

Absence of Local Thermal Equilibrium in Two Models of Heat Conduction

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A crucial assumption in the conventional description of thermal conduction is the existence of local thermal equilibrium. We test this assumption in two simple models of heat conduction: a linear chain of planar spins with nearest neighbor couplings and a Lorentz gas. We look at the steady state of the system when the two ends are connected to heat baths at temperatures T_1 and T_2 . If $T_1 = T_2$, the system reaches thermal equilibrium. If $T_1 \neq T_2$, there is a heat current through the system, but there is no local thermal equilibrium, even in the limit of large system size, when the heat current goes to zero. We argue that this is due to the existence of an infinity of local conservation laws in their dynamics. [S0031-9007(98)08254-4]

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Heat conduction provides a rather elementary example of nonequilibrium steady states (NSS). Here the driving force on the system is an externally applied temperature gradient. Our present understanding of this in terms of nonequilibrium statistical mechanics is not entirely satisfactory. In the traditional treatment of heat conduction, a very important assumption is of a rather quick (in atomic time scales) establishment of local thermodynamical equilibrium (LTE) [1]. This allows one to define thermodynamical quantities such as temperature, pressure, etc. locally. One then writes evolution equations for the slow change in time in these quantities in terms of their small spatial gradients. Thus, in heat conduction, LTE implies that we can define a temperature field $T(x)$ that varies slowly in space. In linear response theory, the local heat current density $\vec{J}(x)$ is given by $\vec{J} = -K(T)\vec{\nabla}T$ (Fourier's law). The well-known Kubo formula determines the thermal conductivity coefficient $K(T)$ in terms of the time-dependent *equilibrium* correlations of the system [2].

However, the question of the necessary (or sufficient) conditions for the fast establishment or nonestablishment of LTE has not been investigated much so far. This is what we study in this paper, in two simple models. The first is a one-dimensional spin model evolving with a Markovian stochastic dynamics. The second model is that of a d -dimensional ($d > 1$) Lorentz gas of noninteracting particles scattering elastically with a set of randomly placed obstacles (e.g., spheres) of finite density. In both these models, we find the unexpected result that the NSS does not show LTE, even in the limit of very small thermal gradients. Thus, one cannot define a local temperature, and the conventional linear response theory does not work. We argue that a sufficient condition for LTE not to occur is the existence of an infinity of locally conserved quantities in the dynamics.

It is obvious that existence of extra conservation laws in an isolated classical mechanical system implies breakdown of ergodicity and, hence, failure to reach thermodynamical equilibrium. Our results are nontrivial

in that we show that this occurs *even in the presence of coupling to heat baths* which leads to breakdown of the conservation laws at the boundaries of the system. Also, the role of conservation laws in a stochastically evolving system is somewhat different from that in deterministic evolution [3], and not so well studied.

Several microscopic models of heat conduction have been studied in the past. The simple model of a harmonic lattice, evolving with classical mechanical equations of motion and coupled to two heat baths at different temperatures T_1 and T_2 at opposite ends of the lattice, is known to show anomalous conduction [4]. It is found that the heat current J across the sample remains finite as the size of the system L goes to infinity, for a fixed T_1 and T_2 . Simulations of harmonic chains with disorder show that J decreases to zero for large L , but only as $L^{-1/2}$ [5]. Several models with nonlinear couplings have been studied numerically: the Fermi-Pasta-Ulam chain with quartic potential [6], the Toda lattice [7], the so-called "ding-a-ling" model [8], the Frenkel-Kontorova model [9], etc. Most of these models are one dimensional, and all do not show the expected $J \sim (T_1 - T_2)/L$ behavior. The uniqueness of the steady state has been proved only for some special models of heat baths and only if the temperature difference is sufficiently small [10]. In this respect models with stochastic dynamics have been more successful. These typically work with local energy-conserving moves and often involve introduction of additional degrees of freedom. Creutz has used an algorithm with Maxwell demons to simulate heat conduction in the Ising model [11]. Lebowitz and Spohn studied heat conduction in the Lorentz model and showed that in the Boltzmann-Grad limit of a large number of scatterers of very small size, one recovers the Fourier law [$J \sim (T_1 - T_2)/L$] [12].

We start with a precise definition of our first model. We consider a linear chain of L planar spins. The spin at site i ($1 \leq i \leq L$) of the lattice is specified by the angle θ_i , $0 \leq \theta \leq 2\pi$. The spins interact with nearest neighbors by ferromagnetic coupling K . The Hamiltonian

of the system is given by

$$\mathcal{H} = -K \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j), \quad (1)$$

where the sum is over all nearest neighbors.

The dynamics is the following: Suppose the instantaneous local field at a site i due to coupling of the neighbors is in the direction ϕ_i and the spin at the site is $\theta_i = \phi_i + \delta\theta_i$. Then the transition $\delta\theta_i \rightarrow -\delta\theta_i$ does not change the energy of the system. We assume that such spin flips occur at all sites stochastically with a constant rate (which may be chosen to be 1). The boundary spins $i = 1, L$ are connected to heat baths. For these spins, the flip rates are the following: A boundary spin θ_i can change to any value θ_i' with a rate α if the energy change $\Delta E \leq 0$, and with a rate $\alpha e^{-\Delta E/T}$, if $\Delta E > 0$, where T is the temperature of the heat bath.

Note that in this model energy is conserved exactly away from the boundaries of the lattice. In the absence of any coupling to heat baths, this dynamics has been studied by one of us earlier [13]. It was found that, in general, the dynamics is not ergodic, and the phase space breaks up into disconnected sectors. We now show that the coupling to heat bath allows transitions between these sectors and makes the system fully ergodic.

Since the rate matrix in our problem satisfies the detailed balance condition, it is sufficient to show that all configurations can be reached from any initial configuration. Consider first the case when a single spin on the lattice, say θ_0 , is coupled to a heat bath at temperature T . Then, θ_0 can be made to take any value, since it can exchange energy with the bath, keeping other spins unchanged. Next consider any spin θ_1 that is nearest neighbor to θ_0 . Then it is easy to see that flipping θ_1 , then changing θ_0 by a small amount $\delta\theta_0$, then flipping θ_1 again, then changing θ_0 back again to its initial value keeps all spins unchanged, except for θ_1 which changes by an amount proportional to $\delta\theta_0$.

We can use a similar argument to change a neighbor of θ_1 , and so on. Thus, there exists an allowed sequence of spin flips by which we can rotate any single spin by an infinitesimal amount. By making many such rotations we can reach any spin configuration. This completes the proof of ergodicity. Note that the proof is valid in all dimensions d and also if more than one spin is in contact with the same heat bath (same T).

In one dimension the equilibrium properties of the XY model are easily determined. We define $\Delta\theta_i = \theta_{i+1} - \theta_i$. Then clearly the $\Delta\theta_i$ are independent random variables. For a mesoscopic description, we define coarse-grained densities by averaging the corresponding microscopic quantity over length scales ℓ , with $1 \ll \ell \ll L$. Let $u^{(n)}(x)$ be the coarse-grained density corresponding to $\cos^n(\Delta\theta_i)$ for i lying in a neighborhood of point x . In equilibrium, at inverse temperature β , there is no dependence on x , and one gets

$$u_i^{(n)} = \frac{\int \cos^n(\Delta\theta) e^{\beta K \cos(\Delta\theta)} d(\Delta\theta)}{\int e^{\beta K \cos(\Delta\theta)} d(\Delta\theta)}. \quad (2)$$

Eliminating βK from these equations we can express $u^{(n)}$, for $n \geq 2$, as explicit nonlinear functions of $u^{(1)}$, i.e., $u^{(n)} = F^{(n)}(u^{(1)})$.

We consider now the case when the two ends are connected to different heat baths, at temperatures T_1 and T_2 . We show that, in the NSS, LTE is not achieved.

In this dynamics, whenever a spin flip occurs, the values of $\Delta\theta$ on the two adjacent bonds get interchanged. This means that the densities $u^{(n)}$ are locally conserved for all positive integers n . For each of these quantities one can write a corresponding current. The current from the $(x-1)$ th bond to the x th bond is given by

$$J^{(n)}(x) = (-\langle \cos^n(\Delta\theta_{x-1}) \rangle + \langle \cos^n(\Delta\theta_x) \rangle), \\ = -\nabla u^{(n)}(x). \quad (3)$$

In the steady state, in one dimension, $J^{(n)}(x)$ must be independent of x , and hence $u^{(n)}$ vary linearly across the chain for all n . Their value at the two ends is determined by the temperatures at the ends. Then, eliminating the coordinate x , $u^{(n)}(x)$ is expressible as a linear function of $u^{(1)}(x)$, for all n . But, as shown above, *in equilibrium*, $u^{(n)}$, for $n \geq 2$ are nonlinear functions of $u^{(1)}$. Thus, we have constructed a simple model in which heat current in the steady state is locally proportional to the gradient of energy density, but there is no LTE (Fig. 1). This result is true even in the limit of system size $L \rightarrow \infty$, when the heat current through the lattice becomes infinitesimal.

For a simple extension of the above result, consider a linear chain in which there is one bond with a different bond strength K' . Then the quantities $u^{(n)}$ ($n \geq 2$) are not

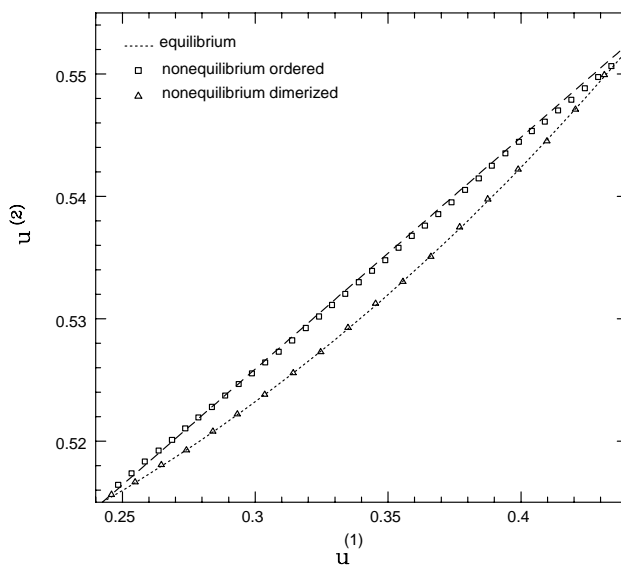


FIG. 1. Plot of $u^{(2)}(x)$ versus $u^{(1)}(x)$ in the steady state of the linear chain ($K = 1$). The results for the dimerized chain ($K' = 2$) agree with the equilibrium curve.

conserved at this “bad” bond. In this case, the currents take different values $J_1^{(n)}$ and $J_2^{(n)}$ to the left and right of the bond, respectively (for $n \geq 2$). In this case, there are no strict conservation laws, but $u^{(n)}$ are still linear functions of $u^{(1)}$ in each (left or right) half of the chain, and LTE is still not obtained. This conclusion has also been checked in simulations (Fig. 2).

In higher dimensions, there are no known locally conserved quantities, other than energy, in the spin model. Hence, we expect LTE to be attained. Indeed, a numerical simulation of a 40×40 lattice with $T_1 = 1.4$ K, and $T_2 = 0.4$ K agrees fully with this conclusion. In this case, we checked that the observed value of $\langle u^{(2)}(x) \rangle$ at any point x in the NSS agrees very well with the value of $u^{(2)}$ in the *homogeneous equilibrium state* having energy density $u^{(1)}(x)$. Similarly, if we consider a dimerized chain with alternating coupling constants K and K' , then there are no conserved quantities other than the energy density. In this case, the results of our simulations (also shown in Fig. 1) confirm that the NSS does show LTE even in one dimension if $K \neq K'$.

Our second example of absence of LTE in heat conduction is provided by the model of the d -dimensional Lorentz gas studied earlier by Lebowitz and Spohn [12]. The model describes a gas of noninteracting point particles moving in a box, undergoing elastic scattering by a random assembly of fixed obstacles of arbitrary shape (Fig. 3). In this model, all collisions with the obstacles are elastic, and energy is conserved. But collisions between the particles and the two walls (at $x = 0$ and $x = L$) are inelastic and lead to the energy after collision being thermalized corresponding to the temperature of the wall.

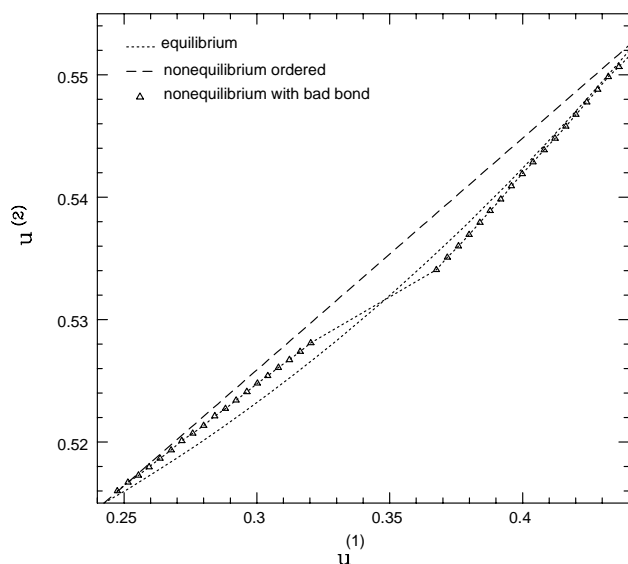


FIG. 2. Plot of $u^{(2)}$ versus $u^{(1)}$ when the middle bond has a different strength $K' = 0.5$ showing the different linear dependences in the left and right halves of the chain. For comparison, the case $K' = 1$ and the equilibrium curve are also shown.

Let $\rho(E, x)dE$ be the average density of particles having energy between E and $E + dE$ in a small volume centered at point x . Then all moments $\mu^{(n)}(x) = \int E^n \rho(E, x) dE$ of this distribution function are locally conserved.

Now consider the effect of coupling it to two different reservoirs at temperatures T_1 and T_2 . Let $p(x)$ be the probability that a randomly chosen particle in the small volume chosen near x was introduced at the left end. Then as collisions with scatterers do not change the energies, clearly $\rho(E, x)$ is given by

$$\rho(E, x) = p(x)\rho(E, x = 0) + [1 - p(x)]\rho(E, x = L). \quad (4)$$

The x dependence of $\rho(E, x)$ comes only from the spatial dependence of $p(x)$. As the linear combination of two Maxwellians is not a Maxwellian, and the distribution must be a Maxwellian *in thermal equilibrium*, it follows that there is no thermal equilibrium in the Lorentz model [14]. Also we expect the heat flow to be diffusive ($J \sim 1/L$) in the limit $L \gg \ell$, where ℓ is the mean free path of the Lorentz particles. Note that an equation similar to Eq. (4) can be written down for the first model also.

If we allow inelastic scattering with local energy conservation (each scatterer can store a small amount of energy, which can be exchanged with the scattered particles), the infinity of conservation laws goes away, and we expect that then the model would show LTE and normal conduction.

To summarize, in this Letter we studied two simple models of heat conduction and showed that local thermal equilibrium is not reached as both the models have an infinity of locally conserved quantities. These counterexamples should help one understand better the mechanism of local thermal equilibration in nonequilibrium systems, in general.

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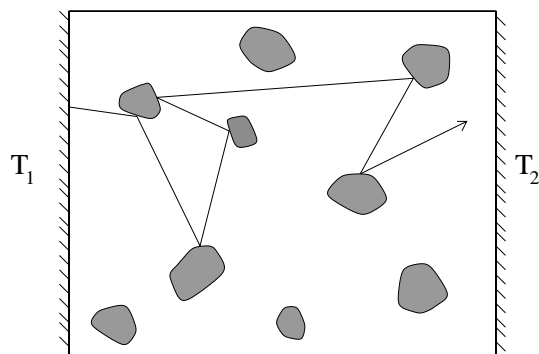


FIG. 3. A schematic representation of the Lorentz model. Particles move ballistically and are scattered elastically, but in a random direction on collision with an obstacle. At the left and right boundaries, they are reflected and are given a new energy randomly from a distribution corresponding to two different temperatures T_1 and T_2 .

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