Abstract

It is argued that a Gibbsian formula for the space-time distribution of microscopic trajectories of a nonequilibrium system provides a unifying framework for recent results on the fluctuations of the entropy production. The variable entropy production is naturally expressed as the time-reversal symmetry breaking part of the space-time action functional. Its mean is always positive. This is both supported by a Boltzmann type analysis by counting the change in phase space extension corresponding to the macrostate as by various examples of nonequilibrium models. As the Gibbsian set-up allows for non-Markovian dynamics, we also get a local fluctuation theorem for the entropy production in globally Markovian models. In order to study the response of the system to perturbations, we can apply the standard Gibbs formalism.

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1 Introduction

A rough and ready distinction between nonequilibrium phenomena can be made by asking whether the system is in a transient state relaxing towards equilibrium or whether the system is in a steady nonequilibrium state. That can depend on the level of description and on the relevant length, time and energy scales. In what follows, we mostly have in mind the ideal steady state scenario where a spatially extended system is driven away from equilibrium via some external forcing or via contacts with unequal reservoirs through which a current is
maintained in the system. This is a vast area of research with many beautiful models and results but it is also characterized by a lack of general guiding principles. This in contrast with equilibrium statistical mechanics where elementary questions (such as to do with the positivity of certain response functions, their relation with fluctuations, weak coupling expansions, etc.) have a general answer mostly because of the power and the generality of the underlying Gibbs formalism. The next section proposes to extend the domain of application of this Gibbs formalism to nonequilibrium situations. First we will state the main ideas in a somewhat formal way and then we will discuss examples and some of the consequences for typical models of nonequilibrium statistical mechanics. This paper is a continuation of [36]; we have discussed other examples and general consequences in [37, 38, 40, 39, 41]. The main motivation and source of inspiration have been on the one hand to try to understand the work of Gallavotti-Cohen in [19, 20] on a general symmetry in the fluctuations of the phase space contraction rate for certain strongly chaotic reversible dissipative dynamical systems, in particular, to interpret their so called chaoticity hypothesis, and on the other hand to apply the theory of space-time Gibbs measures that was started more than a decade ago for probabilistic cellular automata and that has since then been developed way beyond, [1, 7, 23, 25, 44].

2 Main ideas

2.1 Gibbsian hypothesis

By definition, in equilibrium, every region is in equilibrium with the rest of the system. If we imagine a subregion in our big equilibrium system, then we will see there the same equilibrium state as outside for the same microscopic interaction. Mathematically, this can be readily seen from the form \( \exp[-\beta H] \) for equilibrium distributions (here in thermal equilibrium at inverse temperature \( \beta \) for the local and additive microscopic interaction Hamiltonian \( H \)). To be specific, think of the Ising model in the square \( V \) and compute the expectation of a function \( f \) that only depends on the spins \( \sigma_\Lambda \) inside the smaller square \( \Lambda \):

\[
\langle f(\sigma_\Lambda) \rangle_V = \frac{1}{Z_\Lambda(\beta, \sigma_{\partial\Lambda})} \sum_{\sigma_\Lambda} f(\sigma_\Lambda) e^{-\beta H_\Lambda^{\sigma_\Lambda}(\sigma_\Lambda)}
\]  

with \( \sigma_{\partial\Lambda} \) the spin configuration on the external boundary of \( \Lambda \). To appreciate is that the Hamiltonian \( H_\Lambda^{\sigma_{\partial\Lambda}}(\sigma_\Lambda) = H_\Lambda(\sigma_\Lambda) + W_{\partial\Lambda}(\sigma_\Lambda, \sigma_{\partial\Lambda}) \) is just changed at the boundary of \( \Lambda \): \( H_\Lambda \) contains the bulk contribution and \( W_{\partial\Lambda} \) contains the interaction of the spins inside \( \Lambda \) with those outside; for any two boundary conditions \( \sigma_{\partial\Lambda} \) and \( \sigma'_{\partial\Lambda} \), \( |H_\Lambda^{\sigma_{\partial\Lambda}} - H_\Lambda^{\sigma'_{\partial\Lambda}}| \leq c|\partial\Lambda| \). Moreover, upon specifying the boundary condition \( \sigma_{\partial\Lambda} \) the inside and the outside of the region are decoupled. A more general formulation of this is known as the Dobrushin-Lanford-Ruelle equation, see e.g. [12], pages 891–956, for a mathematical introduction to the Gibbs formalism in equilibrium statistical mechanics. Now to nonequilibrium steady states. There is no reason to expect that in general the stationary state, that is the time-invariant distribution, can be described via a sufficiently local Hamiltonian. Even if it is, there does not seem to exist a systematic way of finding it. Typically, if we apply a time-independent constraint (like fixing a rod in running water), we will, unlike in equilibrium,
greatly perturb the system. Think however of letting the rod go with the water. It will do whatever the currents are telling it to do. In order to specify these currents, or, to say how fast what amount of a certain quantity is transported to where, we need space-time. Thus take a space-time window $\Lambda \times [-\tau, \tau]$. If we specify at its borders whatever went inside or outside at what pace, we can expect that the inside is effectively decoupled from the outside, just as in equilibrium. We conclude that the space-time distribution of nonequilibrium steady states may well be sharing the Gibbsian features of equilibrium states.

It is interesting to compare the situation with what happens in the low temperature phases of the two-dimensional Ising model. We can think of it as a space-time distribution corresponding to a 'dynamics' formally specified by the transfer matrix. But the restriction of say the low temperature plus phase to a one-dimensional layer is not a Gibbs distribution for any uniformly and absolutely summable interaction potential, see [51]. That would correspond to the time-invariant or stationary state. There are ways here to restore its Gibbsian characterization by slightly extending the definition of Gibbs measure (as was for example done in [42]) but it remains unclear what aspects of the Gibbsian formalism remain valid and, more to the point, there does not seem an easy way to generalize this in any systematic way. One could object that this Ising example has a major defect as its ‘dynamics’ (imposed by the transfer matrix) is highly nonlocal. There are other examples for a strictly local dynamics, such as in [32] for the voter model, where the invariant measures are not Gibbsian. Yet, the point is that while it is mostly easily seen that the space-time distribution is Gibbsian for some local space-time action functional that can be explicitly constructed from the dynamics, it is in general very hard to get the same thing for the projection on a fixed time layer, that is, for the corresponding invariant distribution. Another mathematical analogy is to think of the difference between the Hamiltonian and the Lagrangian set-up in mechanics.

We now add some formulas. We consider a system in a volume $V$ which is observed over a time-interval $[-\tau, \tau]$. At each time, we have the same microscopic phase space $K$ and a trajectory is denoted by $\omega = (\omega_t, t \in [-\tau, \tau]), \omega_t \in K$; $\omega$ is the history of the microscopic degrees of freedom (for example containing the positions and momenta of all the particles in a box over a certain time-interval). We prepare the system at time $-\tau$ in some macrostate corresponding to a probability distribution $\rho$ on $K$. We write $P = P_\rho$ for the probability distribution of the trajectories $\omega$ given that it started as sampled from $\rho$. How to get this distribution $P$ is another question on which we will soon come back below. Under the Gibbsian hypothesis we assume that $P_\rho$ has a density with respect to a corresponding equilibrium distribution $P_o = P_{o,\rho}$ given as

$$dP(\omega) = e^{-A(\omega)} dP_o(\omega) \quad (2.2)$$

where $A(\omega)$ is the space-time action-functional; it will contain space-time integrals over the microscopic trajectories. The nonequilibrium distribution $P$ is obtained from the equilibrium distribution $P_o$ by adding some external forces or couplings to reservoirs with different thermodynamic parameters. There are various ways then to obtain (2.2). Given a particular dynamics describing an open system it is in general easy to construct $A$ explicitly (modulo space-time boundary terms) and this is what we will illustrate in the next section. We get
the form
\[ A(\omega) = \ln \rho_0(\omega) - \ln \rho(\omega) + \mathcal{H}(\omega) \] (2.3)
where \( \rho, \rho^0 \) are the initial data (at time \(-\tau\)) for the nonequilibrium, respectively, the equilibrium process and the form of \( \mathcal{H} \) depends only on the dynamics. Most important is that \( \mathcal{H} \) is local, and approximately additive for a spatially extended local dynamics. In this way, \( \mathcal{H} \) is like a Hamiltonian in equilibrium statistical mechanics but here for space-time trajectories. In case we consider a steady state process, then \( \rho \), respectively, \( \rho^0 \) should be taken as stationary (i.e., time-invariant) distributions under the nonequilibrium and the equilibrium dynamics. It may seem problematic to assume in general that stationary states have a density with respect to some a priori flat measure, i.e., that they are absolutely continuous with respect to some analogue of the Lebesgue measure on \( K \). In fact, all that is really required here is a local absolute continuity with respect to the Lebesgue measure; since we have in mind macroscopic systems where the macrovariables correspond to sums of local functions, we have every reason to expect that the distribution on \( K \) inferred from their values will indeed have a density.

On the other hand, from the formula (2.2), it is suggestive to forget altogether about the specific dynamics and to concentrate on \( A \) instead. Each \( A \) gives rise to some type of dynamics but it need not be Markovian. The specific form of \( A \) then defines the nonequilibrium model.

The connection between Gibbs measures and nonequilibrium dynamics is not new; the theory has been worked out into considerable detail for various situations, see [25, 44, 36, 30, 7, 1, 23] for examples.

### 2.2 Time-reversal

We are used to forget about time when dealing with equilibrium statistical mechanics. One reason is that, for classical systems, the momenta (entering only in the kinetic energy part of the Hamiltonian) can be integrated out at once from the partition function. Time enters more explicitly in equilibrium dissipative dynamics such as via Langevin equations or Glauber dynamics. Yet, under the condition of detailed balance, the stationary dynamics is microscopically reversible and the past cannot be distinguished from the future. One essential feature of nonequilibrium is that time-reversal invariance is broken.

The time-reversal operation \( \Theta \) acts on path space and it consists of two parts. The first part \( \pi \) is purely kinematical and depends on the nature of the dynamical variables; the second part is just the reflection of the time-axis \( t \to -t \).

So if \( \omega = (\omega_t, t \in [-\tau, \tau]) \) is a trajectory, then its time-reversal is \( \Theta \omega \) with \( (\Theta \omega)_t = \pi \omega_{-t} \) where \( \pi \) is an involution on phase space (for example reversing the sign of the momenta). Since the violation of microscopic reversibility is so essential to the presence of currents and nonequilibrium conditions, it must be clear that important information must be written in the symmetry breaking part \( \Delta \mathcal{H}(\omega) \equiv \mathcal{H}(\Theta \omega) - \mathcal{H}(\omega) \) of the space-time Hamiltonian (2.3). Or, in terms of the Gibbsian distribution \( P = P_\rho^\tau \),

\[ dP_\rho^\tau(\omega) = e^{R_\rho^\tau(\omega)} dP^\tau_{\rho^0, \pi} \Theta(\omega) \] (2.4)

We have the notation \( P^\tau_{\rho^0, \pi} \) for the distribution of the trajectories started at time \(-\tau\) in the state \( \rho_{\tau, \pi} \) where \( \rho_{\tau} \) corresponds to the macrostate in which we
ended up at time \( \tau \) when started at time \(-\tau\) in \( \rho \). More explicitly, from \(2.3\),

\[
R_\rho(\omega) = -\ln \frac{\rho_\tau(\omega_\tau)}{\rho^0(\omega_{\tau})} + \ln \frac{\rho(\omega_{-\tau})}{\rho^0(\omega_{-\tau})} + \Delta \mathcal{H}(\omega) \tag{2.5}
\]

It is physically more convenient to decompose \(\Delta \mathcal{H}\) a bit further and to write

\[
R_\rho(\omega) = -\ln \rho_\tau(\omega_\tau) + \ln \rho(\omega_{-\tau}) + \Delta S_e \tag{2.6}
\]

where \(\Delta S_e\), as we will illustrate, corresponds to the change of entropy in the external world (baths). We will see it in the explicit formula \(3.21\) in example 3.2. As for \(\mathcal{H}\), also \(\Delta \mathcal{H}\) will be a space-time integral of local interaction terms.

This object has some remarkable properties. In fact we will argue in the next section via examples and in Section 4 via some theoretical considerations that \(R_\rho\) is the total variable (space-time-integrated) entropy production but before, there are some simple mathematical facts that are worth observing. First of all, its mean equals

\[
\dot{S}(\rho) \equiv \frac{1}{2} \frac{dR_\rho}{d\tau}(\tau = 0) \tag{2.8}
\]

That is a relative entropy: the path space expectation of the logarithm of the density of that same path space measure with respect to the time-reversed process started at \(\rho_\tau\). We can also look at \(2.7\) as a functional on the fixed time distributions \(\rho\). By making \(\tau\) very small, we then get the entropy production in the transient state \(\rho\). It is thus natural to define the mean entropy production rate in \(\rho\) as

\[
\langle R \rangle = \int dP(\omega) R(\omega) = S(P|P_\Theta) \geq 0 \tag{2.9}
\]

where the right hand side is the relative entropy between the forward and the backward distribution: formally (and in most cases to be understood via a sequence of space-windows),

\[
s(P|P_\Theta) \equiv \int dP(\omega) \ln \frac{dP}{dP_\Theta}(\omega)
\]

It is this quantity that turns out to be the steady state mean entropy production: it is always non-negative and is zero if and only if the dynamics is microscopically reversible (detailed balance). Of course for spatially extended systems \(R\) is an extensive quantity and when divided by the spatial volume, it will take on a definite limiting value as a consequence of the law of large numbers. So its positivity is typical and not only an averaged property.

For the fluctuations we have, almost immediately since \(R(\Theta \omega) = -R(\omega)\),

\[
\int dP(\omega)e^{-zR(\omega)} = \int dP(\omega)e^{-(1-z)R(\omega)} \tag{2.10}
\]
for all complex numbers $z$. This is both for its derivation and for its possible applications very much like a Ward identity (with respect to a discrete symmetry), see e.g. $[52]$. A similar symmetry for the fluctuations of the time-averaged phase space contraction in the so called SRB-measure for a class of strongly chaotic dynamical systems was first observed in $[8]$ and derived in $[19, 20, 22, 49]$. Upon differentiating (2.10) with respect to $z$ and with respect to the parameters hidden in the distribution $P$, we obtain exact relations between space-time correlations. Such derivations have already been explored in $[15, 33, 36]$. This would not be very useful if it were not that the same symmetry remains valid also for local fluctuations. The search for a local fluctuation theorem already started in $[2, 17, 36, 21]$ and a systematic theoretical answer was developed in $[39]$. It is the Gibbsian set-up that saves us: if we take the restriction $P_\Lambda$ of $P$ to a space-time window $\Lambda \times [-\tau, \tau]$ and if we apply the time-reversal $\Theta_\Lambda$ only there, then, by definition, for all functions $f$ of the trajectory in $\Lambda \times [-\tau, \tau]$

$$\int dP(\omega) f(\Theta \omega) = \int dP(\omega) f(\omega) e^{-R_\Lambda(\omega)}$$

(2.11)

where

$$R_\Lambda(\omega) \equiv \ln \frac{dP_\Lambda}{dP_{\Lambda\Theta_\Lambda}}(\omega)$$

and $P_\Lambda \Theta_\Lambda = (P \Theta)_\Lambda$. Therefore, by substituting $f(\omega) = \exp[zR_\Lambda(\omega)]$ in (2.11), we get a local version of (2.10). The important point is now that, due to the locally additive character of $R$, its restriction to $\Lambda$ is exactly equal, modulo space-time boundary terms, to $R_\Lambda$ so that we really get control over the local fluctuations of the entropy production. The only assumption here is that whenever the restriction of a trajectory $\omega$ to $\Lambda \times [-\tau, \tau]$ has positive probability to occur, then the restriction of its time-reversal $\omega \Theta$ to $\Lambda \times [-\tau, \tau]$ is also possible (has positive probability). This is a condition of dynamic reversibility which should not be confused with microscopic reversibility under which the two probabilities would be exactly equal!

We can continue a bit more with (2.11). Suppose we condition the left hand side on a particular value $r$ of the entropy production

$$\langle f(\Theta) | R_\Lambda = r \rangle = \langle f | R_\Lambda = -r \rangle$$

so that, for fixed entropy production in $\Lambda$, the time-reversal operation can be exchanged with conditioning on the opposite entropy production. The local arrow of time is thus decided by the sign of the local entropy production. A similar point was made for the phase space contraction in strongly chaotic dynamical systems in $[13]$.

Finally, another consequence of (2.11) is that by Jensen’s inequality, when $f$ is positive,

$$\langle R_\Lambda \rangle_f \geq \ln \frac{\langle f \rangle}{\langle f(\Theta) \rangle_f}$$

(2.12)

where $\langle R_\Lambda \rangle_f \equiv \langle fR_\Lambda \rangle / \langle f \rangle$ is the expected local entropy production when $P$ is perturbed by the insertion of an extra density $f$. One choice takes $f = R_\Lambda^{n}$ with $n$ even, for which (2.12) implies that $\langle R_\Lambda^{n+1} \rangle \geq 0$ for all $n$. Similar relations can be derived for the transient entropy production. We restrict
us here to the analogue of (2.10) for $z = 1$. We have with no extra effort, upon substituting (2.6),
\[
\int dP^\tau(\omega)e^{-[\ln \rho^\tau(\omega\tau)+\ln \rho(\omega_{-\tau})+\Delta S_e(\omega)]=1}
\]
(2.13)

which expresses just the normalization of the distribution $P^\tau_\rho$. An interesting possibility is that $\rho(\eta) = \exp -\beta H_i(\eta)/Z_i$ and $\rho^\tau(\eta) = \exp -\beta H_f(\eta)/Z_f$ are initial and final equilibrium states at the same inverse temperature $\beta$ but for a different Hamiltonian. As a physical mechanism we can consider the system coupled to a heat bath at constant temperature $T = 1/\beta$ where some parameters (e.g. interaction coefficients) in the interaction of the components of the system are changed. This means that the Hamiltonian $H(t) \equiv H(\lambda(t), \eta)$ is time-dependent and $H_f(\eta) \equiv H(\lambda(\tau), \eta), H_i(\eta) \equiv H(\lambda(-\tau), \eta)$. To change the parameter $\lambda$ from $\lambda(-\tau)$ to $\lambda(\tau)$ some heat must flow from the bath into the system so that the change of entropy of the bath equals $\Delta S_e = -\beta[H_f(\eta_\tau) - H_i(\eta_{-\tau}) - W_\tau]$ where $W_\tau$ is the irreversible work done over the time $[-\tau, \tau]$. The identity (2.13) then becomes
\[
\frac{Z_f}{Z_i} = \int dP^\tau(\omega)e^{-\beta W_\tau}\omega
\]
and the left hand side is the exponential of a change in equilibrium free energy. A similar relation was discussed in [5, 6, 26, 27, 40] where it is also connected with a fluctuation identity for the transient nonequilibrium regime, [9, 3]. The next section illustrates some of the above for some typical models of nonequilibrium statistical mechanics.

3 Examples
We concentrate here on some aspects of two standard models of nonequilibrium physics. More examples of parts of the theory above can be found in [40].

3.1 Reaction-Diffusion process
In a microscopic version of a reaction-diffusion system, particles can disappear or be created on the sites of a regular lattice and they can hop to nearest neighbor vacancies; see [4] for a technical introduction.

We consider variables $\eta(i) = 0, 1$ on the sites $i$ of the square lattice $\mathbb{Z}^2$. We interpret it as meaning that site is empty or occupied by a particle. The phase space is $K = \{0, 1\}^V$ where $V$ is a large square of side length $N$ centered around the origin. The dynamics consists of a reaction part: $\eta \rightarrow \eta^i$ where $\eta^i$ is identical to $\eta$ except that the occupation at the site $i$ is flipped and a diffusion part: $\eta \rightarrow \eta^j$ where $\eta^j$ is the new configuration obtained by exchanging the occupations at sites $i$ and $j$; we take periodic boundary conditions on $V$. We get a driven lattice gas by adding an external field $E > 0$ giving a bias for particle hopping in a certain direction. In formula: first, the probability per unit time to flip from a configuration $\eta$ to the new $\eta^i$ is
\[
c(i, \eta) = \gamma_+ (1 - \eta(i)) + \gamma_- \eta(i)
\]
where $\gamma_+$ is the rate for the transition $0 \rightarrow 1$ and $\gamma_-$ is the rate for $1 \rightarrow 0$. Secondly, the hopping rates over a nearest neighbor pair $\langle ij \rangle$ in the horizontal direction, $i = (i_1, i_2), j = (i_1 + 1, i_2)$:

$$c(i, j, \eta) = e^{E/2}\eta(i)(1 - \eta(j)) + e^{-E/2}\eta(j)(1 - \eta(i))$$

The hopping rate in the vertical direction is symmetric (put $E = 0$ in the above if $j = (i_1, i_2 \pm 1)$). Taking $E$ large, typically, many more particles will be jumping to the right than to the left. In the absence of reaction rates, that is for $\gamma_\pm = 0$, we recover the so called asymmetric exclusion process and particle number is strictly conserved. The stationary state $\rho$ is a product state with uniform density equal to $\gamma_+/\gamma_- + \gamma_+$ corresponding to a chemical potential $\ln \gamma_+ / \gamma_-$ of the particle reservoir.

As reference equilibrium process $P_\alpha$, we take the same model with $E = 0$ and we can take $\rho^\alpha = \rho$. Consider now a trajectory $\omega = (\omega_t, t \in [-\tau, \tau])$. It is then easy to find (2.2) with

$$A(\omega) = -E \sum_{i \in V} \sum_{-\tau \leq t \leq \tau} \omega_t(i)(1 - \omega_t(j)) - \omega_t(j)(1 - \omega_t(i))$$

$$+ \int_{-\tau}^\tau dt \sum_{i \in V} (e^{E/2} - 1)\omega_t(i)(1 - \omega_t(j)) + (e^{-E/2} - 1)\omega_t(j)(1 - \omega_t(i))$$

where $j = (i_1 + 1, i_2)$, the right neighbor of $i = (i_1, i_2)$ and the first sum is over all jump times over the bond $\langle ij \rangle$ in the trajectory $\omega$. Applying the time-reversal $\Theta\omega_i = \omega_{-i}$ we compute that here

$$R(\omega) = \Delta H(\omega) = E \sum_{i \in V} J^i_\tau(\omega)$$

where $J^i_\tau$ is the time-integrated microscopic current over a fixed nearest neighbor pair $\langle ij \rangle$, with $j = (i_1 + 1, i_2)$ to the right of $i$. Explicitly,

$$J^i_\tau(\omega) = \sum_{-\tau \leq t \leq \tau} [\omega_t(i)(1 - \omega_t(j)) - (1 - \omega_t(i))\omega_t(j)]$$

where again the sum is over all jump times $t$ for the bond $\langle ij \rangle$. In other words $\Delta H$ is the variable work done on our system by the external field over the time-interval $[-\tau, \tau]$. Its average in the stationary state equals (up to a temperature factor) the heat dissipated in the environment. In fact we can compute this:

$$\langle \Delta S_c \rangle = \Delta H = 4\tau|V| E \sinh(E/2) \frac{\gamma_+ \gamma_-}{(\gamma_+ + \gamma_-)^2} > 0$$

Let us now fix a rectangle $\Lambda = \{(i_1, i_2) \in V : i_1 = 1, \ldots, \ell, i_2 = 1, \ldots, n\}$ of height $n$ and width $\ell$. To study the fluctuations of the work restricted to $\Lambda$, we follow the set-up of Section 2, equation (2.11), and we introduce the local time-reversal operator $\Theta_\Lambda$ for which $(\Theta_\Lambda \omega)_i = \omega_{-i}(i)$ if $i \in \Lambda$; the other occupation variables are left unchanged. To compute the $R_\Lambda$ of (2.11) we note that the restriction $P_{E,\Lambda}$ of the steady state $P = P_E$ to the volume $\Lambda$ satisfies

$$P_{E,\Lambda}\Theta_\Lambda = (P_E\Theta)_\Lambda = P_{-E,\Lambda}$$
so that (2.11) is verified with
\[
R_\Lambda = \ln \frac{dP_{E,\Lambda}}{dP_{-E,\Lambda}}
\]
Here is the bulk of the formula
\[
R_\Lambda = E \sum_{i \in \Lambda: (i_1+1, i_2) \in \Lambda} J_{\tau}^i \pm c(n + \ell)\tau
\] (3.16)

We have not written out the correction term; we refer to [39] for details and proofs; the important thing is that this correction is of the order of the boundary of \(\Lambda\) times \(\tau\) and the factor \(c\) depends on the field \(E\) and on the chemical potential but it is independent of the big volume \(V\). The first term in \(R_\Lambda\) is of the order of the volume and it is the variable work done on the system in \(\Lambda\) over the time-interval \([-\tau, \tau]\). The main contribution to \(R_\Lambda\) is thus exactly the restriction of (3.15) to \(\Lambda\), as announced in Section 2 (following the identity (2.11)). For the proof of the resulting local fluctuation theorem we refer to [39]. There is one aspect, the analogue of (2.1), that is essential. Suppose we want to compute the expectation at time \(t\) of a function \(f\) that only depends on the particle configuration in \(\Lambda\) given the history of that configuration. That is
\[
\langle f(\omega_t(i), i \in \Lambda) | \omega_s(j) = \eta_s(j), j \in \Lambda, s \leq t - \delta \rangle
\]
Clearly, the evolution restricted to \(\Lambda\) is no longer Markovian, but what are the rates for the elementary transitions, that is taking \(\delta\) very small in the above expectation? The answer is that all the rates remain unchanged except at the boundary. So the restricted process has the same transition rates in the bulk of \(\Lambda\) just as we saw before in (2.1) that in equilibrium the Hamiltonian is unchanged for the restriction to \(\Lambda\).

### 3.2 Nonequilibrium crystal

The previous example was a bulk driven lattice gas. We now take a surface (thermally) driven Hamiltonian system. For large integer \(N\) we consider a linear crystal \(L_N \equiv \{-N, \ldots, 0, \ldots, N\}\) where each site \(i \in L_N\) carries a particle with momentum \(p_i\) and position \(q_i\) (real variables). The Hamiltonian is
\[
H_N(p, q) = \frac{1}{2} \sum_{i=-N}^{N} p_i^2 + U_N(q)
\] (3.17)
with a nearest neighbor potential
\[
U_N(q) = \sum_{i=-N}^{N} V_i(q_i) + \sum_{i=-N}^{N-1} \lambda_i \Phi(q_i - q_{i+1}).
\]
Here we will not care about exposing conditions on the potential which are needed for what follows; the harmonic crystal would correspond to a quadratic potential.

The proposed dynamics is stochastic and generated by Hamilton’s equations of motion in the bulk and by Langevin equations at the boundaries:
\[
dq_i = p_i dt, i \in L_N
\]
\[
\begin{align*}
    dp_i &= -\frac{\partial U_N}{\partial q_i}(q)dt, \ i = -N + 1, \ldots, N - 1 \\
    dp_{-N} &= -\frac{\partial U_N}{\partial q_{-N}}(q)dt - \gamma_{-N}p_{-N}dt + \sqrt{\frac{2\gamma}{\beta_{\ell}}}dW_{\ell} \\
    dp_N &= -\frac{\partial U_N(q)}{\partial q_N}(q)dt - \gamma_{N}p_{N}dt + \sqrt{\frac{2\gamma}{\beta_{r}}}dW_{r}
\end{align*}
\]

where \(\gamma > 0\) and \(\beta_{\ell}, \beta_{r}\), respectively, are the inverse temperatures at the left and the right end of the chain. \(W_{\ell}\) and \(W_{r}\) are independent standard Wiener processes (Itô sense).

\(L_N\) is the generator of the dynamics:

\[
L_N \equiv p \cdot \nabla_q - \nabla_q U_N \cdot \nabla_p - \gamma_{-N} \frac{\partial}{\partial p_{-N}} - \gamma_{N} \frac{\partial}{\partial p_N} + \frac{\gamma_{-N}}{\beta_{\ell}} \frac{\partial^2}{\partial p_{-N}^2} + \frac{\gamma_{N}}{\beta_{r}} \frac{\partial^2}{\partial p_N^2}
\]

Note that if \(\beta_{\ell} = \beta_{r} = \beta\), then the Gibbs measure on \(\mathbb{R}^{4N+2}\) with density

\[
\rho^*(p, q) \equiv \frac{1}{Z_N} e^{-\beta H_N(p, q)}
\]

is reversible in the sense that when \(\beta_{\ell} = \beta_{r} = \beta\), then \(L_N^* = \pi L_N \pi\) on \(L^2(\rho^*)\) where \(\pi f(p, q) \equiv f(-p, q)\).

We are interested in the case \(\beta_{\ell} < \beta_{r}\). We assume that the interaction \(U_N\) is sufficiently well behaved to allow for a unique stationary measure with a smooth density with respect to \(dpdq\). To actually prove this, requires some specific assumptions on the potential; here we take this for granted and we refer to \([10, 11]\) for mathematical results. We denote this unique stationary measure by \(\rho\). The corresponding (stationary) path space measure \(\pi\) in the time-interval \([-\tau, \tau]\) is the law of the stationary Markov diffusion process \(\omega \equiv (\omega(t) \equiv (p(t), q(t)), t \in [-\tau, \tau])\) described by the dynamics above with invariant measure \(\rho\). In this nonequilibrium steady state heat will flow from the left end (hot) to the right (cold) and entropy will be produced. This nonequilibrium model has frequently appeared, see \([45, 48]\) for the harmonic crystal, and see \([10, 11]\) for anharmonic examples.

In order to describe the process \(\pi\) via a space-time action functional \(A\), as in \((2.2)-(2.3)\), we need a reference process. In fact there are many choices. Consider the dynamics

\[
\begin{align*}
    dq_i &= p_i dt, \ i \in L_N \\
    dp_i &= -\frac{\partial U_N}{\partial q_i}(q)dt, \ i = -N + 1, \ldots, N - 1 \\
    dp_{-N} &= -\frac{\partial U_N}{\partial q_{-N}}(q)dt - \gamma_{-N}p_{-N}dt + \sqrt{\frac{2\gamma}{\beta_{\ell}}}dW_{\ell} \\
    dp_N &= -\frac{\partial U_N(q)}{\partial q_N}(q)dt - \gamma_{N}p_{N}dt + \sqrt{\frac{2\gamma}{\beta_{r}}}dW_{r}
\end{align*}
\]

where the only difference with the original dynamics sits in the drift term by the insertion of factors \(\kappa_{-N}, \kappa_{N} > 0\). If we choose \(\beta_{\ell}\kappa_{-N} = \beta_{r}\kappa_{N} = \beta\), then this reference process \(\pi\) is reversible with respect to the same stationary measure.
\( \rho^\circ \) as before with \( \beta_\ell = \beta = \beta_r \). These laws are mutually absolutely continuous and, applying the Girsanov formula (taking it from [35]), we find for (2.2)-(2.3):

\[
dP(\omega) = \frac{\rho(\omega_{-\tau})}{\rho^\circ(\omega_{-\tau})} e^{-\mathcal{H}(\omega)} dP_\circ(\omega)
\]

where

\[
- \mathcal{H}(\omega) = \frac{1}{2} \int_{-\tau}^{\tau} \left((\beta - \beta_\ell)p_{-N}(t) dp_{-N}(t) + (\beta - \beta_r)p_N(t) dp_N(t)\right)
\]

\[
+ \frac{\beta - \beta_\ell}{2} \int_{-\tau}^{\tau} \frac{\partial U_N}{\partial q_{-N}}(q(t)) p_{-N}(t) dt + \frac{\beta - \beta_r}{2} \int_{-\tau}^{\tau} \frac{\partial U_N}{\partial q_N}(q(t)) p_N(t) dt
\]

\[
+ \frac{\gamma}{4} \int_{-\tau}^{\tau} dt ((\beta_{\kappa_{-N}} - \beta_\ell)p_{-N}(t)^2 + (\beta_{\kappa_N} - \beta_r)p_N(t)^2)
\]

Write \( \Theta_{\omega} \) for the time-reversal of the trajectory \( \omega \), that is: if \( ((p(t), q(t)), t \in [-\tau, \tau]) \), then \( \Theta_{\omega} = ((-p(-t), q(-t)), t \in [-\tau, \tau]) \). In order to obtain (2.4)-(2.6), we must compute \( \Delta \mathcal{H} \equiv \mathcal{H}\Theta - \mathcal{H} \), the relative action under time-reversal of \( P \). The result is

\[
\Delta \mathcal{H}(\omega) = (\beta - \beta_\ell) \int_{-\tau}^{\tau} (p_{-N}(t) \circ dp_{-N}(t) + \frac{\partial U_N}{\partial q_{-N}}(q(t)) p_{-N}(t) dt)
\]

\[
+ (\beta - \beta_r) \int_{-\tau}^{\tau} (p_N(t) \circ dp_N(t) + \frac{\partial U_N}{\partial q_N}(q(t)) p_N(t) dt)
\]

where the stochastic integral (indicated by the \( \circ \)) is now in the Stratonovich-sense. Finally, we have (2.4)-(2.4) with

\[
R(\omega) = -\ln \rho(\omega_{\tau}) - \ln \rho(\omega_{-\tau}) - \beta_\ell \frac{1}{2} p_{-N}^2(\tau) - \frac{1}{2} h_{-N}(\tau)
\]

\[
+ \int_{-\tau}^{\tau} \frac{\partial U_N}{\partial q_{-N}}(q(t)) p_{-N}(t) dt - \beta_r \frac{1}{2} p_N^2(\tau) - \frac{1}{2} h_N(\tau) + \int_{-\tau}^{\tau} \frac{\partial U_N}{\partial q_N}(q(t)) p_N(t) dt
\]

The first two terms give the change \( \Delta S \) (between time \( \tau \) and time \( -\tau \)) of the entropy of the system. The other terms give \( \Delta S_c \) of (2.6). Corresponding to the right end of the chain, we have

\[
\frac{1}{2} p_{-N}^2(\tau) - \frac{1}{2} p_N^2(\tau) + \int_{-\tau}^{\tau} \frac{\partial U_N}{\partial q_N}(q(t)) p_N(t) dt =
\]

\[
h_N(\omega_\tau) - h_N(\omega_{-\tau}) - \int_{-\tau}^{\tau} J^+(t) dt
\]

where

\[
h_N(p, q) \equiv p_N^2/2 + V_N(q_N)
\]

and \( J^+ \) is the flow of energy per unit time into the right reservoir:

\[
J^+(t) \equiv \lambda_{N-1} p_N \Phi'(q_{N-1}(t) - q_{N}(t))
\]

and similarly for the current into the left reservoir:

\[
J^-(t) = -\lambda_{-N} p_{-N} \Phi'(q_{-N}(t) - q_{-N+1}(t))
\]
and
\[ h_{-N}(p, q) \equiv p^2_{-N}/2 + V_{-N}(q_{-N}) \]
As required, for all \( k \geq -N + 1, \)
\[ \frac{d}{dt} \sum_{k=1}^{N-1} \frac{1}{2} p_i^2(t) + V_i(q_i(t)) + \lambda_i \Phi(q_i(t) - q_{i+1}(t)) = J_k(t) - J^+(t) \]
and
\[ J_{-N+1}(t) = -J^-(t) - \lambda_{-N} \frac{d}{dt} \Phi(q_{-N}(t) - q_{-N+1}(t)) \]
with
\[ J_k(t) \equiv \lambda_{k-1} p_k(t) \Phi'(q_{k-1}(t) - q_k(t)) \]
the current over the bond \( k-1 \to k, \) and \( J^+(t) = J_N. \) Hence, the second contribution to the entropy production comes from the energy transfers to the left and the right reservoirs due to the very presence of the reservoirs (the energy of the system is not conserved): it equals the sum of \( -\beta_\ell \Delta h_{-N} \equiv -\beta_\ell [h_{-N}(\omega_\ell) - h_{-N}(\omega_r)] \) and \( -\beta_r \Delta h_{N} \equiv -\beta_r [h_N(\omega_r) - h_N(\omega_\ell)] \) and this will be part of \( \Delta S_e \) even when the crystal is decoupled (\( \Phi \equiv 0 \)). Finally, the remaining third contribution consists of the heat current to the left and to the right multiplied by the respective inverse temperatures. We can then summarize (3.21) as
\[ R(\omega) = \Delta S - \beta_\ell \Delta h_{-N} - \beta_r \Delta h_{N} + \beta_\ell \int_{-\tau}^{\tau} J^-(t) dt + \beta_r \int_{-\tau}^{\tau} J^+(t) dt \]
From (3.23), in the steady state, \( -\langle J^- \rangle = \langle J^+ \rangle = \langle J_k \rangle \) and upon taking the steady state average of (3.21), as in (2.9), only this third contribution
\[ 2\tau (\beta_r - \beta_\ell) \langle J_0 \rangle \geq 0 \]
survives and we see explicitly that the heat current goes from larger (at the left) to smaller (at the right) temperatures. While this result is elementary from a thermodynamic perspective, the derivation above from a statistical mechanical model, is, to our knowledge and taste, the simplest and most natural one (compare e.g. with [10, 11, 31]). Dividing the left hand side of (3.23) by the total time \( 2\tau \) gives the standard expression for the mean entropy production rate \( \dot{S}. \) This example will be continued in Section 5.3.

4 Entropy production

In the previous scheme of Section 2.2, entropy production was identified with the time-reversal symmetry breaking part in the space-time action functional governing the nonequilibrium space-time distribution, see (2.4)-(2.6). Of course, this is the total entropy production, that is the change of the entropy of system plus reservoirs. Looking at (2.6) the first two terms give the change in entropy of the system and the rest corresponds to exchanges with the reservoirs or to external work. It is very well possible that in some transient regime, the entropy of the system decreases but the total entropy change is always positive, see (2.7), (2.3). In the steady state, entropy is constantly produced in the system but is carried away to the reservoirs. The mean entropy production \( \langle R \rangle \) is always
time-reversal invariant (same entropy production in original as in time-reversed steady state) and thermodynamic equilibrium is characterized by zero mean entropy production (the absolute minimum).

The easiest way to justify this mechanism is to look at classes of examples as in the above and just observe that it works. For more examples, see [40]. But there are also more general answers.

The first one looks a bit easy but it is essential. Consider a closed system of particles subject to a Hamiltonian dynamics. The entropy of a macrostate $M$ is given via Boltzmann’s formula $S(M) = \ln W(M)$ where $W(M)$ ‘counts’ the number of microstates giving rise to the macrostate $M$; we refer to the recent [24] for details. Suppose now that we condition on starting in this macrostate; what is the probability of a given microscopic trajectory? Since the trajectory is completely decided by the initial microstate, this probability is given by $1/W(M)$.

The trajectory ends in some microstate giving rise to a new macrostate $M'$. The time-reversed trajectory must thus be conditioned on starting somewhere in the phase space corresponding to $M'$ and it has therefore a probability $1/W(M')$. Hence, the ratio of these probabilities is $W(M')/W(M) = \exp[S(M') - S(M)]$ and its logarithm, that is $(2.4)-(2.5)$, thus gives the change of entropy as required.

A second answer is to look in the literature for motivated ‘general’ expressions for the entropy production, see [3]. There exists a standard expression for the entropy production rate in stochastic Markov dynamics. For a finite state space and a nicely behaving continuous time Markov chain with transition rate $k(\eta, \eta')$ for the probability per unit time to change configuration $\eta$ to the new $\eta'$, we consider

$$\dot{S}(\rho) \equiv \sum_{\eta, \eta'} \rho(\eta)k(\eta, \eta') \ln \frac{\rho(\eta)k(\eta, \eta')}{\rho(\eta')k(\eta', \eta)}$$

(4.26)

for $\rho$ a measure on the state space. This functional already appeared in [3] where a reference is made to Kirchhoff, [28], and it was discussed again later, for example in the papers [14, 47, 13]. It is called the entropy production rate and we can verify for our examples above or for other similar models that this is a good name. Take say a hopping dynamics on the volume $V$ as in the asymmetric exclusion process of example 3.1 but now with rates

$$c(i, j, \eta) \equiv e^{-\frac{1}{2}[H(\eta') - H(\eta) - E_{ij}(\eta(i) - \eta(j))]$$

where $H(\eta)$ is the energy of $\eta$ and $E_{ij} = E_{ji}$ is an external field. Then, a small computation gives

$$\dot{S}(\rho) = -\frac{d}{dt} \langle H(\eta_t) \rangle_\rho(t = 0) + P_E + \frac{d}{dt} \langle -\ln \rho(\eta_t) \rangle_\rho(t = 0)$$

which is the rate at which, in “state” $\rho$, energy is transferred to the thermal reservoir (we have set the inverse temperature $\beta = 1$) plus the power $P_E$ delivered by the external field on the system plus the rate at which $-\sum_{\eta} \rho(\eta) \ln \rho(\eta)$ (the Shannon entropy) is changed. This is more or less okay and there are more nice properties (like positivity, homogeneity and convexity of the functional $\dot{S}(\rho)$, see [13]). There are however also bad things about this formula for the entropy production rate. First of all it is restricted to Markovian stochastic dynamics. Secondly, it only gives the mean entropy production in the state $\rho$.
while it is not clear in what sense it is the expectation of what variable quantity of which we could study the (local) fluctuations. Above all, it is bad because it seems more or less useless if we do not know the state \( \rho \), e.g. the stationary state of the dynamics, to compute the steady state entropy production (there is only an approximate minimum entropy production principle to guide us here but it is of limited validity).

We can do better if we extend the formula to the space-time domain which is exactly the set-up of (2.4)-(2.8); (2.8) is just our alternative: we can show for the context of (4.26) that

\[
R^*(\rho) = \int_{-\tau}^{\tau} \dot{S}(\rho_t) dt
\]

(4.27)

the total entropy production over \([-\tau, \tau]\). Now that may seem more complicated but there is in fact much gained. To see it, let us consider the steady state. In that case \( \rho_t = \rho \) for all times and \( R^*(\rho) = 2\tau \dot{S}(\rho) \). Now, \( \rho \) is as unknown as before but its extension to the path space measure \( P = P^{\tau}_\rho \) is much more accessible. \( R^*(\rho) \) is the expectation of (2.5) and we can study its fluctuations and derive the symmetries discussed before. Moreover, the formula for \( R^*(\rho) \) is not at all restricted to Markovian dynamics; it is even not restricted to stochastic dynamics.

As a third general motivation, we give a Boltzmann-like space-time counting interpretation of this entropy production. In order to give a microscopic definition we present here only the simplest set-up that mimics the start of equilibrium statistical mechanics but for space-time trajectories.

Suppose we break up our stationary system into \( N \) space-time cells which are very small but still large enough to associate to each of them a value for the current (the nature of which we do not need to specify here). We assume there are \( n \) possible values \( J_k \) with time-reversed value \( J_k' = -J_k \). The system is observed in these little windows and we call the sequence of integers \( (m_1, \ldots, m_n) \) with \( m_1 + \ldots + m_n = N \) a distribution of current values; say, we find \( m_k \) times out of the \( N \) observations the value \( J_k \) so that \( \sum_k m_k J_k \) approximates the space-time integrated current over our system. We will also use the proportions \( P_k \equiv m_k/N \). The distribution \( (P_k) \) will be kept fixed and characterizing the nonequilibrium condition; \( \sum_k P_k J_k \equiv J \neq 0 \) so that the distribution over the values \( (J_k) \) is not time-reversal invariant. We forget about the origin of this distribution and it can be produced from surface or bulk driving conditions.

We select \( M \) space-time cells from the interior of the space-time system and we suppose that out of the corresponding \( M \) observations we find \( r_k \) times the value \( J_k \). We also write \( Q_k \equiv r_k/M \). Let \( W(r_1, \ldots, r_n; m_1, \ldots, m_n) \) denote the number of ways we can achieve such a distribution. It is given as a product of two multinomial coefficients:

\[
W(r_1, \ldots, r_n; m_1, \ldots, m_n) = \frac{M!(N-M)!}{\prod_k r_k!(m_k - r_k)!}
\]

Therefore, the relative weight for observing the sequence \( (r_1, \ldots, r_n) \) versus the sequence \( (r'_1, \ldots, r'_n) \) for given fixed distribution \( (m_1, \ldots, m_n) \) is

\[
\frac{W(r_1, \ldots, r_n; m_1, \ldots, m_n)}{W(r'_1, \ldots, r'_n; m_1, \ldots, m_n)} = \prod_k \frac{r_k^{!}(m_k - r_k)!}{r'_k!(m_k - r'_k)!}
\]
If we take the limit of this expression for \( N \) very large while fixing the distribution \((P_k)\) and we also let \( M \) be very large, we obtain as relative probabilities for two trajectories \( \omega, \omega' \) of the (internal) subsystem

\[
\frac{\text{Prob}[\omega]}{\text{Prob}[\omega']} = e^{M[S(Q) - S(Q') - \sum (Q'_k - Q_k) \ln P_k]}
\]

with \( S(Q) \equiv -\sum_k Q_k \ln Q_k \) and \( \omega \) and \( \omega' \) empirically corresponding to the distribution \((Q_k)\), respectively \((Q'_k)\). We see therefore that those \( \omega \) are most plausible that have their \( Q_k = P_k \). On the other hand, among two trajectories with equal (equilibrium) entropy \( S(Q) = S(Q') \), the one with larger dissipation \( \varphi(Q, P) \equiv \sum_k Q_k \ln P_k \) gets largest probability. Note that we can rewrite the last term in the exponent above as

\[
\sum (Q'_k - Q_k) \frac{\partial S(P)}{\partial P_k}
\]

which is the product of the displacement \( Q'_k - Q_k \) and the force \( \partial S(P)/\partial P_k \). This term is not time-reversal invariant if the distribution \((P_k)\) is not and in this way the condition of microscopic reversibility is broken. More precisely, by taking \( \omega' = \Theta \omega \) where \( \Theta \) again denotes time-reversal, we get

\[
\frac{\text{Prob}[\omega]}{\text{Prob}[\Theta \omega]} = \exp M \sum_k Q_k \ln \frac{P_k}{P'_k}
\]

where \( P' \) is the time-reversal of the original \( P \). In the exponent we recognize the difference in dissipation

\[
\varphi(Q, P) - \varphi(Q', P) \equiv \sum_k Q_k \ln \frac{P_k}{P'_k}
\]

It is this function of the distribution \((Q_k)\) for the internal system that we have called the (variable) entropy production

\[
R(Q, P) \equiv \sum_k Q_k \ln \frac{P_k}{P'_k}
\]

in the nonequilibrium state \( P \). Through the distribution \((Q_k)\), the entropy production is also a function \( R(\omega) \) of the space-time trajectory \( \omega \) and the fluctuations in the internal system will always satisfy the symmetry

\[
\text{Prob}[R(\omega) = a] = \text{Prob}[R(\omega) = -a] \exp[M a]
\]

on which we wrote before, see (2.11). Of course, we will typically observe the mean entropy production

\[
\langle R \rangle \equiv \sum_k P_k \ln \frac{P_k}{P'_k}
\]

which is in fact the relative entropy between the forward and the backward nonequilibrium state that we introduced before. Furthermore, if we choose \( P_k \sim \exp[\lambda(J) J_k/2] \) with \( \sum_k P_k J_k = J \) fixed, then this becomes

\[
\langle R \rangle = \lambda(J) J
\]

the standard product of force and current. The same scenario can be applied to the case where coriolis or magnetic forces are present (but then the time-reversal operation must take into account the parity of the observables).
5 Consequences

Some of the general consequences of the Gibbsian hypothesis have already been discussed in Section 2.2. and have been illustrated in Section 3. Here we give some additional considerations.

5.1 Local fluctuation symmetry

The expressed symmetry in (2.10) first appeared in the context of dynamical systems, in simulations with thermostated dynamics in [8], for strongly chaotic systems in [19, 21, 22, 19] and in stochastic dynamics in [23, 25, 36, 10]. An experimental verification was sought in [4]. The reason why it got so much attention is that there are indications that it provides a far from equilibrium relation hopefully extending close to equilibrium theory. One can for example base on it a derivation of Green-Kubo relations with the close to equilibrium Onsager reciprocities, see [15, 16, 33, 36]. Our way of looking at it is that it plays a similar role to that of Ward identities in field theory. What is new in (2.11)-(3.16) is the local aspect of the symmetry relation. That makes more physical sense for spatially extended systems because no fluctuations will ever be observed that take the size of the whole macroscopic system. This local aspect was already studied in [17, 21, 36] but now we have a systematic control over it. The results that we obtained in [39] for the asymmetric exclusion process follow exactly the Gibbsian scheme. The distribution $P$ is there the restriction of the steady state process to the subvolume $\Lambda$. This is a non-Markovian process but our Gibbsian set-up is verified and does not care about that. The corresponding $R_{\Lambda}$ for this local process is, up to a space-time boundary term, exactly equal to the local irreversible work and that is why we got a local fluctuation theorem as explained in Section 3.1.

This set-up is very reminiscent of the Onsager-Machlup theory except that there one starts from a linear dynamics for the macroscopic variables. The bulk of their paper is the construction of the associated action functional $A$. All that is said here is that we can do the same starting from a non-linear dynamics on a more microscopic level for the dynamics. Then $A$ is not quadratic but the fluctuation symmetry still holds.

5.2 Positivity of entropy production

From (2.9) it is rather easy to obtain the positivity of the entropy production. When this is a simple product of field and current, it will give also the average direction of the current, as in (3.25). For example, in the example of heat conduction above, it is easy to establish that the heat current will flow from the hot towards the cold reservoir. That is not new, see [10, 11, 31], but our approach seems more general. In particular, all this remains largely unchanged for non-Markovian dynamics, [36].

What is not so clear a priori is whether this situation is stable under taking thermodynamic limits. That is, whether we could have a non-vanishing current even when there is no entropy production. The answers are given in [17, 35, 11]. The opposite is rather easy: you can have a zero net current and still $\langle R \rangle > 0$, see an example in [40].
5.3 Response relations

We restrict us here to nonequilibrium steady states. One of the most important consequences of (2.2) is that we can express the expectation of a function in the stationary state \( \rho \) (at a fixed time) as the expectation in a Gibbsian ensemble

\[
\int f(\eta) d\rho(\eta) = \int dP(\omega) f(\omega)
\]

because \( \rho \) is the restriction of the steady state distribution \( P \) to any fixed time layer. As already announced after (2.10) we can in principle derive exact identities between derivatives of space-time correlation functions via the differentiation of the Ward identity. That was already explored in [15, 33, 34] but it has not been made out whether for example a standard Green-Kubo relation as it should appear in Fourier’s law, is within reach now, see [14]. We will not repeat here the scheme of the approach starting from (2.10) or from fluctuation symmetry but instead, we give here an idea of how close we can get via a direct Gibbsian approach. One should compare it with the usual formal perturbation theory applied to the nonequilibrium dynamics, [14].

We have a steady state \( P \) and a stationary measure \( \rho \) which is obtained by perturbing an equilibrium dynamics with corresponding \( P_o \) and \( \rho_o \). Let us denote by \( \varepsilon \) the small parameter. For example 3.2, in the case of heat conduction in a crystal with stochastic reservoirs, \( \varepsilon \equiv (T_ℓ - T_r)/2 \) with \( T_r = 1/β_r \), \( T_ℓ = 1/β_ℓ \). We also write \( T \equiv (T_ℓ + T_r)/2 = 1/β \). Take a function \( f \) that is antisymmetric under time-reversal, \( f(\Theta) = -f \). A good example is a current, e.g. the sum of heat currents \( J_k \) of (3.24) at the oriented bonds \( \langle k - 1, k \rangle \subset L_N \) in our crystal: we take some \( 0 < M = M(N) < N \) and put

\[
f(\omega) = \frac{1}{N} \sum_{-M}^{M} J_k(0)
\]

The idea is now very simple. Simply write the expectation in the stationary state as

\[
\int f(p, q) \rho(p, q) dpdq = \int dP(\omega) f(\omega)
\]

where \( P \) is as always the steady state process over a time interval \([-τ, τ]\). This is indeed very cheap; all what happens is that we imbed the stationary distribution in the larger Gibbsian distribution \( P \). \( P \) depends on \( \varepsilon \) and for \( \varepsilon = 0 \) it just equals \( P_o \), our reference process. Yet, now we can apply (2.2) and write

\[
\int f(p, q) \rho(p, q) dpdq = \int dP_o(\omega) e^{-A(\omega)} f(\omega)
\]

and we can take the derivative with respect to \( \varepsilon \) at \( \varepsilon = 0 \) to find the linear response behavior. To be specific we turn to the formula (3.18), (3.19) and (3.21). The computation gives

\[
\frac{d}{d\varepsilon} \int f(p, q) \rho(p, q) dpdq \big|_{\varepsilon = 0} = \frac{d}{d\varepsilon} \int dP_o(\omega) \rho(\omega - \tau) f(\omega) \big|_{\varepsilon = 0}
\]

\[
= \int dP_o(\omega) f(\omega) \left\{ \frac{1}{2} \rho_N^2(\tau) - \frac{1}{2} \rho_N^2(-\tau) + \int_{-\tau}^{\tau} \left[ \frac{\partial U_N}{\partial q_N}(q(t)) \rho_N(t) dt \right] \right\} \tag{5.28}
\]
We can still rewrite this using (3.23) as
\[
\frac{d}{d\varepsilon} \int f(p, q)\rho(p, q)d\rho dq (\varepsilon = 0) = I_1 + I_2
\]  
(5.29)
with
\[
I_1 = \frac{d}{d\varepsilon} \int \frac{dP_\omega(\omega)}{\rho^0(\omega-\tau)}\rho(\omega-\tau)f(\omega) (\varepsilon = 0) - \frac{d}{d\varepsilon} \int \frac{dP_\omega(\omega)}{\rho^0(\omega-\tau)}\bar{\rho}(\omega-\tau)f(\omega) (\varepsilon = 0)
\]
\[
I_2 = \int dP_\omega(\omega) \int J_k(0)J_0(t)
\]
Equation (5.29) is valid for all \(\tau, N, M\) and it describes the linear response. At this moment, it would be interesting to consider the various possible limits (and possible exchanges with the \(\varepsilon\)-derivative) but we can only make some general comments. The first term \(I_1\) is the \(\varepsilon\)-derivative of a difference of two expectations. The expectations are under the equilibrium dynamics of the current \(f\) at time 0 started at time \(-\tau\) in the nonequilibrium stationary state \(\rho\), respectively the nonequilibrium state \(\bar{\rho}\). Even though there is a non-vanishing current at time \(-\tau\), we expect that for sufficiently large \(\tau\) the current will be arbitrarily small at time 0: the expectation of an antisymmetric function will go to zero under the equilibrium dynamics. The remaining term \(I_2\), of the form \(I_2 = \kappa/N\), should give rise to a Green-Kubo formula for the thermal conductivity \(\kappa\), see e.g. [31], in the limits \(N, \tau \uparrow +\infty\). Note however that the reservoirs are still present in the time-evolution for \(J_0(t)\). It appears therefore that the correct limit is to first take \(M, N \uparrow +\infty\) before \(\tau \uparrow +\infty\) in the equilibrium current-current correlation function. In this way the bulk Hamiltonian dynamics, having a finite horizon of propagation, should dominate the time-evolution and the correct Green-Kubo formula should appear, see [14]. This however requires an analysis that goes much beyond the generalities that have been the subject of the present paper. After all, the above rigorous derivation for finite space-time extension holds also in the harmonic case, while we know that there the current \(\langle J_0 \rangle\) is proportional to the temperature difference \(\varepsilon\) (non-vanishing as the size \(N\) of the system tends to infinity). The problem of estimating the current-current correlations in the thermodynamic limit remains therefore essential and open.

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