FOURIER LAW: A CHALLENGE TO THEORISTS

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We present a selective overview of the current state of our knowledge (more precisely of our ignorance) regarding the derivation of Fourier's Law, $\mathbf{J}(\mathbf{r}) = -\kappa\nabla T(\mathbf{r})$; $\mathbf{J}$ the heat flux, T the temperature and κ, the heat conductivity. This law is empirically well tested for both fluids and crystals, when the temperature varies slowly on the microscopic scale, with κ an intrinsic property which depends only on the system's equilibrium parameters, such as the local temperature and density. There is however at present no rigorous mathematical derivation of Fourier's law and ipso facto of Kubo's formula for κ, involving integrals over equilibrium time correlations, for any system (or model) with a deterministic, *e.g.* Hamiltonian, microscopic evolution.

1 Introduction

There are at least two distinct situations in which Fourier's Law is observed to hold with high precision:

1. An isolated macroscopic system which is prepared at some initial time, say $t = 0$, with a nonuniform temperature $T_0(\mathbf{r})$, *e.g.* a fluid or solid in a domain Λ surrounded by effectively adiabatic walls. At $t > 0$, the temperature will change, due to the heat, *i.e.* energy, current, with the energy density satisfying the conservation equation:

$$c_v(T)\frac{\partial}{\partial t}T(\mathbf{r},t) = -\nabla\cdot\mathbf{J} = \nabla\cdot[\kappa\nabla T]\,, \tag{1}$$

where $c_v(T)$ is the specific heat per unit volume and we have assumed that there is no mass flow or other mode of energy transport beside heat conduction (we also ignore for simplicity any variations in density or pressure). Eq.(1) is to be solved subject to the initial condition $T(\mathbf{r},0) = T_0(\mathbf{r})$ and no heat flux across the boundary of Λ. The stationary state, achieved as $t \to \infty$, is then one of uniform temperature $\bar{T}$ determined by the constancy of the total energy. For our purposes we can also think of Λ as a torus, *i.e.* having periodic boundary conditions.

2. We consider the system in contact with heat reservoirs which specify a time invariant temperature T_α at points of the boundary $\mathbf{r} \in (\partial\Lambda)_\alpha$ in contact with the α-th heat reservoir, $\alpha \geq 1$. When the system has come to a stationary state (again assuming no matter flow) its temperature will be given by the solution of Eq.(1) with the left side set equal to zero,

$$\nabla \cdot \tilde{J}(\mathbf{r}) = \nabla \cdot (\kappa \nabla \tilde{T}(\mathbf{r})) = 0, \tag{2}$$

subject to the boundary condition $\tilde{T}(\mathbf{r}) = T_\alpha$ for $\mathbf{r} \in (\partial\Lambda)_\alpha$ and no flux across the rest of the boundary which is insulating or periodic in the direction perpendicular to the heat flow. A simple example of this situation is the usual set up for a Benard experiment in which the top and bottom of a fluid in a cylindrical slab of height h and cross sectional area A are kept at different temperatures T_h and T_b respectively. (To avoid convection one has to make $T_h > T_b$ or keep $|T_h - T_b|$ small). Assuming uniformity in the direction parallel to the vertical x-axis one has in the stationary state a temperature profile $\tilde{T}(x)$ with $\tilde{T}(0) = T_b$, $\tilde{T}(h) = T_h$ and $\kappa(\tilde{T})\frac{d\tilde{T}}{dx}$ =Const. for $x \in (0, h)$.

From a physical point of view, which is how we presented them, the two cases are conceptually very similar (some physicists would even say identical). We have implicitly assumed that the system is described fully by specifying its temperature $T(\mathbf{r}, t)$ everywhere in Λ. What this means on the microscopic level is that we imagine the system to be in local thermal equilibrium (LTE). To make this a bit more precise we might think of the system as being divided up (mentally) into many little cubes, each big enough to contain very many atoms yet small enough on the macroscopic scale to be accurately described, at a specified time t, as a system in equilibrium at temperature $T(\mathbf{r}_i, t)$, where $\mathbf{r}_i$ is the center of the i-th cube. For slow variation in space and time we can then use a continuous description $T(\mathbf{r}, t)$.

This notion is made precise in the so called hydrodynamic scaling limit (HSL) where the ratio of micro to macro scale goes to zero[47,79,57]. The macroscopic coordinates $\mathbf{r}$ and t are related to the microscopic ones $\mathbf{q}$ and τ, by $\mathbf{r} = \epsilon\mathbf{q}$ and $t = \epsilon^\alpha \tau$, *i.e.* if Λ is a cube of macroscopic sides l, then its sides, now measured in microscopic length units, are of length $L = \epsilon^{-1} l$. We then suppose that at $t = 0$ our system of $N = \rho L^d$ particles with Hamiltonian

$$H(P,Q) = \sum_{i=1}^{N} \left[\frac{\mathbf{p}_i^2}{2m} + \sum_{j \neq i} \phi(\mathbf{q}_j - \mathbf{q}_i) + u(\mathbf{q}_i) \right] = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \mathcal{V}(Q) \tag{3}$$

is described by an equilibrium Gibbs measure with a temperature $T(\mathbf{r}) = T(\epsilon\mathbf{q})$: roughly speaking the phase space ensemble density has the form,

$$\mu_0(P,Q) \sim \exp\left\{ -\sum_{i=1}^{N} \beta_0(\epsilon\mathbf{q}_i) \left[\frac{{\mathbf{p}_i}^2}{2m} + \sum_{j \neq i} \phi(\mathbf{q}_j - \mathbf{q}_i) + u(\mathbf{q}_i) \right] \right\}, \tag{4}$$

where $Q = (\mathbf{q}_1, \ldots, \mathbf{q}_N) \in \Lambda^{dN}$, $P = (\mathbf{p}_1, \ldots, \mathbf{p}_N) \in \mathbb{R}^{dN}$, $\phi(\mathbf{q})$ is some short range inter particle potential, $u(\mathbf{q}_i)$ an external potential and $\beta_0^{-1}(\mathbf{r}) = T_0(\mathbf{r})$[79].

In the limit $\epsilon \to 0$, ρ fixed, the system at $t = 0$ will be macroscopically in LTE with a local temperature $T_0(\mathbf{r})$ (as already noted we suppress here the variation in the particle density $n(\mathbf{r})$). We are interested in the behavior of a macroscopic system, for which $\epsilon << 1$, at macroscopic times $t \geq 0$, corresponding to microscopic times $\tau = \epsilon^{-\alpha} t$, $\alpha = 2$ for heat conduction or other diffusive behavior. The implicit assumption then made in the macroscopic description given earlier is that since the variations in $T_0(\mathbf{r})$ are of order ϵ on a microscopic scale, then for $\epsilon << 1$, the system will, also at time t, be in a state very close to LTE with a temperature $T(\mathbf{r}, t)$ that evolves in time according to Fourier's law, Eq.(1).

¿From a mathematical point of view the difficult problem is proving that the system stays in LTE for $t > 0$ when the dynamics are given by a Hamiltonian time evolution. This requires proving that the macroscopic system has some very strong ergodic properties, *e.g.* that the only time invariant measures locally absolutely continuous w.r.t Lebesgue measure are, for infinitely extended spatially uniform systems, of the Gibbs type [30,70,63]. This has only been proven so far for systems evolving via stochastic dynamics, *e.g.* interacting Brownian particles or lattice gases. In these systems the relevant conserved quantity is usually the particle density rather than the energy density. We shall not discuss such stochastic evolutions here but refer the reader to [79,47] for a mathematical exposition.

The only Hamiltonian system for which a macroscopic transport law has been derived is a gas of noninteracting particles moving among a fixed array of periodic convex scatterers (periodic Lorentz gas or Sinai billiard). For this system one can prove a diffusion equation like Eq.(1) for the density of the particles, both for the initial value and the suitably defined stationary state problem, with the (self)diffusion constant given by the Einstein-Green-Kubo formula [10,56]. Unfortunately, the absence of interactions between particles makes this system a poor model for heat conduction in realistic systems. In particular there is no mechanism for achieving LTE. The speed of each particle $|\mathbf{v}|$ does not change in the course of time and the diffusion constant for each particle is proportional to its speed. The diffusion equation for the density mentioned above are therefore in fact separate uncoupled equations for particles with specified speeds. It corresponds to the usual diffusion equation only when all the particles have the same speed.

To remedy this problem it would be necessary to add interactions between the moving particles, *e.g.* instead of points make them little balls, and then derive coupled equations for the diffusion of both particle and energy densities. This is what we would consider a satisfactory answer to the challenge in the title of this article and we offer a bottle of very good wine to anyone who provides it. We believe that this system, with only two conservation laws and an external source (the fixed convex scatterers) for chaotic dynamics may be the simplest Hamiltonian system for which such results could be proven rigorously.

Just how far we are from such results will become clear as we describe our current mathematical understanding of the stationary nonequilibrium state (SNS) of macroscopic systems whose ends are, as in the example of the Benard problem, kept at fixed temperatures T_1 and T_2. The heat conductivity in this situation can be defined precisely without invoking LTE. To do this we let $\tilde{J}$ be the expectation value in the SNS, *i.e.* we assume that the SNS is described by a phase-space measure (whose existence we discuss later), of the energy or heat current flowing from reservoir 1 to reservoir 2. We then define the conductivity κ_L as $\tilde{J}/(A\delta T/L)$ where $\delta T/L = (T_1 - T_2)/L$ is the effective temperature gradient for a cylinder of microscopic length L and uniform crossection A and $\kappa(T)$ as the limit of κ_L when $\delta T \to 0$ ($T_1 = T_2 = T$) and $L \to \infty$[54]. The existence of such a limit with κ positive and finite is what one would like to prove.

2 Heat Conduction in Gases

Before going on to a mathematical discussion of heat conducting SNS, we turn briefly to the "kinetic theory" analysis of heat conduction in gases. This is historically the first example of a microscopic description of this macroscopic phenomenon. It goes back to the works of Clausius, Maxwell and Boltzmann [9] who obtained a theoretical expression for the heat conductivity of gases, $\kappa \sim \sqrt{T}$, independent of the gas density. This agrees with experiment (when the density is not too high) and was a major early achievement of the atomic theory of matter[9].

Clausius and Maxwell used the concept of a "mean free path" λ: the average distance a particle (atom or molecule) travels between collisions in a gas with particle density ρ. Straightforward analysis gives $\lambda \sim 1/\rho\pi\sigma^2$, $\sigma \sim$ an "effective" hard core diameter of a particle. They considered a gas with temperature gradient in the x-direction and assumed that the gas is (approximately) in local equilibrium with density ρ and temperature $T(x)$. Between collisions a particle moves a distance λ carrying a kinetic energy proportional to $T(x)$ from x to $x + \lambda/\sqrt{3}$, while in the opposite direction the amount carried is proportional to $T(x + \lambda\sqrt{3})$. Taking into account the fact that the speed is proportional to $\sqrt{T}$ the amount of energy transported per unit area and time across a plane perpendicular to the x-axis J is approximately,

$$J \sim \rho\sqrt{T}\left[T(x) - T(x + \lambda\sqrt{3})\right] \simeq -\sigma^{-2}\sqrt{T}\frac{dT}{dx}\,, \tag{5}$$

and so $\kappa \sim \sqrt{T}$ independent of ρ, in agreement with experiment.

It was clear to the founding fathers that starting with a local equilibrium situation (corresponding to a Maxwellian distribution of velocities) there will develop, as time goes on, a deviation from LTE. They reasoned however that this deviation from local equilibrium will be small when $(\lambda/T)dT/dx << 1$, the regime in which Fourier's law is expected to hold, and the above calculation should yield, up to some factor of order unity, the right heat conductivity. In fact if one computes the heat flux at a point x by averaging the microscopic energy current at x $j = \rho\mathbf{v}(\frac{1}{2}mv^2)$ over the one particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$ then it is only the deviation from local equilibrium which makes a contribution. The result however is essentially the same as Eq.(5). This was shown by Boltzmann who derived an accurate formula for κ in gases by using the Boltzmann equation to compute κ. If one takes κ from experiment the above analysis yields a value for σ, the effective size of an atom or molecule, which turns out to be close to other determinations of the characteristic size of an atom[9]. This gave evidence for the reality of atoms and the molecular theory of heat.

Using ideas of hydrodynamical space and time scaling described earlier it is possible to derive a controlled expansion for the solution of the stationary Boltzmann equation describing the steady state of a gas coupled to temperature reservoirs at the top and bottom[23,24,25]. The coupling is implemented by the imposition of "Maxwell boundary conditions": when a particle hits the left (right) wall it get reflected with a distribution of velocities

$$f_\alpha(d\mathbf{v}) = \frac{m^2}{2\pi(kT_\alpha)^2}|v_x| \exp\left[-\frac{m\mathbf{v}^2}{2kT_\alpha}\right] d\mathbf{v} \qquad \alpha = 1,2 \tag{6}$$

corresponding to a temperature T_1 (T_2) at the left (right) wall. One then shows[23,24,25] that for $\epsilon << 1$, ϵ being now the ratio λ/L, the Boltzmann equation for f in the slab has a time independent solution which is close to a local Maxwellian, corresponding to LTE, (apart from boundary layer terms) with a local temperature and density given by the solution of the Navier-Stokes equations which incorporates Fourier's law as expressed in Eq.(2). The main mathematical problem is in controlling the remainder in an asymptotic expansion of f in power of ϵ. This requires that the macroscopic temperature gradient, *i.e.* $|T_1 - T_2|/h$, where $h = \epsilon L$ is the thickness of the slab on the macroscopic scale, be small.

Even if this apparently technical problem could be overcome we would still be left with the question of justifying the Boltzmann equation for such steady states and of course it would not tell us anything about dense fluids or crystals. In fact the Boltzmann equation itself is really closer to a macroscopic then to a microscopic description. It is obtained in a well defined kinetic scaling limit in which in addition to rescaling space and time the particle density goes to zero[79], *i.e.* $\lambda >> \sigma$.

3 Heat conduction in insulating crystals

Excellent accounts of the historical development of the theory of heat conduction in solids exist [72,51] so we will content ourselves here with some brief remarks. In (electrically) insulating solids, heat is transmitted through the vibrations of the lattice (in conductors the electronic contribution is in general much larger then the contribution due to the lattice vibrations). In order to use concepts of kinetic theory, it is useful to picture a solid as a gas of phonons which can store and transmit heat. In a perfectly harmonic crystal, the phonons behave like a gas of noninteracting particles and therefore the thermal current will not decrease with the length of the crystal placed between two thermal reservoirs. Thus a perfectly harmonic crystal has an infinite thermal conductivity: in the language of kinetic theory $\sigma = 0$ and the mean free path λ is infinite. A real crystal is not harmonic and, in the phonon picture, any thermal current will be degraded by the anharmonic forces in the lattice. Another source of finite thermal conductivity may be the lattice imperfections and impurities which will scatter the phonons and degrade the thermal current too.

Debye [18] devised a kind of kinetic theory for phonons in order to describe thermal conductivity. One assumes that a small gradient of temperature is imposed and that the collisions between phonons maintain local equilibrium. An elementary argument [2] gives a thermal conductivity analogous to Eq.(5) obtained in Section 2 for gases, (remembering however that the density of phonon is itself a function of T)

$$\kappa \sim c_v c^2 \tau \,. \tag{7}$$

Comparing Eq.(7) and Eq.(5) we see that ρ has been replaced by c_v the specific heat of the phonons, $\sqrt{T}$ by c the (mean) velocity of the phonons, and λ by $c\tau$, where τ is the effective mean free time between phonon collisions. The thermal conductivity depends on the temperature via τ and a more refined theory is needed to account for this dependence. Peierls [71] used a Boltzmann type equation for phonons to investigate this problem. The Peierls theory singles out one phenomenon which gives rise to a finite thermal conductivity[72]. The momentum of phonons in collisions is conserved only modulo a vector of the reciprocal lattice. One can therefore classify the collisions of phonons into two classes: the ones where phonon momentum is conserved (the normal processes) and the ones where the initial and final momenta differ by a non-zero reciprocal lattice vector (the umklap processes). Peierls theory may be summarized (very roughly) as follows: in the absence of umklap processes the mean free path and thus the thermal conductivity of an insulating solid is infinite.

A success of Peierls theory is to describe correctly the temperature dependence of the thermal conductivity [2]. Furthermore, on the basis of this theory, one does not expect a finite thermal conductivity in 1-dimensional mono-atomic lattices with pair interactions: this seems so far a correct prediction, see Section 10.

The justification of the Boltzmann equation for phonons has been questioned [46]. Various alternative mechanisms have been proposed which would give rise to a finite thermal conductivity, but it seems fair to say that, so far, no better theory of heat conduction in insulators has been proposed. As Peierls himself puts it [72]: "It seems there is no problem in modern physics for which there are on record as many false starts, and as many theories which overlook some essential feature, as in the problem of the thermal conductivity of [electrically] non-conducting crystals".

To find a mathematical description of thermal conduction in crystals we need to specify the Hamiltonian of the system or at least some appropriately idealized version of it. A model crystal is characterized by the fact that all atoms oscillate around given equilibrium positions. The equilibrium positions can be thought of as the points of a regular lattice in $\mathbb{R}^d$. For simplicity we will assume that the lattice is simply $\mathbb{Z}^d$. Although $d = 3$ is the physical situation one can be interested also in the case $d = 1, 2$. (The $d = 1$ system may show finite thermal conductivity without violating the Peierls criteria if we admit one particle, non momentum conserving interactions.)

Let $\Lambda \subset \mathbb{Z}^d$ be a finite set and denote by N its cardinality. Each atom is identified by its position $\mathbf{x_i} = \mathbf{i} + \mathbf{q_i}$ where $\mathbf{i} \in \Lambda$ is the equilibrium position and $\mathbf{q_i} \in \mathbf{R}^d$ is the displacement of the particle at lattice site $\mathbf{i}$ from this equilibrium position, and we denote by $\mathbf{p_i}$ its momentum and m its mass. Since inter atomic forces in real solids have short range, it is reasonable to assume that the atoms interact only with their nearest neighbors via a potential that depends only on the relative distance with respect to the equilibrium distance.

As already noted it is useful to allow an external confining 1-body potential which breaks the translation invariance. Accordingly the Hamiltonians that we consider have the general form

$$H(P,Q) = \sum_{\mathbf{i}\in\Lambda} \frac{\mathbf{p}_{\mathbf{i}}^2}{2m} + \sum_{|\mathbf{i}-\mathbf{j}|=1} V(\mathbf{q}_{\mathbf{i}} - \mathbf{q}_{\mathbf{j}}) + \sum_{\mathbf{i}} U_{\mathbf{i}}(\mathbf{q}_{\mathbf{i}}) = \sum_{\mathbf{i}\in\Lambda} \frac{\mathbf{p}_{\mathbf{i}}^2}{2m} + \mathcal{V}(Q)\,, \qquad (8)$$

where $P = (\mathbf{p}_{\mathbf{i}})_{\mathbf{i}\in\Lambda}$ and analogously for Q. We shall further assume that as $|\mathbf{q}| \to \infty$ so do $U_{\mathbf{i}}(\mathbf{q})$ and $V(\mathbf{q})$. The addition of $U_{\mathbf{i}}(\mathbf{q})$ pins down the crystal and ensures that $\exp[-\beta H(P,Q)]$ is integrable with respect to $dPdQ$ and thus the corresponding Gibbs measure is well defined. Observe that for many purpose it is enough to put the potential $U_{\mathbf{i}}$ on only some of the atoms, *e.g.* the ones on the boundary of Λ[75,67]. We note finally that when $\Lambda \subset \mathbb{Z}^d$ one can still consider that $\mathbf{p}_{\mathbf{i}}$ and $\mathbf{q}_{\mathbf{i}} \in \mathbb{R}^\nu$, $\nu \neq d$, but we will generally assume that $\mathbf{q}_{\mathbf{i}} \in \mathbb{R}^d$.

Remark: While the Hamiltonian in Eq.(8) looks similar to that in Eq.(3) the meaning and domain of the Q variables is entirely different. In a fluid all the particle are identical and the particle with label i interacts with any other particle whose position $\mathbf{q}_j$ is close to $\mathbf{q}_i$, $\mathbf{q}_l \in \Lambda \subset \mathbb{R}^d$, $l = 1, \ldots, N$. The pair interaction potential $\phi(\mathbf{q})$ is of finite range, *e.g.* hard balls, or decays rapidly with distance. For the crystal in Eq.(8) $\mathbf{q}_i$ is the *deviation* from an equilibrium position $\mathbf{i} \in \Lambda \subset \mathbb{Z}^d$, etc.

4 Microscopic models of heat reservoirs

To produce a stationary heat flow in a system, be it a gas or a crystal, the system must be coupled to at least two heat reservoirs at different temperatures. A physical coupling is one which acts only at the boundary of the system leaving the dynamics in the bulk purely Hamiltonian.

Since a realistic description of heat reservoirs and coupling is out of the question various model reservoirs have been used in analytical and numerical studies. We give here some examples which will be used later (other choices are of course possible). The expectation is of course that the different models will give the same behavior away from the boundary when the system is macroscopic. This has not been proven in any example, see [32,33]

4.1 Stochastic reservoirs.

We have already discussed one such model of reservoirs commonly used for fluids in Section 2. This corresponds to Maxwell boundary condition discussed in Eq.(4) for a gas in a rectangular slab. More generally given a fluid in a domain $\Lambda \subset \mathbb{R}^d$ a particle hitting the wall of the container confining the system at a point $\mathbf{r} \in \partial\Lambda$ will bounce back into Λ with a Maxwellian distribution of momenta

$$f_{\mathbf{r}}(d\mathbf{p}) = \frac{\beta(\mathbf{r})^2}{2\pi m^2} \mathbf{p} \cdot \hat{n}(\mathbf{r}) e^{-\beta(\mathbf{r})\frac{\mathbf{p}^2}{2m}} d\mathbf{p}\,, \qquad (9)$$

where $\hat{n}(\mathbf{r})$ is the inward directed unit vector normal to $\partial\Lambda$ at $\mathbf{r}$ and $\beta^{-1}(\mathbf{r})$ is the preassigned temperature at $\mathbf{r}$.

For solids, which are usually not confined to any fixed spatial region by external walls, it is sometimes mathematically convenient to use Langevin type reservoirs which act on the atoms at the "edge" of the crystal. For definiteness we will choose Λ to be a chain of particles or a parallelepiped in higher dimension (with suitable boundary conditions), $\Lambda = \{\mathbf{i} \in \mathbb{Z}^d\,;\, 1 \le i_k \le N_k\,,\, 1 \le k \le d\}$. We assume that the particles at the "left" boundary $\{\mathbf{i} \in \Lambda\,;\, i_1 = 1\}$ are coupled to a heat reservoir at temperature T_L and that the particles at the "right " boundary $\{\mathbf{i} \in \Lambda\,;\, i_1 = N_1\}$ are coupled to a heat reservoir at temperature T_R. We set $\mathcal{L} \equiv N_1$ the length of the crystal and $A \equiv N_2 \cdots N_\nu$ its cross section.

For the particles at the boundary of the crystal in contact with a heat reservoir, the Hamiltonian equations of motion are modified by the addition of an Ornstein-Uehlenbeck process:

$$m_{\mathbf{i}}\dot{\mathbf{p}}_{\mathbf{i}} \;=\; -\nabla_{\mathbf{q}_{\mathbf{i}}}\mathcal{V}(\mathbf{q}) - \lambda_\alpha \mathbf{p}_{\mathbf{i}}/m_{\mathbf{i}} + (2\lambda_\alpha T_\alpha)^{1/2}\xi_\alpha(t)\,. \tag{10}$$

In Eq.(10), $\alpha \in \{L, R\}$ are indices of the reservoirs, λ_α describes the strength of the coupling to the reservoir with temperature T_α of the reservoir, and $\xi_\alpha(t)$ is a white noise, *i.e.* , a Gaussian random processes with covariance $\langle \xi_\alpha(t)\xi_\beta(s)\rangle = \delta_{\alpha\beta}\delta(t-s)$. The form of the coefficients is chosen so that the dynamics satisfy detailed balance. This implies in particular that if the system is coupled to a single reservoir at temperature T, then the Gibbs measure with density $Z^{-1}\exp\left(-T^{-1}H(P,Q)\right)$ is a stationary state of the system.

With any such a choice of stochastic process to model the reservoirs the dynamics is described by a stationary Markov process in the phase space of the system Ω.

4.2 Hamiltonian reservoirs.

In this case the reservoirs themselves are modeled by infinite Hamiltonian systems and the full system consisting of reservoirs+system is Hamiltonian[a]. An alternative but equivalent point of view is to start with an infinite system and to consider a finite subsystem of it as the system and the remaining part as the reservoirs. A non-equilibrium situation is obtained by choosing suitable initial conditions for the part of the total system which describes the reservoirs, *e.g.* the initial conditions of the reservoirs are assumed to be distributed according to a Gibbs measure with corresponding temperatures[b].

Studied in [77,80,69] the simplest version of such a total system consists of an infinite chain. The "left" reservoir consists of the particles with labels in $(-\infty, -N]$ and the right reservoir consists of the particles with labels in $[N, +\infty)$. The system

[a] A series of results has been obtained for systems coupled to a single reservoir, such as non-relativistic atoms coupled to the quantized electromagnetic field at temperature zero [3,4,5], finite level atoms coupled to a boson field at positive temperature [43,44,19], classical particles coupled to a scalar field at temperature zero [49,50] or at positive temperature [45].

[b] For quantum spin systems axioms are formulated in [78] which establish the existence of a stationary state and its mixing property for finite systems coupled to several reservoirs at different temperatures

consists of the particles in the middle. At time $t = 0$, the reservoirs are assumed to be in thermal equilibrium at temperatures T_L and T_R. This is clearly readily generalized to higher dimensions.

4.3 Hamiltonian/Stochastic reservoir.

While Hamiltonian reservoirs are in principle the right ones to use they are totally intractable without further simplifications. When this is done it is actually possible to find examples in which one starts with a Hamiltonian reservoir and by integrating out over the degrees of freedom of the reservoirs, ends up with a stochastic evolution. Many models of this type have been constructed[38,39,28]. We describe here a model considered in [45,21,22,20]. The system is a finite chain of anharmonic oscillators coupled at each end to a reservoir modeled by a linear d-dimensional wave equation, which is the continuum limit of a d-dimensional lattice of harmonic oscillators. The dynamics of the infinite system, crystal+reservoirs, is Hamiltonian. One makes the statistical assumption that, at time $t = 0$, the reservoirs are in thermal equilibrium at temperatures T_L and T_R. Since the reservoirs are linear, one may integrate them out, and, by our assumptions on the initial conditions of the reservoirs, the resulting dynamics for the crystal is stochastic, though in general not Markovian. Nevertheless, the fact that the reservoirs are described by a wave equation, together with special choices of the coupling between the reservoirs and the chain, permits [21] enlarging the phase space of the crystal with a finite number of auxiliary variables so that the dynamics is Markovian on the enlarged phase space.

In the simplest case of coupling one variable per reservoir is enough and the resulting equations for the N oscillators are

$$\begin{aligned}
\ddot{\mathbf{q}}_1 &= -\nabla_{\mathbf{q}_1}\mathcal{V}(Q) + \mathbf{r}_L\,, \\
\ddot{\mathbf{q}}_j &= -\nabla_{\mathbf{q}_j}\mathcal{V}(Q)\,, \quad j = 2,\ldots,N-1\,, \\
\ddot{\mathbf{q}}_n &= -\nabla_{\mathbf{q}_n}\mathcal{V}(Q) + \mathbf{r}_R\,, \\
\dot{\mathbf{r}}_L &= -\gamma_L(\mathbf{r}_L - \lambda_L^2\mathbf{q}_1) + (2\gamma_L\lambda_L^2 T_L)^{1/2}\dot{w}_L(t)\,, \\
\dot{\mathbf{r}}_R &= -\gamma_R(\mathbf{r}_R - \lambda_R^2\mathbf{q}_1) + (2\gamma_R\lambda_R^2 T_R)^{1/2}\dot{w}_R(t)\,,
\end{aligned} \tag{11}$$

In Eqs.(11) λ_L and λ_R describe the coupling strength to the reservoirs, γ_L, γ_R are parameters describing the coupling and $\dot{w}_L$, $\dot{w}_R$ are white noises.

If the temperatures of both reservoirs are the same, $T_L = T_R = T$, then the stationary state is given by the generalized Gibbs measure with density

$$Z^{-1}\exp\left(-\frac{1}{T}G(P,Q,R)\right) \tag{12}$$

where Z is a normalization constant and the generalized "Hamiltonian" G is given by

$$G(P,Q,R) = \left(\frac{\mathbf{r}_L^2}{2\lambda_L^2} - \mathbf{q}_1\mathbf{r}_L\right) + \left(\frac{\mathbf{r}_R^2}{2\lambda_R^2} - \mathbf{q}_N r_R\right) + H(P,Q)\,. \tag{13}$$

If one integrates the generalized Gibbs state, Eq.(12), over the auxiliary variables

$\mathbf{r}_L$ and $\mathbf{r}_R$ one finds

$$\int d\mathbf{r}_L d\mathbf{r}_R\, Z^{-1} \exp\left(-\frac{1}{T}G(P,Q,R)\right) \;=\; \tilde{Z}^{-1} \exp\left(-\frac{1}{T}H_{\rm eff}(P,Q)\right), \qquad (14)$$

where $H_{\rm eff}(P,Q) = H(P,Q) + \lambda_L^2 \mathbf{q}_1/2 + \lambda_R^2 \mathbf{q}_n/2$ and $\tilde{Z}$ a normalization constant. In view of this it is natural to consider $H_{\rm eff}(P,Q)$ as the energy of the chain.

4.4 Thermostats.

A fourth way of modeling the reservoirs is by deterministic (non-Hamiltonian) forces[27,31]. Such models of reservoirs are usually called thermostats. An example of such reservoirs which are widely used in numerical work, are the so called Nosé-Hoover[68,41] thermostats. Imposing these thermostats on small parts of the system[c] (on the left and on the right) Λ_L and Λ_R, the equations of motion of particles in those region of the box are respectively

$$\begin{aligned} m\ddot{\mathbf{q}}_{\mathbf{i}} &= -\nabla_{\mathbf{q}_{\mathbf{i}}}\mathcal{V}(Q) - \zeta_L \dot{\mathbf{q}}_{\mathbf{i}} \\ m\ddot{\mathbf{q}}_{\mathbf{i}} &= -\nabla_{\mathbf{q}_{\mathbf{i}}}\mathcal{V}(Q) - \zeta_R \dot{\mathbf{q}}_{\mathbf{i}} \end{aligned} \qquad (15)$$

where $\mathbf{q}_i \in \Lambda_\alpha$ for a fluid and $\mathbf{i} \in \Lambda_\alpha$ for a crystal, $\alpha \in \{L,R\}$. The variable ζ_α model the action of the thermostat and satisfy the equations

$$\dot{\zeta}_\alpha \;=\; \frac{1}{\Theta^2}\left(\frac{1}{T_\alpha}\sum_{\mathbf{i}\in\Lambda_\alpha}\frac{\mathbf{p}_{\mathbf{i}}^2}{2m} - 1\right). \qquad (16)$$

In Eq.(16), Θ is interpreted as the response time of the reservoir and T_α is the temperature of the α-th reservoir.

A limiting case of Eqs.(15)(16) is when we let $\Theta \to 0$. This limit can be formally taken and the model becomes equivalent to the so called Gaussian thermostat. This means that one computes ζ_α as a function of P and Q in such a way that the kinetic energy of the particles in Λ_L or Λ_R is a constant of the motion. After a simple calculation one gets for the chain:

$$\zeta_L(Q,P) = \frac{\sum_{i<I_L}\mathbf{p}_{\mathbf{i}}(\mathbf{f}(\mathbf{q}_{\mathbf{i}} - \mathbf{q}_{\mathbf{i}+1}) - \mathbf{f}(\mathbf{q}_{\mathbf{i}-1} - \mathbf{q}_{\mathbf{i}})) + \mathbf{f}_l(\mathbf{q}_{\mathbf{i}}))}{\sum_{i<I_L}\mathbf{p}_{\mathbf{i}}^2}, \qquad (17)$$

and similarly for $\zeta_R(Q,P)$. Here $\mathbf{f}_l(\mathbf{q}) = -\nabla U_{\mathbf{i}}(\mathbf{q})$. One may also prescribe Gaussian thermostat in which the total energies, instead of just the kinetic energies, in Λ_L and Λ_R are kept fixed.

5 Existence and Nature of Heat Conducting SNS

Suppose we are given a system described by a Hamiltonian of the form Eq.(3) or Eq.(8) and that we have chosen a given model of heat reservoirs. We shall now

[c]It is also possible to give "mechanized" models of heat transport in which one imposes the presence of a heat flow through the application of a particular force on the bulk of the system. This strong modification of the Hamiltonian character of the dynamics seems unnatural to us, although it can be useful for numerical simulations, and we will not discuss these models here [27,81].

formulate a sequence of statements (of increasing mathematical difficulty) on the properties of the resulting dynamical system.

5.1 Existence, Uniqueness and approach to the Stationary State.

The first property that we want to prove is existence and if possible also uniqueness of a stationary state. For the case when all reservoirs are at the same temperature T existence is generally obvious - after all the reservoirs are chosen so that they leave the canonical Gibbs distribution or some variation of it invariant under the time evolution. Uniqueness and approach to this equilibrium state presents more of a problem and may not even be true for certain type of reservoirs and initial states.

The real problem of interest for us is when the reservoirs are at different temperatures. We expect that if the dynamics is stochastic (*e.g.* for models 4.1 and 4.3 of reservoirs) then "almost any" initial distribution of the state of the system converges to a unique stationary state which is mixing. This is however, in general, a mathematically non-trivial problem. The isolated system has a non-compact phase space and has many invariant states. The coupling to the reservoirs induces a drift towards a state determined by the reservoirs. Since however the coupling to the reservoirs occurs only at the boundary, the proof of the existence of an invariant measure requires a good understanding of how energy is transmitted through the system. There are in fact only few examples (to be discussed in Section 6) where this behavior has been proven.

For general Hamiltonian or thermostated reservoirs the problem seems to be mathematically out of reach at the present time. Starting in a state that corresponds to the product of two equilibrium states for the reservoirs times a generic initial distribution for the crystal we then expect, that in the long time limit the marginal distribution for the system will approach some limit. When the two infinite reservoirs are initially at different temperatures, the limiting state should describe a system having a temperature gradient and a heat flow. Observe that in general the state for each reservoir at times $t > 0$ will not be the invariant state at a given temperature which is stationary for the isolated reservoir. It is this fact which makes the problem of general Hamiltonian reservoirs much more difficult that than of stochastic reservoirs. It is only in very special cases (essentially no interaction inside the reservoir) such as that discussed in subsection 4.3 where this can be dealt with.

For thermostated systems the temperature of the reservoirs is already given by the equations of motion so we expect again to have a unique invariant distribution. Moreover these systems have the property that the phase space volume is not conserved by the dynamics so that, in general, no invariant measure will be absolutely continuous with respect to Lebesgue measure. In this case we need a criterion to chose the "physical" invariant distribution. A natural choice are the so called SRB states. These can be characterized by assuming that the system was in equilibrium in the very distant past and that at some point a forcing was switched on and this drove the system to a steady state distribution. More mathematically this means that we consider the weak limit of a probability distribution absolutely continuous with respect to Lebesgue, *e.g.* the canonical distribution that characterize the system when all thermostats have the same temperature, under the time evolution, *i.e.* if Φ^t is the flow describing the evolution of the thermostated system then a state μ is called SRB if it has the property that

$$\mu_{SRB}(dX) = \lim_{t\to\infty} \bar{\Phi}^t \lambda(dX)\,, \qquad X = (P, Q) \tag{18}$$

where $\bar{\Phi}^t$ indicates the adjoint and $\lambda(dX)$ is the given initial distribution. We observe that we often cannot choose directly the Lebesgue distribution because the phase space of our system in not compact like for the Nosé-Hoover thermostat Eq.(16).

Although the definition Eq.(18) is interesting for its similarity to the ones used in the previous system+reservoirs models another characterization of these measure is obtained by saying that they represent the statistics of the motion. More precisely, given any observable, the average of this observable with respect to the SRB distribution is equal to its time average along a trajectory starting from almost every point (with respect to Lebesgue measure). In formulae we can say that if μ is the SRB distribution then

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t dt \delta_{\Phi^t(X)} \;=\; \mu_{SRB}(dX) \tag{19}$$

for a set of X of full (or at least positive) Lebesgue measure. In Eq.(19) the limit is to be understood as a weak limit[d].

5.2 Heat Flow and Entropy Production in Reservoirs.

Since our interest here is specifically in Fourier's law our next question about the stationary state of the system coupled to two reservoir at different temperatures is the existence and nature of the heat flux across the system. It is clear that even existence is not automatic: most trivially just imagine that our system is composed of two noninteracting parts each coupled to a single reservoir.

To study the heat flux through the system we first define a local energy density. For a fluid let $\mathbf{q} \in \Lambda \subset \mathbb{R}^d$ then

$$h(\mathbf{q}; P, Q) = \sum_{i=1}^{N} \delta(\mathbf{q} - \mathbf{q}_i) \left[\frac{{\mathbf{p}_i}^2}{2m} + \sum_{j\neq i} \phi(\mathbf{q}_j - \mathbf{q}_i) + u(\mathbf{q}_i) \right] \tag{20}$$

where the square bracket is identical to that in Eq.(4). For a crystal with nearest neighbor interactions we define the local energy density at site $\mathbf{i}$ as

$$h(\mathbf{i}; P, Q) = \frac{\mathbf{p}_\mathbf{i}^2}{2m} + U(\mathbf{q}_\mathbf{i}) + \frac{1}{2d} \sum_k \left(V(\mathbf{q}_\mathbf{i} - \mathbf{q}_{\mathbf{i}-1_k}) + V(\mathbf{q}_{\mathbf{i}+1_k} - \mathbf{q}_\mathbf{i}) \right) \tag{21}$$

where 1_k is the d-dimensional vector with all components 0 except the k-th equal to 1.

---

[d]The only thermostated "physical" model for which a SNS corresponding to an SRB measure with the desired properties has been proven is the Moran-Hoover model of a single particle moving among fixed periodic scatterers (see Section 1) to which is added an external electric field and a Gaussian thermostat[14].

Given the local energy density we can define a local microscopic heat flow Ψ through the continuity equation. To avoid repetition we shall do so only for the crystal. Writing

$$\frac{dh(\mathbf{i};P,Q)}{dt} = \tilde{\nabla}\Psi(\mathbf{i}) \tag{22}$$

where $\tilde{\nabla}\Psi(\mathbf{i}) = \sum_k \tilde{\partial}_{i_k}\Psi_k(\mathbf{i})$ with $\tilde{\partial}_{i_k}\Psi_j(\mathbf{i}) = (\Psi_j(\mathbf{i}+1_k) - \Psi_j(\mathbf{i}))/2$. It easy to verify that

$$\Psi_k(\mathbf{i}) = \mathbf{f}(\mathbf{q_i} - \mathbf{q}_{\mathbf{i}+1_k})\frac{\mathbf{p_i} + \mathbf{p}_{\mathbf{i}+1_k}}{2} \tag{23}$$

where $\mathbf{f}(\mathbf{q}) = -\nabla V(\mathbf{q})$. We will usually be interested in the heat flow $\Phi(j)$ through the plane $\{\mathbf{i}\in\Lambda\,;\, i_1 = j\}$. It is clear that we can integrate eq.(22) and obtain

$$\Phi(j) \;=\; \sum_{\substack{\mathbf{i}=(j,i_2,\ldots,i_d),\\ 1\le i_l\le N_l}} \Psi_1(\mathbf{i}). \tag{24}$$

Of course the heat current inside the system in the steady state is just the energy flux from one reservoir to the other, presumably from the one with the higher temperature to the one with the lower one. Let S^t be the time evolution for observables (averaged over the realizations if the evolution is stochastic). Since the equations of motion are Hamiltonian except at the boundary, one finds that the time derivative of the energy is given by

$$\frac{d}{dt}S^t H(P,Q) \;=\; -S^t\left(\Phi_L + \Phi_R\right) \tag{25}$$

where Φ_L (Φ_R) depends only on the variables of the left (right) boundary of the system. It is natural to interpret Φ_L as the flow of energy from the system to the left heat reservoir and similarly for Φ_R. We suppose that a stationary state μ exists, and, for any observable f, we set $\mu(f) = \int f d\mu$. One obtains

$$-\mu\left(\Phi_L + \Phi_R\right) \;=\; \mu\left(\frac{d}{dt}S^t H(p,q)\right) \;=\; 0\,, \tag{26}$$

and therefore

$$\mu(\Phi_L) \;=\; -\mu(\Phi_R)\,. \tag{27}$$

To check that the heat flux is indeed as expected it is useful to define the entropy production σ of the reservoirs as[6]

$$\sigma \;=\; \frac{\Phi_L}{T_L} + \frac{\Phi_R}{T_R}\,, \tag{28}$$

i.e., σ is the sum of the energy flows into the reservoirs divided by the temperatures of the reservoirs. This (microscopic) definition of the reservoirs entropy production is in accordance with our notion of heat reservoir at specified temperature. It does not require that the system itself be close to equilibrium. A convenient way of proving that if $T_L > T_R$ then heat is flowing through the system from left to right is to show that in the steady state

$$\mu(\sigma) \;=\; \left(\frac{1}{T_R} - \frac{1}{T_L}\right)\mu(\Phi_R) \;\ge\; 0\,, \tag{29}$$

and

$$\mu(\sigma) = 0 \quad \text{if and only if} \quad T_L = T_R \,. \tag{30}$$

(One may also consider the heat flow $\Phi(i)$ (or the corresponding $J(\mathbf{q})$ for a fluid) inside the system and formally define a corresponding entropy production $\sigma_i = (T_R^{-1} - T_L^{-1})\Phi(i)$. One obviously has that $\mu(\Phi_L) = \mu(\Phi_i)$ in the stationary state but σ_i is not the macroscopic entropy production density inside the system[27,15,16].)

If T_L and T_R are close, one expects linear response theory to be valid. Setting $T = (T_L + T_R)/2$ and $\delta T = (T_L - T_R)$, formal perturbation theory gives

$$\mu(\sigma) = \int_0^\infty dt\, \mu_0(\sigma S_0^t \sigma) + \text{ lower orders in } \delta T \,, \tag{31}$$

where μ_0 is the equilibrium Gibbs state at temperature T and S_0^t the time evolution for observables with $T_L = T_R = T$. For the heat flux $\Phi = \Phi(j)$ one obtains

$$\mu(\Phi) = \frac{T_L - T_R}{T^2} \int_0^\infty dt\, \mu_0(\Phi S_0^t \Phi) + \text{ lower orders in } \delta T \,. \tag{32}$$

It is important to note that in Eqs.(31) and (32), the reservoirs are still present via the time evolution S_0^t. Although very similar this is not the Green-Kubo formula which will be discussed below.

5.3 Fourier's Law.

Assuming that 1. and 2. have been proved, we can then define the heat conductivity $\kappa_{\mathcal{L}}$ as in Section 1, where $\mathcal{L}$ the length of the system (fluid or crystal) in microscopic units and A the area of its crossection. Since $\delta T/\mathcal{L}$ is the average temperature gradient the heat conductivity at temperature T should then be given by

$$\kappa = \lim_{\mathcal{L}\to\infty} \mathcal{L} \lim_{\delta T \to 0} \frac{1}{\delta T} \left(\mu(\Phi)/A\right) \,, \tag{33}$$

i.e., $\kappa = \kappa(T)$ is the heat flux per unit area divided by the temperature gradient. One might also have taken the limit $A \to \infty$ in Eq.(33). As might be expected it is the limit $\mathcal{L} \to \infty$ which is the crux of the matter.

6 Summary of Exact Results

We now summarize briefly the limited number of results relating to points 1-3 of the last section.

6.1 Fluid systems.

Consider a system of N particle in $\Lambda \subset \mathbb{R}^d$, $d \geq 2$, with Hamiltonian given in Eq.(3), such that $u(\mathbf{q}_i) = 0$ and the pair potential $\phi(|\mathbf{q}|)$ is positive, with $\phi(0) = C_1$, and $-C_2 < \phi'(|\mathbf{q}|) < 0$, $0 < C_1, C_2 < \infty$, for $|q| > 0$. Then it was shown in [36,37,35] that, using Maxwell boundary conditions Eq.(9) with temperature $T(\mathbf{r}) > 0$, $\mathbf{r} \in \partial\Lambda$ (Λ a regular domain) there exists a unique stationary μ. Furthermore this μ is absolutely continuous with respect to Lebesgue measure on $\Omega = \Lambda^N \times \mathbb{R}^{dN}$ and is approached, as $t \to \infty$, from almost any initial (P, Q), *i.e.* the set Ω' for which the approach may fail has Lebesgue measure zero.

The argument makes use of the boundedness of the force acting on any particle in the interior of Λ. This assures that any particle with a sufficiently high speed will hit the boundary with only little deviation from a straight path. This and the fact that the force $-\phi'(|\mathbf{q}|)$ is everywhere positive insures effective contact between the system and the stochastic boundaries which, according to Eq.(9), "spread" the velocity of particles which hit it. This yields something like a "Harris condition" which guarantees existence, uniqueness and approach to the stationary state.

Using general technique developed in [6] Eq.(29) for systems in contact with stochastic reservoirs satisfying detailed balance is immediate. It is probably also possible to prove inequality (30) for such systems but the latter has not been done generally as far as for we know; see below.

6.2 Harmonic Crystal.

A system with Hamiltonian given by Eq.(8) in which both V and $U_{\mathbf{i}}$ (when it does not vanish) are quadratic functions of their arguments is an ideal harmonic crystal. When such a system is placed in contact with stochastic reservoirs of the Langevin type the resulting process and thus also the stationary measure is Gaussian and one only needs to compute the covariances. This was done essentially explicitly for a chain in [75]. The most important difference with the equilibrium state is that there are now non-vanishing covariances between position and momentum variables proportional to δT. One finds uniqueness and approach to the stationary measure μ that satisfies Eqs.(29) and (30)

As already mentioned however the heat flux $\mu(\Phi)$ is essentially independent of $\mathcal{L}$ and $\kappa_{\mathcal{L}}$ defined in Eq.(33) grows as $\mathcal{L}$. (For the case of "random masses" $\kappa_{\mathcal{L}}$ grows as $\sqrt{\mathcal{L}}$[13,69,76]). The solution of [75] was extended to $d > 1$ in [67] where there were also considered various possibilities for $U_{\mathbf{i}}$, *e.g.* pinned down everywhere, only at the boundary or nowhere. Looking at the invariant measure in the limit $\mathcal{L} \to \infty$ one finds that the decay of the position-momentum covariance is rapid when $U_{\mathbf{i}} \neq 0$ (at least on the boundary) but does not decay at all when $U_{\mathbf{i}} = 0$.

The case of an infinite harmonic chain with left and right portions acting as Hamiltonian reservoirs was investigated in [80]. The results are qualitatively the same as for the stochastic reservoirs: the heat current remain proportional to the initial temperature difference as $t \to \infty$ and the system approaches its stationary state which is again a Gaussian measure[e].

6.3 Anharmonic Crystals.

The anharmonic crystal coupled to Hamiltonian/Stochastic reservoirs described by Eq.(11) has been investigated in [21,22,20]. Technical conditions on the growth at infinity of the potential are needed: either [21] that $\mathcal{V}$ is quadratic at infinity or [20] more general polynomial growth. (In the latter case, the one-body potential U

[e] For an infinite quantum harmonic chain with a special particle subject to a sufficiently small non harmonic potential, the existence of stationary states and their mixing property has been established, both for KMS states [29,65] and for SNS [29].

grows more slowly at infinity then the two-body potential V). One assumes also that the two-body potential is strictly convex, and this condition alone implies [22] that the stationary state is unique. Under these conditions the following results hold:

1. Existence and uniqueness of the stationary state μ. The stationary state is mixing, *i.e.* any initial distribution will converges to the stationary state as $t \to \infty$. The stationary state has a $\mathcal{C}^\infty$ density which decays at infinity at least as fast as a Gibbs state with temperature equal to the maximum of the temperature of the reservoirs.

2. The stationary state is conducting: One has $\mu(\Phi_R) = 0$ if and only if $T_L = T_R$ and $\mu(\Phi_R) > 0$ if $T_L > T_R$. Linear response theory is valid: For a large class of observables f, the expectation value $\mu(f)$ is a real-analytic function of the temperature difference δT. In particular, near equilibrium, one obtains, with $T = (T_L + T_R)/2$

   $$\mu(\Phi_R) \; = \; \frac{\delta T}{T^2} D + O(\delta T^2)\,, \tag{34}$$

   Eq.32 for the coefficient D has not been proved, but rather the slightly weaker form

   $$D = \mu_0(\Phi_R(L_0^{-1}\Phi_R))\,, \tag{35}$$

   where μ_0 is the Gibbs state Eq.(12) with temperature T and L_0 is the generator of the Markovian semi-group S_0^t associated with the stochastic differential equations (11) with $T_L = T_R = T$. Notice that, formally, one has

   $$L_0^{-1} = \int_0^\infty dt S_0^t \tag{36}$$

   and, inserting Eq.(36) into Eq.(35) yields Eqs.(32). In order to prove Eq.(36), one needs presumably some information on the decay of correlations. This has not been obtained so far. Nothing is known about the dependence of D on $\mathcal{L}$ and thus ipso facto about the validity of Fourier's law.

7 The Green-Kubo Formula

It is clear that, aside from the case of the harmonic crystal, which does not satisfy Fourier's law, none of the exact results quoted in the last section says anything about the local structure, *e.g.* about local equilibrium in the SNS. This means in particular that at this time we have no rigorous way of relating the local heat flux $\mu(\Phi)$ to the gradient of the local temperature as defined in Eq.(4). Even in the absence of LTE one can define a local kinetic temperature by means of the average local kinetic energy. Thus for the crystal at site $\mathbf{i}$, $T(\mathbf{i}) = \mu(\mathbf{p}_\mathbf{i}^2/m)/d$. For the harmonic crystal $T(\mathbf{i})$ in found to be uniform away from the ends, *i.e.* there is no temperature gradient. Even accepting such a definition of temperature (in numerical simulation, to be discussed later, $T(\mathbf{i})$ is one of the most directly measured quantities) we are completely lacking at this point any rigorous or even formal connection between the κ defined in Eq.(33) and the usual Green-Kubo formula for the conductivity which is defined in terms of the time evolution of an isolated system in equilibrium. Denoting by $\hat{S}_0^t$ the Hamiltonian evolution of the isolated system the thermal conductivity κ_{GK} is given by [53,66]

$$\kappa_{GK} = \lim_{L\to\infty} \frac{L}{A}\frac{1}{T^2}\int_0^\infty dt\, \langle \Phi \hat{S}_0^t \Phi\rangle \tag{37}$$

where $\langle\cdot\rangle$ denotes the microcanonical average and the energy density is chosen such that it corresponds to the thermodynamic energy at temperature T (since we are in equilibrium this is the same as the kinetic temperature). If the total momentum Π is conserved it has to be set equal to zero. Alternatively one may use in Eq.(37) truncated correlation functions $\langle \Phi \hat{S}_0^t \Phi\rangle_{E,\Pi}^T = \langle \Phi \hat{S}_0^t \Phi\rangle_{E,\Pi} - \langle\Phi\rangle_{E,\Pi}^2$ and then average over E and Π using the canonical distribution[f]. One expects that the equivalence of equilibrium ensembles will extend also to this case.

The Green-Kubo formula, Eq.(37), also makes sense for a system with a few degree of freedom where it can be related to the variance in the fluctuation of the current; see the article of Bunimovich and Spohn [11] for a discussion. There is no clear connection however between the integral in Eq.(37) for a small system and the κ in Fourier's law. From a mathematical point of view it is not even clear how to prove equivalence for macroscopic systems, *i.e.* show that $\kappa = \kappa_{GK}$. It would be nice to find even a formal argument establishing the equivalence.

8 Entropy Production and Large Deviations

The proper definition of microscopic entropy production has attracted much attention in recent years. The interest comes from the observation of an interesting symmetry property in the large deviation functional associated to the phase space volume contraction rate in thermostated systems. This property was first observed numerically in [26] and then proved under strong hyperbolicity condition in [31]. For such systems the phase space volume contraction has strong connection to the entropy production in Section 5. Using this connection the fluctuation theorem has been extended to large deviations of the entropy production of various stochastic systems[52,58]. For crystals with stochastic reservoirs or for the model considered in Section 4.3, only formal proofs of the Gallavotti-Cohen fluctuation theorem are available so far.

The Gallavotti-Cohen fluctuation theorem can be formulated as follows: In both deterministic and stochastic systems one identifies an observable $\sigma(X)$ as the "entropy production" although its identification with the thermodynamic entropy production is not always clear. If one now considers the ergodic average,

$$\sigma_t(X) = \frac{1}{t}\int_0^t ds \sigma(X(s)) \tag{38}$$

where for deterministic dynamics $X(t)$ is trajectory of the system while for stochastic dynamics $X(t)$ is a particular realization of the random process. Then by the

[f] If one does not fix Π in an equilibrium ensemble for which the total momentum is conserved then the integral in Eq.(37) is divergent[74] but this does not say anything about κ_{GK}.

large deviation principle (assumed to hold) there exists an $e(p)$ such that for any interval I

$$\lim_{t\to\infty} \log \mathrm{Prob}(\sigma_t(x) \in I) = \inf_{p\in I} e(p)\,. \tag{39}$$

The fluctuation theorem asserts that the odd part of $e(p)$ is linear with slope -1, *i.e.* $e(p) - e(-p) = -p$.

In the deterministic case the entropy production variable that one consider is, as already mentioned, the phase space contraction rate which, in the case of Gaussian thermostats, coincides with entropy production as we defined it in Subsection 5.2. This can be easily seen by computing the divergence of the equations of motion quoted at the end of Subsection 4.4. Already for the case of the Nosé-Hoover thermostat the phase space contraction and the entropy production are not the same quantities although their average value in the SNS are the same. For anharmonic chains with a two body potential given $V(x) = x^2 + \beta x^4$ the validity of the fluctuation theorem has been checked numerically in [59] for the entropy production (but not for the phase space contraction).

The connection between the Gallavotti-Cohen fluctuation theorem and its various generalizations can be related to the following observation: For a stochastic model described by a Markov process one can consider the measure P on the path space induced by the evolution. Let ϕ be a path leading from X to Y in phase space in the time interval $[0,t]$ and consider now the transformation which maps the path ϕ into the time reversed path leading from IY to IX, where I is the involution on phase space which reverses the velocities of all particles. This transformation maps the measure P into a new measure $\overline{P}$ which is absolutely continuous with respect to P with Radon-Nykodym derivative given by

$$\frac{dP}{d\overline{P}}(\phi) \;=\; \exp\left(R(\phi(t)) - R(\phi(0)) + \int_0^t \sigma(\phi(s))ds \right)\,, \tag{40}$$

where σ is the entropy production defined in Eq.(28). Eq. (40) states, roughly speaking, that the probability of a time reversed path is equal (up to a boundary term) to the probability of taht path times the exponential of the integrated entropy production along this path. This property can be assumed as a general definition of entropy production[64] and can be seen as a generalization of detailed balance. In fact in the equilibrium case ($T_L = T_R = T$), the right hand side of Eq.(40) depends on ϕ only through its endpoints and is equal to $\exp\left(T^{-1}(H(\phi(t)) - H(\phi(0)))\right)$ and this is precisely detailed balance.

For thermostated systems the above calculation is quite delicate because, although one can still consider the measure P on the path space, it will not be absolutely continuous with respect to the time reversed measure $\overline{P}$. The original proof of the fluctuation theorem in [31] can be thought of as based on the construction of a series of approximants to the measure P which satisfies a relation formally similar to Eq.(40).

9 Local equilibrium

Since we have nothing to say about LTE in Hamiltonian heat conducting systems we discuss briefly some models where the Hamiltonian dynamics in the bulk is modified by the addition of stochastic forces. These models show that a mechanism sufficiently strong to destroy the coherence of the phonons does indeed produce both a temperature gradient and a normal thermal conductivity, even in one dimensional systems.

The first such model [7,76] is a harmonic chain coupled to self-consistent reservoirs. Each particle of the chain is coupled to its own stochastic reservoir at temperature T_i, $i = 1, \cdots, N$, modeled by Langevin dynamics. The reservoirs coupled to the particles in the bulk supposedly simulate the effect of strong anharmonic interactions. The temperature of the reservoirs coupled to the first and last particles are at fixed temperature $T_1 = T_L$ and $T_N = T_R$. The temperature of the remaining reservoirs is fixed by a self-consistency condition: one requires, that in the stationary state there is no net energy exchange between the reservoirs and the particles in the bulk. It is argued [7] that in the limit of large N, the system exhibits a temperature gradient and Fourier's law is indeed satisfied[76].

Another model [17] is a one-dimensional chain of quantum mechanical atoms (each of which has a finite number of energy levels). The first and the last atoms of the chain are each coupled to heat reservoirs at temperatures T_L and T_R. The atoms in the chains are not directly coupled to each other, but each pair of nearest neighbors in the chain is coupled to a heat reservoir. Since each atom has only a finite number of energy levels, it is possible to choose the coupling to the intermediate reservoirs in such a way that no energy is exchanged between the particles in the bulk and the reservoirs. Compared to the previous model, no self-consistency condition is needed and the transfer of energy between the intermediate reservoirs and the system always vanishes, not only in the stationary state. The model is studied in the weak coupling (or Van Hove) limit, where the coupling between the chains and all reservoirs goes to zero and the time is suitably rescaled. In this limit the evolution is described by a quantum semigroup. For a suitable choice of couplings the model can be solved exactly and it exhibits a temperature gradient and Fourier's law.

Another model considered [48] consists of a chain of uncoupled harmonic oscillators ($U_i(q_i) = q_i^2/2$, $V(q_i - q_j) = 0$). The oscillators at the boundary are coupled to heat reservoirs modeled by Glauber processes which thermalize the oscillators according to the Gibbs distribution at temperatures T_L and T_R. The energy is exchanged between the oscillators in the chain according to the following (microcanonical procedure): at each pair of nearest neighbor sites, there is a clock with exponential law, when it rings the energy of the pair of particle is redistributed in a uniform way, keeping the total energy of the system constant. This model is exactly solvable and satisfies Fourier's law.

10 Numerical results

The availability of fast computers has permitted the investigation of heat current carrying SNS via numerical simulations. Many such simulations have been performed, see e.g. [12,73,59,60,42,40,1,34] for recent works on various models. Earlier works were not always consistent but recently careful simulations of both one and two dimensional crystals have become available[62]. A coherent picture now seems to emerge from the numerical results[62]. We describe this briefly and refer the reader to [61] for a more complete overview.

For obvious reasons, it is convenient in numerical works to keep the number of degrees of freedom as low as possible. On the other hand stochastic differential equations, like the ones used in the Langevin stochastic reservoirs require very good random number generators and present numerical problems connected with the singularity of the covariance of the white noise. For this reason the simulations done using the deterministic thermostat are easier and likely more reliable. In any case there is good agreement (in the data if not always in the interpretation) between simulations with different thermostats.

Since it is not easy to look for invariant measures with numerical simulations one typically computes the time average of a few interesting observables along a given trajectory. Assuming the validity of Eq.(19) this represents averages with respect to the invariant measure. This permits investigation of questions like the temperature profile in a chain in the steady state or the value of the conductivity for which, as we have seen, there is no analytical result at this time. We will focus mainly on this last question.

1. In one dimension, where most of the simulations have been conducted, the conductivity, when $U_{\mathbf{i}}(\mathbf{q}) = 0$, appears to behave, as a function of the length $\mathcal{L}$ of the chain, as $\mathcal{L}^\alpha$ with α a positive exponent, $\alpha = 0.4$ for the anharmonic chain. On the other hand if $U_{\mathbf{i}}(\mathbf{q}) \neq 0$ (typically one consider $U_{\mathbf{i}}(\mathbf{q}) = \frac{1}{2}\omega^2\mathbf{q}^2$) one finds a finite conductivity if some nonlinearity is present in the system (for the linear case $\alpha = 1$[75]). In this situation the exact form of the non linearity seems irrelevant, analogous result are found adding a 4-th order term to $U(\mathbf{q})$ as well as to $V(\mathbf{q})$. Similar results are obtained if one compactifies the configuration space of Q, *e.g.* by considering each $\mathbf{q}$ as a point on a torus, obtaining what can be called a chain of rotators. In all cases the system has a well defined, approximately linear, temperature profile, although there can be a finite jump between the temperature of the first and last oscillator and the temperature of the respective thermostats. Moreover for one dimensional systems simulations using different kinds of reservoirs appear to yield similar values of the exponent α.

2. Recent simulations seem to show that the conductivity in two dimensions is logarithmically divergent if $U_{\mathbf{i}}(\mathbf{q}) = 0$. Although it is not easy to see a logarithm is such a situation the simulation in [62] strongly suggests this conclusion. Moreover in this case one can try to compute the thermal conductivity κ_{GK} as given in Eq.(37)[g] and compare it with the κ obtained from Eq.(33) (without

[g] In this case the equilibrium ensemble used is $\langle\cdot\rangle_{E,\pi}$ described in the comments after Eq.(37)

the limit $\mathcal{L} \to \infty$). The agreement obtained from the numerical data support the validity of the equality $\kappa = \kappa_{GK}$. Although we do not know any results on this direction we believe that adding a confining $U(\mathbf{q})$ to this system will make the conductivity finite.

3. We further expect that the conductivity in three dimensions will be finite, with or without any on site potential.

The above picture can be interpreted in term of the Peierls theory which, as mentioned in Section 4 relies on umklap processes to produce a finite conductivity. We also note that in one and two dimension, there is no stable crystal without an on site potential, but there is localization in $d \geq 3$. The variance in the deviation of an atom near the center from its equilibrium position, when the boundary atoms are tied down, grows like $\mathcal{L}$ in $d = 1$, like $\log \mathcal{L}$ in $d = 2$ and is finite in $d = 3$[8].

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