Unraveling the Fourier Law for Hamiltonian Systems

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We exhibit simple Hamiltonian and stochastic models of heat transport in non-equilibrium problems. Theoretical arguments are given to show that, for a wide class of models, the temperature profile obeys a universal law depending on a parameter α. When $\alpha = 1$, the law is linear, but, depending on the nature of the energy exchange mechanism by tracer particles, we find that α is, in many cases, different from 1. When $\alpha \neq 1$, the temperature profile is not linear, although translation invariance and, in some models, local thermal equilibrium, hold.

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The Fourier law states that for a 1D object composed of homogeneous material, heat flux is proportional to temperature gradient times heat conductivity. In a non-equilibrium steady state, since heat flux is constant along the conductor, temperature profiles are linear, assuming the heat conductivity is constant. In statistical mechanics, one seeks to validate – or refute – this law for chains of interacting systems. Issues surrounding this topic have fascinated physicists for many years and are summarized in excellent reviews, such as [1–3]. The basic conjecture, however, remains largely unanswered.

We consider Hamiltonian systems made up of coupled chains of identical constituent cells, subjected to heat baths at the ends. One of the main thrusts of our work is that under fairly general conditions *not* depending on details of the system, all steady-state temperature profiles (TP) obey a *universal law* with a parameter. More precisely, we let E_i be the energy at site i, and assume the interaction is 1) *nearest-neighbor*, so that in a steady state, E_i is determined entirely by E_{i-1} and E_{i+1}, 2) *translation invariant*, and 3) *energy-scale invariant*, meaning if we multiply E_{i-1} and E_{i+1} by λ, then E_i is also multiplied by λ. We assume also 4) as the number of cells goes to infinity, the limit steady state is a 3-times differentiable function. We show that these assumptions imply that the energy density in 4) is necessarily of the form

$$T(x) = \left(T_{\mathrm{L}}^{\alpha} + (T_{\mathrm{R}}^{\alpha} - T_{\mathrm{L}}^{\alpha})x\right)^{1/\alpha} , \qquad (1)$$

where α is a so-far undetermined constant. Here, T_{L} and T_{R} are the temperatures at the left and right ends, and x is the coordinate along the system (normalized to $x \in [0,1]$).

In this Letter, we discuss two very natural scenarios, one in which $\alpha = 1$ while in the other $\alpha \neq 1$, *i.e., the temperature profile is nonlinear in spite of the fact that the system is made up of identical constituents* [12]. The issue here is that because of the Hamiltonian nature, the varying speeds of transmission of information lead to a *temperature dependent heat conductivity*. We are concerned here primarily with the TP, and will comment on the more delicate issue of local thermal equilibrium (LTE) only at the end of the Letter [13].

We consider models for which there is a sharp distinction between *communicating agent(s)* – which we call **tracers** – and *energy storing devices* (ESD). One should think of the tracers as "light" particles interacting with the ESD, which in our case are turning disks with fixed centers. *The value of α will depend on whether the tracers can wander about or are confined to specific regions between the ESD.* The value of α in (1) also depends crucially on the *time-of-flight* of the tracers. In a real-world conductor, all these aspects are of course mixed, but for a good theoretical understanding it is useful to separate them. The concepts above are distilled from the following beautiful model:

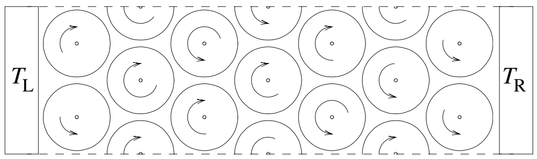

FIG. 1: A typical arrangement of disks in Model H1. The simulations in [4] were done with 2 rows and periodic boundary conditions in the vertical direction, and zig-zag reflecting walls of temperature T_{L}, resp. T_{R}, at the two ends.

Model H1 [4]: This is a purely Hamiltonian model, for which very careful simulations show that the Fourier law holds, with $\alpha = 1$. The system consists of an arrangement of disks of radius 1, and a little point particle of mass 1 (the tracer) which wanders around the playground, bouncing off the disks [14]. While Fig.1 suggests a Lorentz gas [5], there is a crucial difference here: Each disk is "nailed down" in its center, around which it turns freely: The phase space of this model is $X_{\mathrm{H1}} = (-\infty,\infty)^N \times \Omega \times \mathbf{R}^2$ where Ω is the playground for the tracer, *i.e.*, the physical space occupied by the system minus the disks. We denote the phase points $x \in X_{\mathrm{H1}}$ by $x = (\omega_1, \ldots, \omega_N, q, v)$ where ω_i is the angular velocity of disk i, $q \in \Omega$ is the position of the tracer, and v is its velocity. The disks serve as ESD. When the tracer collides with a disk, the rule of interaction is that of "sticky reflection": Suppose the angular velocity of the disk is ω, and v_{n} and v_{t} are the normal, resp. tangential, component of v relative to the impact point. Then the values of v and ω after the collision are given by

$$v'_{\rm n} = -v_{\rm n}\,, \quad v'_{\rm t} = v_{\rm t} - \frac{2\varepsilon}{1+\varepsilon}(v_{\rm t}-\omega)\,,$$
$$\omega' = \omega + \frac{2}{1+\varepsilon}(v_{\rm t}-\omega)\,. \qquad (2)$$

Here, $\varepsilon \in \mathbf{R}^+$ is proportional to the moment of inertia of the disk divided by the mass of the tracer. [4] treats mostly the case $\varepsilon = 1$, where $v'_{\rm t} = \omega$ and $\omega' = v'_{\rm t}$, *i.e.*, the two quantities are simply exchanged. Of particular interest to us is the case $\varepsilon \ll 1$, which from the tracer's point of view resembles the classical Lorentz gas.

Remark. *The Model H1, and the variants we are going to describe later, have the following important property: Since there is only a hard-core potential, the time evolution of the system is* rescaled *(by $\sqrt{\lambda}$ when the energy of the particle and the disks are rescaled by λ). In this respect, the model in [4] is very different from models such as the ding-a-ling and ding-dong models [6, 7]. Most importantly, the time-of-flight between collisions of the tracer with the disks does* **not** *depend on the state of the disks, but only on the energy of the tracer.*

We still need to say what happens when the tracer hits one of the ends. In [4], many variants are considered, but for our purpose, the following process is assumed: When the tracer hits one of the ends, it exits the system, and a new tracer is injected into Ω to take its place. The new tracer enters Ω at the point of exit of the old one. Its direction is arbitrary, and its speed is given by the Maxwell distribution for the temperature of the end in question.

Model H2: We start with Model H1, and increase the radii of the disks simultaneously until they exactly touch each other. It is assumed that they do not exert friction on each other, and that there is exactly one tracer in each of the "holes" that have formed (and similarly at the ends). Each little tracer rattles in its hole, exchanging energy with the turning disks via the mechanism described in (2). We further modify the model so that the channel is exactly 1-disk wide, *i.e.*, the disks are linearly ordered, and argue that in this case $\alpha = \frac{3}{2}$, a result we have checked numerically [15].

Abstracting Model H1. We approach the problem in the following way: First we identify those dynamical properties of Model H1 that are responsible for the outcome, and build a new Hamiltonian system that, on the conceptual level, is an idealization of these properties. Here we briefly outline one such model, which we call H1' (see [8]). We consider a chain of boxes separated by walls each one of which has a tiny hole that allows the tracer to pass between boxes. Inside each box are $M_1 \gg 1$ turning disks and $M_2 \gg M_1$ fixed disks. As in H1, the turning disks serve as ESD. Having a large number of them is conducive to attaining a local equilibrium. The fixed disks serve as *bona fide* Lorentz scatterers, and because there are many between the rotating disks, we infer that the sequence of rotating disks hit by the tracer as well as the angles of incidence are random. A single tracer wanders from box to box, exchanging energy with the rotating disks according to the rules in Eq.(2) [16]. The small holes in the separating walls prevent the tracer from leaving a box without having interacted "enough" with the rotating disks inside.

We argue in [8] that H1' reduces to the stochastic model below. This reduction is supported by reasoning in agreement with current understanding of dynamical systems, but the technology for rigorous proofs is not available at this time.

Model S1: In this model, there are N sites on a 1-D lattice, each with its random variable ξ_i, $i = 1,\ldots,N$. The variable ξ_i represents the energy at site i and takes values in $[0,\infty)$. The heat baths at the ends are modeled by stochastic variables $\xi_{\rm L}$ and $\xi_{\rm R}$ which take values in $[0,\infty)$ with a distribution $T_{\rm L}\exp(-\xi_{\rm L}/T_{\rm L})$, resp. $T_{\rm R}\exp(-\xi_{\rm R}/T_{\rm R})$ (the Boltzmann constant $k_{\rm B}$ being set to 1). We assume here and in all other models that $T_{\rm L} \le T_{\rm R}$, so that the cold reservoir is on the left and the hot on the right (and therefore heat is always expected to flow from right to left). We will also identify $\xi_{\rm L}$ with the variable ξ_0, and $\xi_{\rm R}$ with ξ_{N+1}. There is another random variable, η, to be thought of as the energy of the tracer, and finally j, which gives the location of the tracer at any given time. The phase space of the system is thus $X_{\rm S1} = \{0,\ldots,N+1\}\times[0,\infty)\times[0,\infty)^N$, with $x \in X_{\rm S1}$ given by $x = (j,\eta,\xi_1,\ldots,\xi_N)$. We assume that when the tracer is at site j, it interacts with ξ_j. At a site j, $j \notin \{0,N+1\}$, the action is as follows: There is an exponential clock with rate $f(x)$, for example $f(x) = \eta^{-1/2}$ or $(\eta+\xi_j)^{-1/2}$, representing the time it takes for the tracer to make its way around the jth box, but basically any (integrable) function not involving the heat baths is allowed here. When the clock rings, we assume the following mixing of energies has taken place: Choose a random variable p with uniform distribution in $[0,1]$. Then,

$$\eta' = p(\xi_j+\eta), \quad \xi'_j = (1-p)(\xi_j+\eta)\,. \qquad (3)$$

If $j=0$, η is replaced by a value chosen from the exponential distribution of temperature $T_{\rm L}$. The rule at the right end ($j = N+1$) is similar. After these operations, the tracer jumps with probability $\frac{1}{2}$ to $j-1$ or $j+1$, except when it is at the ends, in which case it stands still with probability $\frac{1}{2}$ and moves into position 1 (resp. N) from the boundary. *We show in [8] that this model leads to a linear TP, and that this is independent of the waiting function f.*

The gist of this argument is that the tracer serves as an agent with several crucial properties: 1) It transports energy from "site" j to site $j\pm1$, performing an unbiased random walk among the sites. 2) It exchanges energy in a random way with that "stored" at site j (preserving, of course, total energy). 3) When it is at site j, all ξ_i with $i \neq j$ are unaffected. (An interesting issue is what happens in the case of multiple tracers, particularly when the number of tracers per site is positive in the limit $N \to \infty$. When several tracers share the same site for varying durations, mixing rules are model-dependent and, to be realistic, necessarily more complex.)

This part of our work is inspired by [9, 10], in which the authors considered a model – **Model S0** – similar to S1, but without the variable η. Its random process is as follows: Choose with uniform probability a bond $i \leftrightarrow i+1$, with $i \in \{0,\ldots,N\}$,

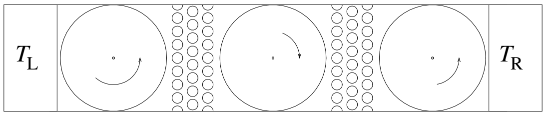

FIG. 2: A sketch of Model H2'. Between the rotating disks, there are disks serving as Lorentz scatterers. The tracers are not shown. The horizontal walls are reflecting.

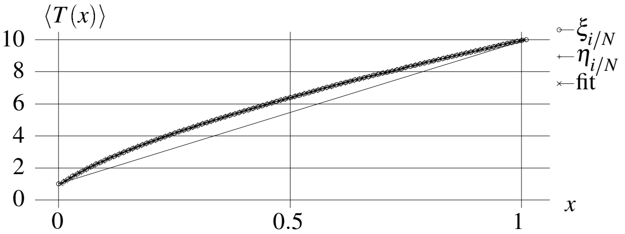

FIG. 3: The mean values of ξ and η, as a function of $x = i/N$, with $T_L = 1$, $T_R = 10$, $N = 100$, averaged over $2 \cdot 10^9$ exchanges of energy according to Model S2. Superposed is the theoretical curve of Eq.(1). Note that the temperature profile is *not* linear and that its curvature is more pronounced at the cold end. Here, $\alpha = \frac{3}{2}$. We have obtained the same profile for many variants of model S2.

and independently a second random variable p with uniform distribution in $[0,1]$. Then, if $i \neq 0, N$, replace the pair (ξ_i, ξ_{i+1}) by $\xi_i' = p(\xi_i + \xi_{i+1})$, $\xi_{i+1}' = (1-p)(\xi_i + \xi_{i+1})$. At the ends the rule is as above, with mixing to take place between ξ_0, resp. ξ_N, and the baths. For this model, the authors of [10] showed all the properties of the Fourier law for fixed T_L and T_R, including a linear TP and LTE.

Abstracting Model H2. We proceed as with H1, proposing first some Hamiltonian models H2' that idealize H2. The simplest version of H2' consists of a channel with turning disks at fixed distances apart. As in H2, these disks turn freely, but they block the channel completely, separating it into individual cells. Inside each cell, there is a single tracer, which moves back and forth, transferring energy between the turning disks as before. If the turning disks are relatively far apart, the length of the corridor will serve to randomize the position and angle of the next collision. Another variant of H2' has a similar configuration, but has additionally many fixed disks inside each cell, simulating a Lorentz gas. After hitting one turning disk, the tracer "gets lost" in this array of scatterers, to emerge at some random moment to hit the turning disk at either side; see Fig.2. In both cases, the time-of-flight of the tracer between hitting the turning disks is *independent* of the state of the disks; it depends only on the speed of the tracer.

The variants of H2' lead to the following stochastic models:

Models S2: These models are similar to Model S1, but now there is one independent tracer η_j for *each* pair $(j, j+1)$, $j = 0, \ldots, N$. Thus, the phase space X_{S2} is $[0,\infty)^{N+1} \times [0,\infty)^N$, where the first $N+1$ coordinates are the ξ_i and the last N are the η_i. Each η_j is equipped with an (independent) clock which rings at an exponential rate proportional to $\eta_j^{-1/2}$. When this clock rings, an exchange of energy involving η_j takes place. In the first variant of H2' above, η_j exchanges energy alternately with ξ_j and ξ_{j+1}. In the second, η_j chooses with probability $\frac{1}{2}$ its left or right partner (*i.e.*, ξ_j or ξ_{j+1}), and performs the usual mixing: For example, if ξ_j has been chosen, then

$$\eta_j' = p(\xi_j + \eta_j)\ , \xi_j' = (1-p)(\xi_j + \eta_j)\ . \tag{4}$$

When the clock at site 0 rings, η_0 is replaced by a value chosen from the exponential distribution of temperature T_L as in Model S1. The rule at the right end ($j = N+1$) is similar.

In both cases, numerical simulations show clearly profiles deviating strongly from linearity. They are in perfect agreement with Eq.(1) with $\alpha = \frac{3}{2}$ (see Fig.3), and the local distributions of the ξ_i are canonical. This nonlinear profile is caused by a *biasing* of temperatures that can be seen by considering 3 successive sites, say ξ_{j-1}, ξ_j, and ξ_{j+1}. Since $\xi_{j-1} < \xi_{j+1}$, η_{j+1} rattles faster than η_j (the rate being given by $\eta^{-1/2}$). Thus ξ_j equilibrates more often, and better, with ξ_{j+1} than with ξ_{j-1}. Therefore, ξ_j is closer to ξ_{j+1} than to ξ_{j-1}, which explains the concavity of the TP. Indeed, if the rates were independent of the η_j, one would recover again a linear profile.

Sketch of theoretical arguments: **I. Computing the temperature profile.** Here, we show how Eq.(1) is obtained. We start by performing a perturbative analysis at a point $x = i/N$ where N is very large. Let t_-, t, t_+ denote the temperatures at sites $i-1$, i, and $i+1$. For illustration we consider Model S2, assuming (i) the tracer visits alternately the left and right disks and (ii) the mixing of energies at each collision is exactly half-and-half. The stationarity condition means that the speed of the tracer is equilibrated as well. Let the energy of the left tracer be $\eta_{-,\rightarrow}$ as it heads toward site i, $\eta_{-,\leftarrow}$ as it goes away from site i. By the rule of mixing, we have $\eta_{-,\rightarrow} = (\eta_{-,\leftarrow} + t_-)/2$, $\eta_{-,\leftarrow} = (\eta_{-,\rightarrow} + t)/2$, $\eta_{-,\rightarrow} = (2t_- + t)/3$, $\eta_{-,\leftarrow} = (t_- + 2t)/3$.

We assume the speed of the tracer is E^γ where E is its energy. The value of γ for Model H2 (and many other models without potential) is $\gamma = \frac{1}{2}$, while for potential interactions, the time is given by an integral of the form $\int dq\,(E - V(q))^{-1/2}$, which for large E and $V(q) \sim |q|^m$ behaves like $\mathcal{O}(E^{-1/2+1/m})$, so that $\gamma = \frac{1}{2} - \frac{1}{m}$ [17]. Fixing γ, the average time for a round-trip of the tracer between sites $i-1$ and i is $\tau_- = \eta_{-,\rightarrow}^{-\gamma} + \eta_{-,\leftarrow}^{-\gamma}$, and the rate at which site i gets information from the left is the inverse of this quantity. An entirely analogous reasoning applies on the "+" side.

From the stationarity condition, we get

$$t = \frac{\tau_-^{-1}(t + \eta_{-,\rightarrow})/2 + \tau_+^{-1}(t + \eta_{+,\leftarrow})/2}{\tau_-^{-1} + \tau_+^{-1}}\ . \tag{5}$$

Let $\varepsilon = 1/N$. Then, to second order in ε, $t_\pm = T(x) \pm \varepsilon T'(x) + \frac{1}{2}\varepsilon^2 T''(x)$, and (5) leads to

$$t = T(x) + \varepsilon^2 \frac{T''(x)T(x) + \gamma\big(T'(x)\big)^2}{4T(x)} + \mathcal{O}(\varepsilon^4)\ .$$

Since $t = T(x)$, we find

$$T''(x)T(x) = -\gamma\big(T'(x)\big)^2 ,$$

the solution of which with boundary conditions $T(0) = T_L$ and $T(1) = T_R$ is Eq.(1) with $\alpha = 1+\gamma$. Thus, for the cases considered in Model S2, we have $\gamma = \frac{1}{2}$ and $\alpha = \frac{3}{2}$. One also checks that the energy flux is given by $T'(x)\sqrt{T}(x)$ (which is constant along the profile, but *not* proportional to the temperature difference.).

Generalization. Note that when $\gamma = 0$, *i.e.*, when the rate at which information is exchanged is independent of energy, then $\alpha = 1$, which indeed leads to a linear TP. Note also that our derivation is quite general: if E^γ is replaced by $1/F(E)$, the profile is given by $T''(x)F(T(x)) = \big(T'(x)\big)^2 F'(T(x))$.

Remark. Many authors have done careful simulations of models that are close to (Hamiltonian) versions of Model S2, and have observed linear TPs. It should be noted that the profile predicted by (1) is, in fact, very close to linear in some of these cases. Note, however that deviations from linearity grow with T_R/T_L.

II. Linear profile in Model S1. Consider again the space X_{S1} and $x \in X_{S1}$. Given an initial condition x_0, the sample paths of the stochastic process are parametrized by (Σ,μ) where $\Sigma = (\{+,-\}\times[0,1])^\infty$ and μ is the product measure on Σ. Here $\{+,-\}^\infty$ tells us the sequence of "jumps" made by the tracer: $\pm$ means it goes from site j to $j\pm1$, (at the ends it is only allowed to go in the direction that makes sense, or stand still); and the sequence of $p \in [0,1]$ are the random variables in the mixing rule in Eq.(3) [18].

Consider first a *fixed time model*, meaning the tracer makes one jump with the passage of each unit of time. In this case the variable j performs a standard random walk on $\{1,2,\ldots,N\}$ (except at the ends), and it is easy to see that it spends an equal amount of time at each of the N sites. Reasoning as above, we see that in the stationary measure, site i is affected equally by the sites $i+1$ and $i-1$, resulting in a linear profile (that is, $\alpha = 1$).

Model S1 as described earlier is a *skewed time model*, in the sense that the jumps occur at exponential rates depending on a certain waiting time f. A crucial observation here is that the mixing rule, and hence the outcome of the mixing process, *does not depend on the duration of this waiting time*. Although the tracer may spend a great deal more time at one site than at another, since it leaves site i with equal probability to each side, it must also return to i with equal probability from both sides, and hence the TP is linear in this case as well.

Remarks on LTE. In [11], the authors exhibited simple stochastic examples without LTE. Their setup is similar to that in Model S0, except that the rule of mixing is a simple flip: $\xi_i' = \xi_{i+1}$, $\xi_{i+1}' = \xi_i$ in general, and $\xi_1' = \xi_0$, $\xi_N' = \xi_{N+1}$ at the ends. They show that while the energy profile of this model is linear, the distribution of ξ_i is $xT_L\exp(-\xi_i\cdot T_L) + (1-x)T_R\exp(-\xi_i\cdot T_R)$ where $x = i/N$. This is *not* an exponential when $T_L \neq T_R$.

On the positive side, a rigorous proof of LTE for Model S0 is given by the authors of [9, 10]. This together with [11] suggests that some form of randomness in the sharing of energies is essential for LTE. The rules of mixing in our stochastic models are the same as those in S0. For S1, we believe that a proof along the lines of [9, 10] gives LTE provided we assume the exponential clock depends only on "local" coordinates, such as $f = f(\eta,\xi_j)$; see [8]. For S2, we have observed numerically exponential distributions for ξ_i in a number of cases.

For Hamiltonian systems, chaotic behavior is the simplest way to provide the needed randomness. We have tried to arrange that through the use of Lorentz scatterers in Models H1' and H2'. Rigorous results on LTE for Hamiltonian systems, however, seem out of reach at the present time.

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[12] It should be noted that the law (1) can be very close to linear when the *ratio* of the temperatures is close to 1, which is the case for many numerical simulations found in the literature. See discussion in text.
[13] Because of LTE, measuring the mean energy is equivalent to measuring the temperature.
[14] More than one tracer is sometimes used in [4], but we will limit ourselves to the single tracer case.
[15] Mejía-Monasterio has performed numerical simulations when the disks are as in Fig.1 ([4]) but touching each other, and has found in this case the TP to be linear (private communication).
[16] In [4] several of the considerations above are implemented in a very good compromise between practical feasibility and reasonable mixing between the collisions.
[17] The case of the hard disks of Model H1 corresponds to $m = \infty$.
[18] At the ends, we take the exponential distribution.