On the local space-time structure of non-equilibrium steady states.

Raphaël Lefevere[1]
Laboratoire de Probabilités et modèles aléatoires
UFR de Mathématiques Université Paris 7,
Case 7012, 75251 Paris Cedex 05, France

Abstract

We consider the Gibbs representation over space-time of non-equilibrium dynamics of Hamiltonian systems defined on a lattice with local interactions. We first write the corresponding action functional as a sum of local terms, defining a local action functional. We replace the local system by a translation-invariant system whose dynamics has an identical space-time characterization. We study in details the irreversible properties of the new dynamics, define the local conductivity and show its equivalence with the Green-Kubo formula. Given the definition of the local heat conductivity and using conservation of energy, we derive the shape of the temperature profile. Next we apply our scheme to various approximations of anharmonic Hamiltonian models, show how to compute their thermal conductivity and recover results confirmed in numerical simulations.

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[1]lefevere@math.jussieu.fr

1 Introduction.

Non-equilibrium stationary states (NESS) of systems of classical Hamiltonian oscillators located on a lattice coupled to heat baths at their boundaries have been extensively studied over recent years [7, 9, 24]. Numerous global results concerning those NESS have been obtained, including existence and uniqueness of the stationary probability measure. The positivity of the entropy production and the validity of the Gallavotti-Cohen fluctuation theorem has also been established [8, 20, 26]. They have also been abundantly studied with the help of numerical simulations, see [5, 17] for a review of those and a general overview of the subject.

However, in contrast to equilibrium states for which the explicit Gibbs formula may be used, the effective computation of correlation functions of the stationary states out of equilibrium remains a challenging problem. Conceptually, one may distinguish two different reasons for that. The first one is common with the equilibrium situation and has to do with the difficulty of dealing with nonlinear interactions between the components of the system. The second one has to do with the lack of translation invariance which is, in a sense built-in in the non-equilibrium set-up. This paper adresses the second issue for Hamiltonian systems defined on a lattice with local interactions. The difficulties we have just mentioned are particularly obvious when one tries to identify the physical mechanism giving rise to a finite thermal conductivity in non-linear Hamiltonian systems and compute its dependance on the microscopic interactions. The conductivity is a local property of the system that relates local quantities like the current and the local temperature gradient. The goal of this paper is to outline a method which, by dealing with the lack of translation invariance of the system, allow to focus on the effect of nonlinearities on the non-equilibrium steady states and perform concrete computations of their correlation functions. The method is a priori independent of any approximation scheme and apply to any local Hamiltonian lattice system out of equilibrium.

As we will argue later, what matters locally and away from the boundaries in a non-equilibrium set-up is not so much the spatial geometry but rather the specific way in which the time reversal symmetry of the equilibrium dynamics is broken. It turns out that heuristically, the non-equilibrium dynamics may be characterized locally in a simple, universal and translation-invariant way, see (25) below. This follows from local (on the lattice) conservation of energy and the characterization of NESS in terms of probabilities over pathspace introduced by Maes [18]. Therefore, in order to study the local dynamics, we will consider a spatially homogeneous Hamiltonian chain of oscillators coupled to a stochastic thermostat at a fixed temperature T and, in order to recover the time-reversal symmetry breaking induced locally by the heat baths located at the boundaries, we include an additional term in the deterministic part of the dynamics. The construction of the dynamics is very similar in spirit to the Evans heat flow algorithm [10] but ours proceeds through the introduction of a *stochastic* thermostat, which makes analytical computation straightforward. In particular, the proof that the dynamics satisfy the Gallavotti-Cohen fluctuation theorem is simple and the equations for the correlation functions in the stationary state may be easily written down. Systems with Langevin stochastic thermostats and non-conservative forces producing entropy have been considered in [13, 19]. We shall also see how to recover the linear response theory's Green-Kubo formula in a natural way. However, our scheme hopefully also allows to describe the behaviour of systems far from equilibrium. We shall also see how to reconstruct the

temperature profile on the original chain coupled to heat baths at different temperatures. The basic assumption that is made is that two systems having the same time-reversal symmetry breaking functional will have basically the same average heat current.

In the last section, we consider a concrete anharmonic Hamiltonian model, generic of models having a normal heat conduction behaviour. The Hamiltonian is given by,

$$H(\underline{q}, \underline{p}) = \sum_{i=1}^{N} [\frac{p_i^2}{2} + \omega^2 \mu^2 \frac{q_i^2}{2} + \frac{\lambda}{4} q_i^4 + \frac{\omega^2}{2} (q_i - q_{i-1})^2] \tag{1}$$

On that example, we will see how to implement our strategy and study the problem with the help of the non-equilibrium translation invariant dynamics we have defined before. We will show that this dynamics provides a source term, absent in equilibrium, in the equation for the evolution of the average heat current j in the chain. This is of course what should be expected because the dynamics is built so as to break the time-reversal symmetry of the equilibrium dynamics in a proper way. Roughly speaking we get an equation of the form,

$$\frac{d}{dt} j(t) = -\gamma j(t) + \lambda \mathcal{N}(t) + S(t). \tag{2}$$

The first term on the RHS of this equation is a damping term coming from the coupling of the chain to an external friction represented by the coefficient γ. The second term comes from the Hamiltonian evolution and vanishes when the anharmonic part of the interaction is zero, i.e., when $\lambda = 0$. The third term represents an external "creation" of current and comes from the action of the non-equilibrium dynamics. Equation (2) will therefore yield a balance equation for the heat current in the stationary state. First, we review the linear case ($\lambda = 0$) and next we study two approximations which have been used recently to analyze the effect of the anharmonic terms on the non-equilibrium properties of the Hamiltonian system. The first one [2, 12] amounts to replace the effects of the anharmonic terms by a random exchange of energy between nearest-neighbours, this gives rise to a normal heat conductivity and to a linear profile of temperature.

The second one has been derived and used over the years since Peierls [6, 11, 14, 15, 22, 27]. It amounts to a closure assumption on the hierarchy of correlations and to a derivation of a stationary Boltzmann-type equation with a collision kernel representing the interaction between the phonons due to the nonlinearity of the system. The basic mechanism which gives rise to a normal heat conductivity has been known to physicists for a long time, it was postulated to be the result of some particular resonances in the collision between phonons. However, the lack of explicit localization and of a proof of the existence of those resonances prevented the effective computation of the thermal conductivity in terms of the physical microscopic parameters. The localization of the resonances in the model (1) for large pinning μ has been achieved in [15], where a similar translation invariant dynamics has been devised, and the value

$$\kappa = \alpha \frac{\omega^9 \mu^3}{\lambda^2 T^2} \tag{3}$$

for the thermal conductivity was obtained. The value of $\alpha = 0.275637$ was computed in [1] where the expression (3) was also tested and numerically confirmed. The localization of the resonances at $\mu = 0$ was obtained by Pereverzev [23] who used it to discuss anomalous heat conduction in a related anharmonic model.

2 Local time-reversal in models for heat conduction.

In order to explain the behaviour of the thermal conductivity in crystalline solids, one often modelizes the solid by a chain (or lattice in higher dimension) whose ends are coupled to heat baths maintained at different temperatures. The coupling can be taken stochastic and more precisely of Langevin type. In one dimension, the set-up is as follows. At each site i of a lattice $\{1, \ldots, N\}$ is attached a particle of momentum p_i and position q_i. The dynamics is hamiltonian in the bulk and stochastic through the Langevin coupling to heat baths at the boundaries. The Hamiltonian is of the form,

$$H(\underline{p}, \underline{q}) = \sum_{i=1}^{N} \left(\tfrac{1}{2} p_i^2 + V(q_i) \right) + \sum_{i=2}^{N} U(q_i - q_{i-1}) + U(q_1) + U(q_N). \tag{4}$$

The equations of motions are given by,

$$dq_i = p_i dt, \quad i = 1, \ldots, N,$$
$$dp_i = -\frac{\partial H}{\partial q_i}(p, q) dt, \quad i = 2, \ldots, N-1, \tag{5}$$

and,

$$dp_1 = -\frac{\partial H}{\partial q_1}(p, q) dt - \gamma p_1 dt + \sqrt{2\gamma k T_L}\, dw_l,$$
$$dp_N = -\frac{\partial H}{\partial q_N}(p, q) dt - \gamma p_N dt + \sqrt{2\gamma k T_R}\, dw_r. \tag{6}$$

T_L and T_R stand for the temperature of the left and right reservoirs, respectively, whereas w_l and w_r are two independent standard Wiener processes.

It is an easy fact to check that when $T_L = T_R = T = \beta^{-1}$, the equilibrium measure on the configuration space $\mathbf{R}^{2N}$ whose density with respect to the Lebesgue measure is given by

$$\rho(\underline{p}, \underline{q}) = Z^{-1} e^{-\beta H(\underline{p}, \underline{q})} \tag{7}$$

is invariant (stationary) for the stochastic dynamics defined above. In the case of two different temperatures, existence, uniqueness and exponential convergence to an unique invariant state has been established under fairly general conditions on the potentials U and V [7, 9, 24]. In the case of harmonic coupling, the covariance of the stationary state has been exactly computed in [21, 25].

In order to describe the conduction of heat in the crystal, one defines a local energy function,

$$h_i(\underline{p}, \underline{q}) = \frac{p_i^2}{2} + V(q_i) + \tfrac{1}{2}(U(q_{i+1} - q_i) + U(q_i - q_{i-1})) \tag{8}$$

for $i \neq 1, N$,

$$h_1(\underline{p}, \underline{q}) = \frac{p_1^2}{2} + V(q_1) + U(q_1) + \tfrac{1}{2}U(q_2 - q_1) \tag{9}$$

and similarly for h_N. The heat current is defined through the time evolution of the local energy,

$$\frac{dh_i}{dt} = j_i^+ - j_i^- \tag{10}$$

for $i \neq 1, N$ and where,

$$j_i^+ = \tfrac{1}{2}F(q_i - q_{i+1})(p_i + p_{i+1}), \tag{11}$$

$$j_i^- = \tfrac{1}{2}F(q_{i-1} - q_i)(p_i + p_{i-1}), \tag{12}$$

where $F = -U'$ and j_i is defined to be the microscopic current of energy or heat between atom i and $i+1$, i.e the rate of energy transfer between those atoms. We observe that $j_{i-1}^+ = j_i^-$ and in the following we shall use the shorthand notation, $j_i \equiv j_i^+$.

We use the notation $\langle . \rangle$ to denote average with respect to the stationary state. And define the local temperature in the chain to be

$$\left\langle p_i^2 \right\rangle \equiv T_i \tag{13}$$

and the average heat current is,

$$j \equiv \langle j_i \rangle = \frac{\omega^2}{2} \left\langle F(q_i - q_{i+1})(p_i + p_{i+1}) \right\rangle \tag{14}$$

which must be constant throughout the chain due to conservation of energy.
This follows from,

$$\left\langle \frac{dh_i}{dt} \right\rangle = \left\langle j_i^+ \right\rangle - \left\langle j_i^- \right\rangle = 0 \tag{15}$$

and $j_{i-1}^+ = j_i^-$.

Fourier law states that,

$$j = \kappa(T_i)(T_{i+1} - T_i) \tag{16}$$

where κ is the conductivity of the crystal, a major problem is to understand how the anharmonic part of the Hamiltonian makes this constant finite and to compute its value from the microscopic parameters.

An elegant and systematic way of describing non-equilibrium dynamics was devised by Maes [18]. For stochastic processes, it amounts to compare the probability of trajectories of the non-equilibrium process at hand and of its time-reverse. By the Girsanov formula, the ratio of the two probabilities is given by the exponential of an "action functional". Then the part of the action functional which breaks the time-reversal invariance is identified with the entropy production. Let P_μ^t the pathspace measure on trajectories $\xi = ((\underline{q}(s), \underline{p}(s)), s \in [-t, t])$ obtained from the dynamics (5,6) started from initial conditions which are distributed according to some measure μ. We define the time-reversal operator on trajectories as follows, $(\Pi\xi)_s = (\underline{q}(-s), -\underline{p}(-s))$ and let $P_\mu^t \Pi$ be the pathspace distribution of the time-reverse process. In [20, 26], it has been show that the ratio of the two measures may be written as,

$$\frac{dP_\mu^t}{dP_\mu^t \Pi} = \exp(R^t(\xi)) \tag{17}$$

modulo temporal boundary terms involving the distribution μ.
The action functional R^t is given by,

$$R^t(\xi) = \beta_L (\int_{-t}^t j_1(s)ds - (h_1(\xi_t) - h_1(\xi_{-t}))$$

$$+ \beta_R (\int_{-t}^t -j_{N-1}(s)ds - (h_N(\xi_t) - h_N(\xi_{-t})), \tag{18}$$

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with $\beta_L = T_L^{-1}$ and $\beta_R = T_R^{-1}$. We observe now that for any collection K_i, $i = 1, \ldots, N$, such that $K_1 = T_L$ and $K_N = T_R$,

$$R^t(\xi) = \sum_{i=1}^{N-1} \int_{-t}^{t} \sigma_i(s) ds - \sum_{i=1}^{N} \frac{1}{K_i} (h_i(\xi_t) - h_i(\xi_{-t})), \tag{19}$$

where we defined the local entropy production σ_i,

$$\sigma_i = \left(\frac{1}{K_i} - \frac{1}{K_{i+1}} \right) j_i. \tag{20}$$

This follows from *local* energy conservation inside the chain written under the integral form,

$$h_k(\xi_t) - h_k(\xi_{-t}) = \int_{-t}^{t} (j_k(s) - j_{k-1}(s)) ds \tag{21}$$

Except for the arbitrariness of the K_i's, this shows that the conservation energy imposes strict conditions on the representation of the action (18) in terms of the local variables j_i and h_i.

Among all the equivalent representations for the action difference (19), we now *choose* one which is useful because it allows detailed local analysis of the dynamics. Let us take $K_i = T(\frac{i}{N})$, with $T(.)$ a smooth function over the interval $[0, 1]$. Now, at lowest order in N^{-1}, (19) becomes,

$$R^t(\xi) = \frac{1}{N} \sum_{i=1}^{N-1} \int_{-t}^{t} j_i(s) \frac{\nabla T(\frac{i}{N})}{T^2(\frac{i}{N})} ds - \sum_{i=1}^{N} \beta(\frac{i}{N})(h_i(\xi_t) - h_i(\xi_{-t})). \tag{22}$$

In the limit $N \to \infty$ and around a fixed point x of the interval $[0, 1]$, the variation of the coefficient in front of the integral of the current and the local energy goes to zero. So we subdivide the interval $[0, 1]$ in subintervals of size ϵ, with ϵ small but $N >> \epsilon^{-1}$, each interval being centred about some point that we denote by x_k. Now, at lowest order in ϵ, we write,

$$R^t(\xi) = \sum_k R_{x_k}^t(\xi) \tag{23}$$

The local action functional $R_x^t(\xi)$ is given by,

$$R_x^t(\xi) = \frac{\nabla T(x)}{T^2(x)} \frac{1}{N} \sum_{i \in B_\epsilon(x)} \int_{-t}^{t} j_i(s) ds - \beta(x) \sum_{i \in B_\epsilon(x)} (h_i(\xi_t) - h_i(\xi_{-t})) \tag{24}$$

where $B_\epsilon(x) = \{j | |j - Nx| \leq \frac{1}{2} N \epsilon\}$. Note that $|B_\epsilon(x)| = \epsilon N$. So locally around the point x, we get the following characterization of the non-equilibrium dynamics.

$$Q_x = \exp\left(\frac{\nabla T(x)}{T^2(x)} \frac{1}{N} \sum_{i \in B_\epsilon(x)} \int_{-t}^{t} j_i(s) ds - \beta(x) \sum_{i \in B_\epsilon(x)} (h_i(\xi_t) - h_i(\xi_{-t})) \right). \tag{25}$$

with,

$$\frac{dP_\mu^t}{dP_\mu^t \Pi} = \prod_k Q_{x_k} \tag{26}$$

The important feature of (24) is that the original problem has become locally (in the box $B_\epsilon(x)$) translation invariant. For a given x, we now fix $T \equiv T(x)$ and

$\tau \equiv N^{-1}\nabla T(x)$, $M = [N\epsilon]$ and in the next section, we define a dynamics which has exactly the property (25) for those parameters, see (56). Then, in the last section, we will write the equations that the correlations of the stationary state satisfy in a concrete model. This amounts to ask *local* stationarity in the original non-translation invariant chain and allows on one hand to interpret the parameter T as a local temperature because it gives the average kinetic energy. On the other hand, it fixes the current as a function of the temperature gradient ∇T and local temperature T. Going back to the original problem, the fact that the average current in the stationary state is constant in position then fixes the kinetic energy (i.e. temperature) profile as we shall see at the end of section 5. We have derived (25) for Hamiltonian containing only nearest-neighbour interactions. Presumably the same identity may be derived for systems with sufficiently local interactions. And in the next section, we devise a dynamics which include more general interactions.

3 The dynamics and its entropy production.

We consider a periodic lattice hamiltonian system described by the Hamiltonian,

$$H(\underline{q}, \underline{p}) = \sum_{i=1}^{M} \left[\frac{p_i^2}{2} + V(q_i) + \frac{1}{2} \sum_{k=1}^{M-1} (U^k(q_i - q_{i+k}) + U^k(q_i - q_{i-k})) \right] \quad (27)$$

with the convention $i + M = i$. Note that the form of the Hamiltonian is slightly more general than in the previous section but is the same when $U^k = 0$, for $k \neq 1$. Proceeding exactly as in (8,10), one computes the local energy variation rate, and by analogy,

$$j_i = \frac{1}{2} \sum_k (p_i + p_{i+k}) F^k(q_i - q_{i+k}), \quad (28)$$

where $F^k = -(U^k)'$. j_i is interpreted as the total heat current entering the site i coming from the "right" of the chain. We shall use below the spatial average of the energy current,

$$J = \frac{1}{M} \sum_{i=1}^{M} j_i \quad (29)$$

Our dynamics is,

$$dq_i = p_i dt$$
$$dp_i = -\gamma p_i dt - \frac{\partial H}{\partial q_i} dt + \frac{\tau}{2T} \sum_k (F^k(q_{i-k} - q_i) + F^k(q_i - q_{i+k})) dt + \sqrt{2\gamma T} dw_i$$
$$(30)$$

and the w_i are standard independent Brownian motion $i = 1, \ldots, M$. The term proportional to τ is the non-equilibrium part of the dynamics and is responsible for the breaking of the time-reversal symmetry of the equilibrium dynamics (at $\tau = 0$). We will see that its particular form allows to show the validity of (25) and thus the validity of the fluctuation theorem and of the Green-Kubo formula for the thermal conductivity. The generator of the dynamics is,

$$L = L_0 + L_\tau \quad (31)$$

with,

$$L_0 = \sum_i -\gamma p_i \frac{\partial}{\partial p_i} - \frac{\partial H}{\partial q_i}\frac{\partial}{\partial p_i} + \frac{\partial H}{\partial p_i}\frac{\partial}{\partial q_i} + \gamma T \frac{\partial^2}{\partial p_i^2} \qquad (32)$$

and

$$L_\tau = \frac{\tau}{2T}\sum_{i,k}(F^k(q_{i-k} - q_i) + F^k(q_i - q_{i+k}))\frac{\partial}{\partial p_i} \qquad (33)$$

We note the basic identity,

$$-L_\tau^T H = L_\tau H = \frac{MJ\tau}{T} \qquad (34)$$

where L_τ^T is the adjoint of the operator L_τ with respect to the Lebesgue measure. We assume the existence, uniqueness, smoothness and regularity in the parameter τ of a stationary measure satisfying, $L^T \rho^\tau = 0$.

Remark. The structure of the additional force proportional to the parameter τ is chosen so that (34) is satisfied, or more generally so that the generalized detailed balance relation holds, see (52) below. This in turn implies the validity of the time-reversal characterization of the non-equilibrium dynamics (25) (and (56), see below). The only degree of freedom left is the value of the friction parameter γ which does not enter in (25) and (56) as it does not in the stationary measure at equilibrium either. It should be seen as a regularizing parameter. Indeed as we shall see explicitly in the last section, its main role is to provide an "external" degradation mechanism for the energy current in the chain. The physical degradation should come however from the nonlinearity of the chain and we shall take the friction $\gamma \to 0$ in order to evaluate the conduction properties of the chain. But *before* taking the limit $\gamma \to 0$, we will always take the limit $M \to \infty$. By doing this, we will be able to discriminate between normal heat conduction and anomalous conduction, in one case the conductivity is infinite in the other it is not. It is in the limit of $\gamma \to 0$ that we should expect the system defined by the dynamics (30) and the local dynamics of the original non-equilibrium problem to be equivalent.
We first study the evolution of the Shannon entropy under the evolution defined by the generator L. To any measure with a smooth density f on the phase space $\mathbf{R}^{2M}$ we associate the Shannon entropy,

$$S(f) = -\int dx f \log f \qquad (35)$$

with the notation $x = (\underline{p}, \underline{q})$. Compute its derivative with respect to time for a density whose evolution is given by

$$\partial_t f_t = L^T f_t \qquad (36)$$

Next,

$$\partial_t S(f_t) = -\int dx(1 + \log f_t)(\partial_t f_t) \qquad (37)$$

$$= -\int dx(1 + \log f_t)L^T f_t \qquad (38)$$

$$= -\int dx f_t L \log f_t \qquad (39)$$

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$$\partial_t S(f_t) = -\int dx\, f_t L(\log \frac{f_t}{\rho^0}) + \int dx\, f_t LH \tag{40}$$

where $\rho^0 = Z^{-1}\exp(-\beta H)$. For the first term, we note the identity,

$$L(\log h) = h^{-1}Lh - \Gamma(h, h) \tag{41}$$

where Γ is the Dirichlet form associated to the generator L,

$$\Gamma(h, g) = \sum_i \gamma T \frac{\partial h}{\partial p_i}\frac{\partial g}{\partial p_i} \tag{42}$$

So that (40) becomes,

$$\partial_t S(f_t) = -\int dx\, \rho^0 L((\rho^0)^{-1}f_t) + \int dx\, f_t \Gamma((\rho^0)^{-1}f_t, (\rho^0)^{-1}f_t) + \int dx\, f_t LH \tag{43}$$

Integration by parts of the first term yields,

$$\partial_t S(f_t) = -\int dx\, ((\rho^0)^{-1}f_t)L^T\rho^0 + \int dx\, f_t(\Gamma((\rho^0)^{-1}f_t, (\rho^0)^{-1}f_t)) + \int dx\, f_t LH \tag{44}$$

Using (34), one gets $L^T\rho^0 = \rho^0\frac{MJ\tau}{T^2}$ and therefore,

$$\partial_t S(f_t) = -\int dx\, f_t \frac{MJ\tau}{T^2} + \int dx\, f_t \Gamma((\rho^0)^{-1}f_t, (\rho^0)^{-1}f_t) + \int dx\, f_t LH \tag{45}$$

When f_t is the density of the stationary measure ρ^τ, the last term drops and one gets,

$$0 = -\int dx\, \rho^\tau(x)\frac{MJ\tau}{T^2} + \int dx\, \rho^\tau(x)\Gamma((\rho^0)^{-1}\rho^\tau, (\rho^0)^{-1}\rho^\tau) \tag{46}$$

It is natural to define the entropy production as

$$\sigma \equiv \frac{MJ\tau}{T^2} \tag{47}$$

And using the fact that the second term of (46) is given by a (positive) Dirichlet form which vanishes iff $\rho^\tau = \rho^0$, one concludes that the average entropy production in the stationary state is positive and that the current $J \neq 0$ iff $\tau \neq 0$.

4 Generalized detailed balance relation.

4.1 Fluctuation theorem for the entropy production.

Consider the ergodic average of the entropy production,

$$\bar{\sigma}_t \equiv \frac{1}{t}W(t) \equiv \frac{1}{t}\int_0^t \sigma(s)ds = \frac{1}{t}\int_0^t \frac{M\tau}{T^2}J(\underline{q}(s), \underline{p}(s))ds. \tag{48}$$

If the process is ergodic one has,

$$\lim_{t\to\infty} \bar{\sigma}_t = \langle\sigma\rangle_{\rho^\tau} \tag{49}$$

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for ρ^τ-almost every initial conditions $\underline{q}(0), \underline{p}(0)$. The fluctuation theorem is concerned with the specific shape of the large deviation functional $e(w)$ of $\bar{\sigma}_t$ defined roughly as,

$$\mathbf{P}(\bar{\sigma}_t \in [w - \epsilon, w + \epsilon]) \sim \exp(-e(w)t) \tag{50}$$

The Gallavotti-Cohen fluctuation theorem states that

$$e(w) - e(-w) = -w. \tag{51}$$

and by standard arguments [8, 13, 16, 26], assuming good properties of the process, the validity of this identity is basically ensured by the *generalized detailed balance relation* which is elementary to check in our case. Indeed, defining the reversal of velocities operator π, $\pi f(\underline{p}, \underline{q}) = f(-\underline{p}, \underline{q})$, one checks, for any α,

$$(\rho^0)^{-1}\pi(L^T - \alpha\sigma)\pi\rho^0 = L - (1 - \alpha)\sigma. \tag{52}$$

4.2 Time-reversal and entropy production.

We now show that the dynamics (30) has the property (25), expressing the fact the time-reversal symmetry is broken in a proper way. In order to compare the space-time probability of a process and of its time-reverse, we first choose a reference process, to which we shall compare both. Let P_μ^t the pathspace measure on trajectories $\xi = ((\underline{q}(s), \underline{p}(s)), s \in [-t, t])$ obtained from the dynamics (30) started from initial conditions which are distributed according to some measure μ. We define the time-reversal operator on trajectories as follows, $(\Pi\xi)_t = \pi\xi_{-t}$, where π as above reverse the sign of the momenta. We want to evaluate the ratio $dP_\mu^t/dP_\mu^t\Pi$, where, as in section 2, $P_\mu^t\Pi$ is the distribution of the time-reverse process. We compute first $dP_\mu^t/dP_{\rho^0}^t$, where $P_{\rho^0}^t$ is the pathspace measure obtained from the dynamics (30) with $\tau = 0$ and as initial distribution the Gibbs measure $\rho^0 = Z^{-1}\exp(-\beta H)$. A direct application of Girsanov formula yields,

$$dP_\mu^t = \exp(A^t(\xi))dP_{\rho^0}^t \tag{53}$$

where,

$$A^t(\xi) = \int_{-t}^t \frac{\tau}{4\gamma T^2}\underline{F}(\underline{q}(s))d\underline{p}(s) - \int_{-t}^t \frac{\tau^2}{16\gamma T^3}\underline{F}^2(\underline{q}(s))ds$$
$$+ \int_{-t}^t \frac{\tau}{4T^2}\underline{F}(\underline{q}(s))\underline{p}(s)ds + \ln\mu(\xi_{-t}) - \ln\rho^0(\xi_{-t}), \tag{54}$$

with, $F_i(\underline{q}) = \sum_k (F^k(q_i - q_{i-k}) - F^k(q_i - q_{i+k}))$ and the first term of (54) is an Ito integral. Using the reversibility of the equilibrium measure, i.e. $P_{\rho^0}^t = P_{\rho^0}^t\Pi$, we write,

$$\frac{dP_\mu^t}{dP_\mu^t\Pi} = \frac{dP_\mu^t}{dP_{\rho^0}^t}\frac{dP_{\rho^0}^t}{dP_\mu^t\Pi} = \exp(A^t(\xi) - A^t(\Pi\xi)) \tag{55}$$

Being invariant under the time reversal operator Π, the second term in (54) does not contribute to the difference in the above (55). The fact that the first term does not contribute is somewhat less obvious, see for instance example 3 in [19] for a proof of this fact in a similar set-up. Finally, using $\underline{F}(\underline{q}(s))\underline{p}(s) = 2MJ(s)$, we get,

$$R^t(\xi) \equiv A^t(\xi) - A^t(\Pi\xi) = \int_{-t}^t \sigma(s)ds + \beta H(\xi_{-t}) - \beta H(\xi_t), \tag{56}$$

modulo the boundary terms involving the distribution μ, this is the same as (25) with the identification $\tau = N^{-1}\nabla T(x)$, $\beta = T^{-1}(x)$ and $M = [\epsilon N]$.

5 Properties of the stationary state.

5.1 Heat conductivity and Green-Kubo formula.

We define the heat conductivity κ as

$$\kappa \equiv \lim_{\gamma \to 0} \lim_{M \to \infty} \lim_{\tau \to 0} \tau^{-1} \langle J \rangle_{\rho^\tau} \tag{57}$$

and show now that it formally coincides with the usual Green-Kubo formula for Hamiltonian systems. The Green-Kubo formula for the thermal conductivity of an Hamiltonian system is,

$$\kappa_{GK} = \lim_{M \to \infty} \frac{M}{T^2} \int_0^\infty \langle J(0) J(s) \rangle_{\rho^0} ds. \tag{58}$$

where $J(s)$ is given by (29) in terms of the coordinates $\underline{q}(s), \underline{p}(s)$, solution of the Hamiltonian *deterministic* equations (i.e (30) with $\tau = 0$ and $\gamma = 0$) with initial conditions $\underline{q}(0), \underline{p}(0)$.
As before, we assume the existence and uniqueness of a smooth (both in space and as function of τ) invariant measure for the process (30), whose density ρ^τ satisfies,

$$L^T \rho^\tau = 0 \tag{59}$$

Developping at first order in τ the density $\rho^\tau = \rho^0 + \tau \rho^1 + \ldots$, we get an equation for the first-order correction to equilibrium (at temperature T) from,

$$L^T \rho^\tau = L_0^T \rho^0 + \tau L_0^T \rho^1 + L_\tau^T \rho^0 + \ldots \tag{60}$$

and thus, formally,

$$\rho^1 = -(L_0^T)^{-1} L_\tau^T \rho^0 \tag{61}$$

We first compute $\lim_{\tau \to 0} \tau^{-1} \langle J \rangle^\tau$. Using (61) and again (34)

$$\rho^1 = -(L_0^T)^{-1} \frac{M}{T^2} J \rho^0. \tag{62}$$

Next, because the expected value of the current is zero in equilibrium and $((L_0^T)^{-1})^T = L_0^{-1}$, we get,

$$\lim_{\tau \to 0} \frac{\langle J \rangle^\tau}{\tau} = -\frac{M}{T^2} \langle J(L_0)^{-1} J \rangle_{\rho^0} = \frac{N}{T^2} \int_0^\infty \langle J(0) \langle J(s) \rangle^{\gamma,T} \rangle_{\rho^0} ds \tag{63}$$

where $\langle J(s) \rangle^{\gamma,T}$ is the solution of

$$\frac{d}{ds} \langle J(s) \rangle^{\gamma,T} = L_0 \langle J(s) \rangle^{\gamma,T} \tag{64}$$

with initial conditions $\langle J(0) \rangle^{\gamma,T} = J(0)$. Formally, the most natural thing to do is to take next the limit of $M \to \infty$ and then the limit $\gamma \to 0$ to recover the Green-Kubo formula (58). So that we get finally our definition of the conductivity (57).

Remark. The discussion of these limits is a bit delicate in the case of *anomalous* conductivity in which case one tries to evaluate the dependance in M of the conductivity κ, proceeding as we do yield $\kappa = \infty$ each time that there is anomalous conductivity. If one wishes to study the size dependance of the conductivity as for instance in [3, 23], it seems that one should take γ scaling as M^{-1} and let go $M \to \infty$. But at the moment, we do not have any justification for that particular scaling of the friction and suspect that it might be model-dependent while the definition (57) is not and does discriminate between normal and anomalous heat conduction.

5.2 Temperature profile.

We come back now to the original problem of the chain heated at its boundaries. As we have seen above, if the conductivity is finite, one may write,

$$\langle J \rangle^\tau = \kappa(T)\tau \tag{65}$$

where κ will in general depend not only on the temperature T but also on the physical parameters of interaction, in the limit of large N and small γ. As we shall illustrate in the next section on a concrete example, one obtains such a relation by simply writing down the stationary Fokker-Planck equation for the dynamics (30) and analyzing the effect of the nonlinearity on the nonequilibrium properties. But now, as we explained at the end of section 2, we do the identification $\tau = N^{-1}\nabla T(x)$, $T = T(x)$, $M = [\epsilon N]$ so that (56) is really identical to (25) . And we get,

$$\langle j_i \rangle = \langle J \rangle^\tau = \kappa(T(x))\frac{1}{N}\nabla T(x). \tag{66}$$

for $i \in B_\epsilon(x)$, the box of size ϵ around the point x. This is where one explicitly uses the assumption of equivalence between the original local dynamics (in the box $B_\epsilon(x)$) and of the dynamics (30) in the limit $\gamma \to 0$ because of their identical time-reversal property (25), (56). As we observed in (15), in the stationary state, the energy current must be constant along the chain and therefore, one gets,

$$\nabla\kappa(T(x))\nabla T(x) = 0, \tag{67}$$

away from the boundaries. The temperature profile is finally fixed by imposing the boundary conditions, which also sets the value of the current as a function of the imposed temperature difference.

6 Models for heat conduction and current degradation.

Having investigated the general properties of the stationary measure of the dynamics (30) and shown that its spacetime extension has the natural characterization (25),(56), we now study the stationary measure of a concrete model by writing down the equations that the correlation functions satisfy. As a generic model for anharmonic systems having a normal conductivity, we consider a lattice system described by the Hamiltonian,

$$H(\underline{q},\underline{p}) = \sum_{i=1}^{M}[\frac{p_i^2}{2} + \omega^2\mu^2\frac{q_i^2}{2} + \frac{\lambda}{4}q_i^4 + \frac{\omega^2}{2}(q_i - q_{i-1})^2] \tag{68}$$

and the non-equilibrium dynamics (30) with periodic b.c. becomes,

$$
\begin{aligned}
dq_i &= p_i dt \\
dp_i &= -\gamma p_i dt - \omega^2((2 + \mu^2)q_i - q_{i-1} - q_{i+1}) - \lambda q_i^3 \\
&\quad + \frac{\omega^2\tau}{2T}(q_{i+1} - q_{i-1}) + \sqrt{2\gamma T}dw_i
\end{aligned}
\tag{69}
$$

As above, one defines a local energy function,

$$h_i(\underline{p}, \underline{q}) = \frac{p_i^2}{2} + \omega^2 \mu^2 \frac{q_i^2}{2} + \frac{\lambda}{4} q_i^4 + \frac{\omega^2}{4}((q_i - q_{i-1})^2 + (q_i - q_{i+1})^2) \tag{70}$$

and the heat current in the chain j_i,

$$j_i = \frac{\omega^2}{2}(q_{i+1} - q_i)(p_i + p_{i+1}). \tag{71}$$

and because of translation invariance, we shall often use the notation,

$$j \equiv \langle j_i \rangle^\tau. \tag{72}$$

for the average microscopic current in the stationary state. Compute now the evolution of the current j_i under the Hamiltonian evolution,

$$\frac{d^h j_i}{dt} = \frac{\omega^2}{2}((p_{i+1}^2 - p_i^2) - (q_{i+1} - q_i)(\omega^2(q_i + q_{i+1}) - (q_{i+1} + q_{i+2}) - (q_{i-1} + q_i)) + \lambda(q_i^3 + q_{i+1}^3)) \tag{73}$$

As the dynamics is translation invariant, we can assume that the unique stationary measure is also translation invariant, which implies that,

$$\left\langle \frac{d^h j_i}{dt} \right\rangle^\tau = \lambda \left(\langle q_i q_{i+1}^3 \rangle^\tau - \langle q_i^3 q_{i+1} \rangle^\tau \right) \tag{74}$$

One obtains in the stationary state,

$$\frac{d}{dt} \langle j_i \rangle = \left\langle \frac{d^h j_i}{dt} \right\rangle^\tau - \gamma \langle j_i \rangle^\tau + \frac{\omega^4 \tau}{4T} \left\langle (q_{i+1} - q_{i-1})^2 \right\rangle^\tau = 0 \tag{75}$$

So that we finally get,

$$-\gamma \langle j_i \rangle^\tau + \frac{\omega^4 \tau}{4T} \left\langle (q_{i+1} - q_{i-1})^2 \right\rangle^\tau + \lambda \left(\langle q_i q_{i+1}^3 \rangle^\tau - \langle q_i^3 q_{i+1} \rangle^\tau \right) = 0 \tag{76}$$

This is the basic equation for the current. The first term is a damping term for the current, the second term is a source term for the current (as we see below) and has the same sign as the parameter τ, it comes directly from the irreversible part of the non-equilibrium dynamics, i.e it is produced by the force proportionnal to τ in (30). The last term comes from the Hamiltonian part of the dynamics. It should be responsible for the "internal" degradation of the current in case of a normal conductivity.

Harmonic case.
We look first at the harmonic case ($\lambda = 0$) and at the lowest-order in τ since we are interested in computing the heat conductivity, i.e we write,

$$-\gamma \langle j_i \rangle^\tau + \frac{\omega^4 \tau}{4T} \left\langle (q_{i+1} - q_{i-1})^2 \right\rangle^0 = 0 \tag{77}$$

where $\langle . \rangle^0$ denotes the expectation value with respect to the equilibrium harmonic measure. This last term is readily computed and (77) yield,

$$\langle j_i \rangle^\tau = \frac{\omega^2 \tau}{\gamma} \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{\sin^2(2\pi x)}{\mu^2 + 4\sin^2(\pi x)} dx \tag{78}$$

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for large N. Here the basic problem of harmonic chains is apparent, when the external friction γ is taken to zero the current becomes infinite, the harmonic chain has no internal mechanism which could degrade the current that is continuously created by the "thermal force" proportional to τ (i.e by the local temperature gradient). According to our definition, the conductivity of the harmonic model is,

$$\kappa = \lim_{\gamma \to 0} \lim_{M \to \infty} \lim_{\tau \to 0} \tau^{-1} \langle J \rangle^\tau = +\infty \tag{79}$$

Let us see now how to deal with the anharmonic interactions. Observe first that if the stationary measure was Gaussian, the conductivity of the system would be infinite, indeed under Gaussian assumption and translation invariance,

$$\left(\left\langle q_i q_{i+1}^3 \right\rangle^\tau - \left\langle q_i^3 q_{i+1} \right\rangle^\tau \right) = 3(\langle q_i q_{i+1}\rangle^\tau \left\langle q_i^2 \right\rangle^\tau - \langle q_i q_{i+1}\rangle^\tau \left\langle q_{i+1}^2 \right\rangle^\tau) = 0 \tag{80}$$

and one gets (77) again. Observe also that $\left\langle q_i q_{i+1}^3 \right\rangle^\tau - \left\langle q_i^3 q_{i+1} \right\rangle^\tau$ is odd under the exchange of the indices i and $i+1$, as is the current, by definition (71).

Stochastic approximation of the non-linearity.
The simplest possible assumption which can be made about the stationary state is to assume,

$$\left\langle q_i q_{i+1}^3 \right\rangle^\tau - \left\langle q_i^3 q_{i+1} \right\rangle^\tau = -\eta j_i \tag{81}$$

for some η. The important point is that such a term may be produced by a dynamics which amounts to randomly exchange energy between nearest-neighbours in the chain and not by an external damping term in the dynamics. This random exchange is responsible for the degradation of the current constantly produced by the "thermal force" proportional to τ. See [2] for details and rigorous results on the model. Now, (76) become

$$-\gamma \langle j_i \rangle^\tau - \eta \langle j_i \rangle^\tau + \frac{\omega^4 \tau}{4T} \left\langle (q_{i+1} - q_{i-1})^2 \right\rangle^0 = 0 \tag{82}$$

and the conductivity is,

$$\kappa = \frac{\omega^2}{\eta} \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{\sin^2(2\pi x)}{\mu^2 + 4\sin^2(\pi x)} dx, \tag{83}$$

when $\mu = 0$, one gets $\kappa = \frac{\omega^2}{2\eta}$ which is the number obtained in [2][2]. As the conductivity does not depend on the temperature T, from (67), one gets a linear profile. More sophisticated models and stochastic approximations have been devised to tackle the problem of anomalous heat conduction [3].

Closure approximation.
We refer to [15] for details about the closure approximation on the model we are considering in this section, but we give the outline of the argument. Observe that (76) involves a four-point correlation function. In order to interpret it as term providing a internal mechanism for the degradation of the current, one would like to show that it is simply proportional to the average current, namely a two-point correlation function. To achieve this, the simplest thing to do is to assume that the

---

[2]There is a slight difference coming from the fact that in [2], the definition of the current contains a part coming from the random exchange itself, for small η this becomes negligible in the computation of the conductivity.

stationary measure is Gaussian. As we observed above, this obviously factorizes the four-point correlation in terms of the two-point correlation but does not produce any significant correction to (76) with respect to the harmonic case. The next simplest thing to do is to write down the hierarchy of equations satisfied by the n-point correlation functions and assume that the six-point correlations factorize in terms of the two-point correlations. After linearizing around the equilibrium harmonic solution, this yields a linear expression of the four-point correlations in terms of the two-point correlations. The main point of the analysis is to identify the resonances in the interactions between the harmonic degrees of freedom (the phonons). To formulate the end result of the closure approximation we need to consider the general set of correlation functions,

$$\hat{J}_l \equiv \omega^2 \langle p_i q_{i+l} \rangle^\tau \tag{84}$$

the fact the RHS does not depend on i follows from translation-invariance. In particular, $\hat{J}_1 = j$. We denote by $\underline{\hat{J}}$ the vector made of the $\hat{J}_l$'s. Now, after closure, the stationary equation for this vector takes the form, for large μ,

$$-\gamma \underline{\hat{J}} - \frac{\lambda^2 T^2}{\omega^7 \mu^5} \mathcal{L}(\underline{\hat{J}}) + \underline{\sigma} = 0 \tag{85}$$

Where $\mathcal{L}$ is a linear operator which does not depend on any physical parameter entering the equations of motion. The components of the vector $\underline{\sigma}$ coming from the thermal force are given by,

$$\sigma_m = \omega^2 \tau \int_{-\frac{1}{2}}^{\frac{1}{2}} \frac{\sin(2\pi x) \sin(2\pi m x)}{\mu^2 + 4\sin^2(\pi x)} dx. \tag{86}$$

When computing $\underline{\sigma}$ we have neglected correction of order λ in the equilibrium measure has been neglected. When $\gamma \to 0$, one inverts $\mathcal{L}$ and gets,

$$\underline{\hat{J}} = \frac{\omega^7 \mu^5}{\lambda^2 T^2} \mathcal{L}^{-1}(\underline{\sigma}) \tag{87}$$

from which one may obtain $\hat{J}_1 = j$ and thus the conductivity which is (for large μ)

$$\kappa = \alpha \frac{\omega^9 \mu^3}{\lambda^2 T^2} \tag{88}$$

The value of $\alpha = 0.275637$ was computed in [1] where the expression (3) was also tested and numerically confirmed. As for the temperature profile, one gets,

$$\nabla \frac{1}{T^2(x)} \nabla T(x) = 0 \tag{89}$$

away from the boundaries. The solution of (89) and the problem of its boundary conditions has been discussed in [1].

Finally, we note once again that our method is not limited to the example we are treating here. Each model will have a particular source term in the equation governing the degradation of the current. This source term can be directly computed from the dynamics (30). In particular, it would be very interesting to study the heat conductivity of the Toda lattice with this method, which we plan to do in a future publication.

7 Appendix: Solution of the Harmonic case.

We take the process defined by (69) with $\lambda = 0$ and solve the equations for the correlations in the stationary state.

It is most convenient to work in coordinates where the equations become diagonal, and we introduce the Fourier coordinates for the periodic harmonic chain by

$$Q_k = \frac{1}{\sqrt{N}} \sum_{j=1}^{N} e^{i\frac{2\pi}{N}kj} q_j \tag{90}$$

with $-N/2+1 \le k \le N/2$. The P_k coordinates are defined in a similar fashion. We note for further purposes that $\overline{Q}_k = Q_{-k}$ and $\overline{P}_k = P_{-k}$. In those coordinates, the Hamiltonian reads,

$$H(\underline{Q}, \underline{P}) = \sum_{k=-N/2+1}^{N/2} [\frac{|P_k^2|}{2} + \omega_k^2 \frac{|Q_k|^2}{2}] \tag{91}$$

where

$$\omega_k^2 = \omega^2(\mu^2 + 4\sin^2(\frac{\pi k}{N})) \tag{92}$$

The spatial average of the energy current in the periodic chain (29) reads now

$$J = \frac{1}{4N} \sum_{k=-N/2+1}^{N/2} \omega(\frac{\pi k}{N})\omega'(\frac{\pi k}{N}) \operatorname{Im}(Q_{-k}P_k) = \frac{1}{N} \sum_{k=-N/2+1}^{N/2} \sin(\frac{2\pi k}{N}) \operatorname{Im}(Q_{-k}P_k). \tag{93}$$

In Fourier coordinates, the equations (69) with $\lambda = 0$ become,

$$dQ_k = P_k dt \tag{94}$$

$$dP_k = -\gamma P_k dt - (\omega_k^2 - i\frac{\tau}{T}\sin(\frac{2\pi k}{N}))Q_k dt + \sqrt{2\gamma T}dW_k \tag{95}$$

The W_k are complex Wiener processes which satisfy $\overline{W}_k = W_{-k}$ and, $\langle W_k, W_l \rangle = \delta(l+k)$.

The equations for the correlations in the stationnary state are,

$$\langle P_k Q_{-k} \rangle + \langle Q_k P_{-k} \rangle = 0 \tag{96}$$

$$\left\langle |P_k|^2 \right\rangle - \omega_k^2 \left\langle |Q_k|^2 \right\rangle = 0 \tag{97}$$

$$2\gamma \left\langle |P_k|^2 \right\rangle + i\omega_k^2 \alpha_k \frac{\tau}{T} \langle P_k Q_{-k} \rangle = 2\gamma T \tag{98}$$

$$2\gamma \langle P_k Q_{-k} \rangle - i\omega_k^2 \alpha_k \frac{\tau}{T} \left\langle |Q_k|^2 \right\rangle = 0 \tag{99}$$

where $\alpha_k = 2\omega^2 \omega_k^{-2} \sin(\frac{2\pi k}{N})$. These are readily solved and yield

$$\left\langle |P_k|^2 \right\rangle = \delta_k T \tag{100}$$

$$\langle P_k Q_{-k} \rangle = \tfrac{1}{2}\gamma^{-1} i \delta_k \alpha_k \tau \tag{101}$$

with, $\delta_k = (1 + \frac{\omega_k^2 \alpha_k^2 \tau^2}{4\gamma^2 T^2})^{-1}$. Keeping the lowest-order in τ and doing a little computation gives (78) again.

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