial and the results so far have not been conclusive. From a mathematically rigorous point of view, very few results have been obtained [1]. From the numerical point of view, the systems considered thus far are either too complicated to shed much light upon the problem, or fail to reproduce the macroscopic phenomenology. Indeed, to our knowledge, the validity of Fourier's law has been proven analytically only for a specific model in the limit of infinite dilution with finite mean free path [2,3]. There have also been attempts to link transport phenomena to the chaotic properties of the underlying classical dynamics [4], and a connection between the rate of entropy production and the rate of contraction of phase space volume has been pointed out [5]. Further results have also been obtained concerning energy transport in the Lorentz gas [6]. However, as was shown in [7], this last system does not satisfy local thermal equilibrium (LTE), which is a fundamental assumption of irreversible thermodynamics. It is therefore not clear what precise meaning should be attached to Fourier's law in this situation. Numerically, attempts have been made, on one side, through the simulation of realistic many-body systems satisfying a thermostatted (non-Hamiltonian) dynamics [8]. These simulations have indeed been able to reproduce nontrivial transport phenomena. However, such studies do not provide a detailed understanding of the microscopic processes involved due to the excessive complexity of the system. The other numerical approach involves the study of transport in "simple systems." Examples of these include chains of anharmonic oscillators [9], for which Fourier's law does not hold; Lorentz gases [6], which, as mentioned above, do not satisfy LTE; and the so-called ding-a-ling and ding-dong models [10,11], which indeed yield normal heat transport, but have geometric constraints that make even their equilibrium properties a complicated affair and cannot be generalized, retaining their simplicity, to obtain the coupled heat and matter transport commonly found in real systems. Under these circumstances, the minimal ingredients required in the microscopic physics of a system to attain normal heat conduction in low dimensions are presently still under discussion [1,12,13].

In this work we introduce the first simple reversible Hamiltonian model system whose steady state is well described by the hypothesis of LTE and supports both normal heat and matter transport. These are nontrivially coupled, satisfying Onsager's reciprocity relations. Furthermore, this system has the advantage that its equilibrium properties are trivial since its description reduces to that of ideal gases. This makes our model an ideal testing ground for theories linking microscopic mechanical properties to transport phenomena. Moreover, this model can be easily modified to study other physical problems from a microscopic approach, such as transport in heterogeneous systems [14] and the effects of applied fields.

Our model consists of noninteracting point particles of mass m scattered by an array of *freely rotating* circular scatterers of radius R with a finite moment of inertia Θ. The only relevant adimensional parameter characterizing the system is

$$\eta = \frac{\Theta}{mR^2}, \tag{1}$$

which determines the amount of energy transfer between disks and particles in a collision. The scattering proceeds according to the rules characterizing perfectly rough collisions, designed to conserve energy and angular momentum. They are given by the following prescription: the normal velocity v_n of the particle changes sign, whereas the tangential velocity v_t of the particle and the angular velocity ω of the disk are transformed as follows:

$$\begin{aligned} v_n' &= -v_n, \qquad v_t' = v_t - \frac{2\eta}{1+\eta}(v_t - R\omega), \\ R\omega' &= R\omega + \frac{2}{1+\eta}(v_t - R\omega). \end{aligned} \tag{2}$$

These rules define a deterministic, time-reversible, and canonical transformation at each collision. For finite values of η, particles in the system may exchange energy among each other through the disks, even though they do not interact directly. It is precisely this disk-mediated energy exchange which permits the systems to reach thermodynamical equilibrium without the necessity of any additional thermostat (a similar idea was proposed in [15] as a model of a deterministic thermostat). It should be noted that both the limits $\eta \to 0$ and $\eta \to \infty$ are exceptional: In the former case the particle dynamics reduces to that of normal elastic scattering by a hard disk, which is the usual Lorentz gas model; in the latter, the state of rotation of the disks is unaffected by the collisions. Thus, in both limits the energy-mediating effect of the disks is suppressed and thermodynamical equilibrium is not reached. In the following, unless the contrary is explicitly stated, we shall always be dealing with the case $\eta = 1$, since that is the value of η for which equilibration is most efficient. We shall also always set m and R to 1.

A peculiarity of this system is that it is homogeneous, i.e., it has no proper energy scale, or, equivalently, no proper time scale. Thus all energies and temperatures reported in this work are rescaled to the lower nominal temperature of the baths.

The geometric disposition of the scatterers is indicated in Fig. 1. The centers of the scatterers are fixed on a triangular lattice, along a narrow channel with periodic boundary conditions in the vertical direction. At the ends, the walls are used to fix both the temperature T and the quantity μ/T, where μ is the chemical potential. This is achieved by ensuring that each particle that hits the right or the left wall is absorbed with probability $1 - \exp(-1/|v_n|)$, where v_n is the normal component to the wall of the particle velocity. Otherwise, the particle is reflected with a velocity chosen from

$$P_n(v_n) = \frac{1}{T}\,|v_n| \exp\left(-\frac{v_n^2}{2T}\right), \qquad P_t(v_t) = \frac{1}{\sqrt{2\pi T}} \exp\left(-\frac{v_t^2}{2T}\right), \tag{3}$$

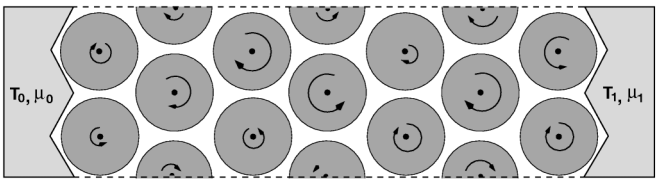

FIG. 1. Schematic illustration of the scatterer geometry: the scatterers are disposed on a triangular array with finite horizon to avoid infinitely long trajectories. For matters of convenience, in this work the separation between scatterers has been set to have the critical horizon. Periodic boundary conditions are used in the vertical direction. To avoid spurious effects arising from multiple scattering off the same disk, we have put two disks on each vertical. To study the dependence with system size, the length L of the sample is varied. The quoted length is the number of disks.

where v_n and v_t are, respectively, the normal and tangential components of the velocity with respect to the wall, and T is the nominal temperature of the wall. Additionally, the walls emit particles with velocities distributed as in (3), at a velocity dependent rate given by $\gamma[1 - \exp(-1/|v_n|)]$. Here, γ determines the nominal value of the chemical potential at the walls through $\mu = T \ln(\gamma/T^{3/2})$. Details will be given in a forthcoming publication [16]. At the level of equilibrium statistical mechanics the system is an ideal gas mixture, with the disks having 1 degree of freedom and the particles 2. We have verified that our model reaches an equilibrium state fulfilling the equipartition theorem in the microcanonical, canonical, and grand canonical ensembles of equilibrium statistical mechanics. Further, the temperature and chemical potential at which the system equilibrates coincides with the nominal values at the walls in the canonical and grand canonical cases. Finally, when the system is subjected to a weak temperature or chemical potential gradient, it reaches a well-defined stationary state after a relaxation time that depends on the length of the system and on the gradients themselves. To show that LTE is indeed achieved in the stationary state attained by our system, we display in Fig. 2 a typical realization of the energy distribution function $P_x(\varepsilon)$ of the particles as they cross a narrow slab centered around position x for three different positions. At each position, $P_x(\varepsilon)$ is consistent with the Boltzmann distribution. Further, if we determine the temperature $T(x)$ by a fit of the $P_x(\varepsilon)$ to the Boltzmann distribution, the agreement with the expected linear temperature profile in the system is satisfactory and coincides with the average energy of the particles measured at that position; see the inset of Fig. 3. Thus, the identification of the average particle energy with the local temperature

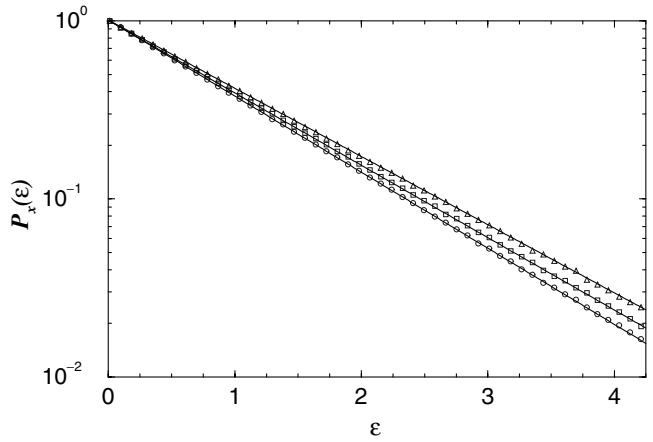

FIG. 2. Semilogarithmic plot of the particle's energy distribution $P_x(\varepsilon)$ at different positions along a channel of length 30 with an end-to-end temperature difference $\Delta T = 1/7$ and $\Delta(\mu/T) = -0.2002$. The different curves correspond to a fit to a Boltzmann distribution for each position. From these fits, we obtain the temperatures $T = 1.0193$ at $x = 3$ (circles), $T = 1.0693$ at $x = 13$ (squares), and $T = 1.1335$ at $x = 27$ (triangles). The curves have been rescaled for clarity.

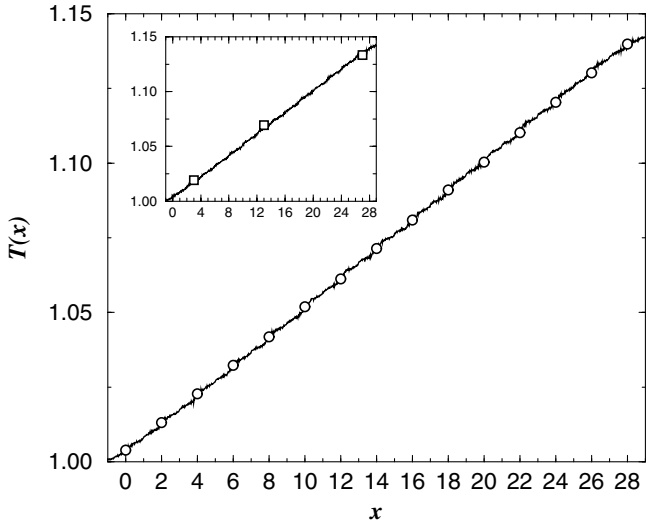

FIG. 3. Temperature profile for the simulation described in Fig. 2. The solid line corresponds to the particle temperature along the channel while the open circles are the temperature of the disks, averaged over 500 realizations. In the inset the particle temperature profile (solid line) is compared with the temperatures obtained from the fits to the Boltzmann distribution of $P_x(\varepsilon)$ in Fig. 2 (open squares).

is justified in this system. In Fig. 3 we show the temperature profiles of both particles and disks, which are found to be linear. The agreement between both values indicates that disks equilibrate with the particles locally along the channel. In the inset, the temperatures obtained in Fig. 2 for three different positions are compared with $T(x)$, measured as the average energy. The agreement reinforces the conclusion that the system establishes a LTE in its steady state. Note again that $T(x)$ reaches the nominal temperatures specified by the walls at both ends. This is in contrast to what is observed in several other models for heat conduction previously proposed [9,11,12]. Moreover, in simulations in which we impose a temperature gradient but the same value of μ/T on both walls, we find that $\rho(x)/T(x)$ is constant along the channel, confirming that the particles in the system can be described as a two-dimensional ideal gas which is locally at equilibrium.

From the general theory of irreversible processes, to linear order the heat and particle currents J_u and J_ρ can be written as follows (see, e.g., [17]):

$$J_u = L_{uu}\nabla\frac{1}{T} - L_{u\rho}\nabla\frac{\mu}{T},$$
$$J_\rho = L_{\rho u}\nabla\frac{1}{T} - L_{\rho\rho}\nabla\frac{\mu}{T}, \tag{4}$$

and the Onsager reciprocity relations read in this case

$$L_{u\rho} = L_{\rho u}. \tag{5}$$

The central feature of the model is that its transport properties are *normal,* meaning that the various transport coefficients appearing in (4) do not depend on the length of the system, and are, thus, well defined in the thermodynamical limit. In Fig. 4 we show the dependence of the currents on the length L of the system, for a typical realization. The $1/L$ dependence observed confirms that transport is normal.

In order to obtain the value of the coefficients in (4), it is enough to perform two simulations: Fixing the value of ∇T and setting $\nabla(\mu/T) = 0$ yields L_{uu} and $L_{\rho u}$ while setting $\nabla T = 0$ and fixing $\nabla(\mu/T)$ gives $L_{u\rho}$ and $L_{\rho\rho}$.

We have performed simulations with temperature and chemical potential differences up to 20% of the minimal nominal values at the walls, and in all cases we have found normal transport consistent with (5). For example, in a simulation in which a temperature difference of $\Delta T = 1/14$ and $L = 30$ at fixed $\mu/T = -5.01$, averaged over 500 realizations, we found that after the steady state has been reached, both a heat current and a particle current were driven by the temperature gradient. The measured value for $L_{\rho u}$ in this case was $0.0054 \pm 0.000\,13$. This implies, through (5), that a heat current will be driven by a gradient in μ/T at fixed T, as is indeed observed. In the complementary simulation with T constant, where $\Delta\frac{\mu}{T} = -0.06$, we found $L_{u\rho} = 0.0055 \pm 0.000\,13$, thus confirming (5) to within our numerical accuracy.

As a consistency check, we have also studied a "canonical" situation, in which we supressed absorption and emission of particles at the walls. In this situation there is no flow of matter in the steady state. The relationship between heat flow and temperature gradient becomes $J_u = \kappa\nabla T$, with κ given by the following expression:

$$\kappa = \frac{L_{uu}L_{\rho\rho} - L_{u\rho}L_{\rho u}}{T^2 L_{\rho\rho}}. \tag{6}$$

This relationship was found to hold to good accuracy, thus confirming the validity of our "grand canonical" simulations by which the L's were evaluated.

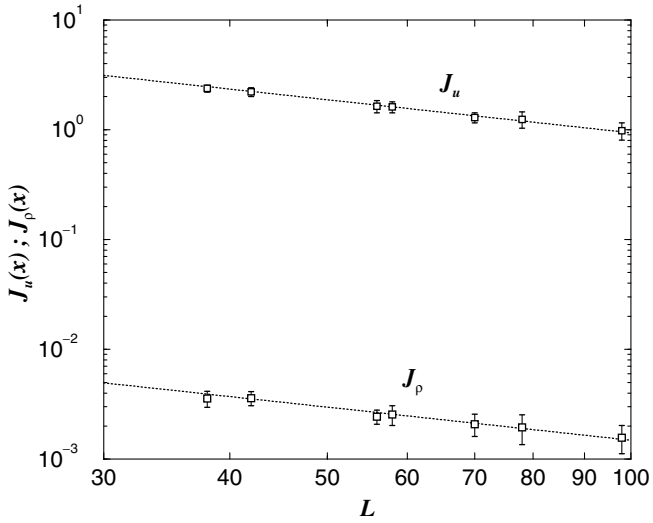

FIG. 4. Size dependence of the heat and matter currents for simulations with a fixed temperature difference, $\Delta T = 1/7$, and μ/T constant. The dotted lines correspond to $1/L$ scaling. From the agreement it follows that the transport coefficients do not depend on the size of the system.

We argue that the coupling between the two currents is nontrivial in the following sense: in a canonical simulation, the simplest assumption for the dependence of the density on the position is that the orbit of each particle covers the sample uniformly. Then the local temperature merely determines the speed at which the orbit is being traversed. This would imply that in such a simulation, the particle density scales inversely with the average velocity that is

$$\rho(x)T(x)^{1/2} = \text{const.} \tag{7}$$

In terms of the transport coefficients defined in (4), Eq. (7) is equivalent to $L_{\rho u} = (d + 1)TL_{\rho\rho}/2$, where d is the dimension of the system. This relation corresponds to a system for which all transport arises from uncorrelated Markovian motion of the particles, as in the Knudsen gas [17].

However, Eq. (7) does not hold in our system as we always find a systematic spatial variation in this quantity, the size and sign of which depend on the value of η. Thus, our system cannot be accurately described in this simple manner. The correct description is, as in all systems showing realistic transport properties, an open problem.

In summary, we have introduced a reversible Hamiltonian system to study transport, with the following desirable properties: Its statistical mechanics is trivial, reducing to that of ideal gases. In the steady state it is well described by the hypothesis of local thermal equilibrium. Its transport properties are normal and it naturally supports coupled matter and heat transport for which Onsager's reciprocity relations are satisfied to within numerical accuracy. This coupling is nontrivial in that it does not reduce to a simple velocity scaling. In view of these properties, we believe that this model provides an ideal framework from which theories for the emergence of macroscopic transport in out-of-equilibrium conditions can be constructed and/or tested. Furthermore, the model opens the possibility to study other phenomena such as thermal junctions (and other kinds of inhomogeneities) by changing the size or moment of inertia of the disks, Joule heating by applying an electric field, broken time reversal symmetry by applying magnetic fields, etc. [18]. Research into some of these extensions is currently underway [16].

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[1] F. Bonetto, J. L. Lebowitz, and L. Rey-Bellet, math-ph/0002052.
[2] J. L. Lebowitz and H. Spohn, J. Stat. Phys. **19**, 633 (1978).
[3] J. L. Lebowitz and H. Spohn, J. Stat. Phys. **28**, 539 (1982).
[4] L. A. Bunimovich and Ya. G. Sinai, Commun. Math. Phys. **78**, 247 (1980); **78**, 479 (1981); P. Gaspard, J. Stat. Phys. **68**, 673 (1992); J. R. Dorfman and P. Gaspard, Phys. Rev. E **51**, 28 (1995).
[5] N. I. Chernov, G. L. Eyink, J. L. Lebowitz, and Ya. G. Sinai, Commun. Math. Phys. **154**, 569 (1993).
[6] D. Alonso, R. Artuso, G. Casati, and I. Guarneri, Phys. Rev. Lett. **82**, 1859 (1999).
[7] A. Dhar and D. Dhar, Phys. Rev. Lett. **82**, 480 (1999).
[8] D. MacGowan and D. J. Evans, Phys. Rev. A **34**, 2133 (1986).
[9] S. Lepri, R. Livi, and A. Politi, Phys. Rev. Lett. **78**, 1896 (1997).
[10] G. Casati, J. Ford, F. Vivaldi, and W. M. Visscher, Phys. Rev. Lett. **52**, 1861 (1984).
[11] T. Prosen and M. Robnik, J. Phys. A **25**, 3449 (1992).
[12] B. Hu, B. Li, and H. Zhao, Phys. Rev. E **57**, 2992 (1998).
[13] T. Prosen and D. K. Campbell, Phys. Rev. Lett. **84**, 2857 (2000).
[14] For an ingenious application of transport in heterogeneous systems, see G. D. Mahan and L. M. Woods, Phys. Rev. Lett. **80**, 4016 (1998).
[15] R. Klages, K. Rateitschak, and G. Nicolis, J. Stat. Phys. **99**, 1339 (2000).
[16] C. Mejía-Monasterio, H. Larralde, and F. Leyvraz (to be published).
[17] L. Reichl, *A Modern Course in Statistical Physics* (University of Texas Press, Austin, 1980).
[18] S. R. de Groot and P. Mazur, *Non-equilibrium Thermodynamics* (Dover, New York, 1984).