Contemporary Mathematics

Statistical Mechanics of Anharmonic Lattices

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Dedicated to Lawrence E. Thomas on the occasion of his 60th birthday

ABSTRACT. We discuss various aspects of a series of recent works on the non-equilibrium stationary states of anharmonic crystals coupled to heat reservoirs (see also [**7**]). We expose some of the main ideas and techniques and also present some open problems.

1. Introduction

As emphasized in [**37**] the study of nonequilibrium stationary states, i.e. the states of systems maintained far from equilibrium by suitable forces and/or reservoirs has seen some progress in the last few years. Unlike in equilibrium statistical mechanics, nonequilibrium stationary states are not given by some apriori formula, and therefore the construction of the stationary states and the study of their properties require in general a thorough understanding of the dynamics. Furthermore exactly solvable models (for example linear ones [**34, 39**]) have pathological transport properties, and this makes the study of nonlinear dynamics even more necessary. There are several ways to model reservoirs: by *thermostats* modeled by deterministic forces, see e.g [**16, 35**], by *stochastic reservoirs* modeled by suitable random forces, see e.g. [**1**], and by *Hamiltonian reservoirs* where the reservoirs are Hamiltonian systems. The last choice is perhaps the most natural and fundamental one, but each of the approaches involves some idealization and all of them should be in some (yet unknown) sense equivalent.

We consider here a class of systems (finite lattice of anharmonic oscillators) interacting, at the boundaries only, with Hamiltonian reservoirs described by free phonon fields. A series of rigorous results has been obtained for such systems [**10, 11, 8, 30, 31, 32, 18, 9**]: existence and uniqueness of the stationary state, exponential rate of convergence, positivity of entropy production and study of its fluctuations (Gallavotti-Cohen Theorem). These results are the most complete ones obtained up to date for a (boundary driven) Hamiltonian system with a nontrivial (i.e. nonlinear) dynamics (see also e.g. [**13, 17, 4**] for classical systems and [**36, 21**] quantum systems). But several basic and fundamental problems remain very poorly understood both at the physical and mathematical levels, such as deriving

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2000 *Mathematics Subject Classification.* Primary 82C; Secondary 60H, 60F.

the transport properties of such systems, for example the Fourier's Law of heat conduction (see e.g. the reviews [**2, 24**] and references therein).

In Section 2, we describe a model of a Hamiltonian reservoir at positive temperature. We also describe how to choose a coupling with the system in such a way that one can reduce the infinite-dimensional Hamiltonian dynamics to a Markovian dynamics on a finite-dimensional phase space.

In Section 3, we consider a chain of oscillators connected to two reservoirs at different temperatures and present our results on the ergodic properties of such systems. We present some conceptual ideas behind the proofs: the analysis of dissipation and fluctuations, the construction of Liapunov functions for the dynamics , and the role of breathers as (possible) obstacles to the existence and/or exponential relaxation of the stationary state.

In Section 4 we study the properties of the entropy production: positivity, fluctuations (Gallavotti-Cohen theorem [**12, 16, 22, 23, 26**]), connection with time-reversal, Green-Kubo formula.

In Section 5 consider stochastic reservoirs modeled by Langevin equations. Our techniques apply to these systems too and we consider higher-dimensional lattice for which similar results as in Sections 3 and 4 can be sometimes proved.

We would like to thank Jean-Pierre Eckmann, Martin Hairer, Joel Lebowitz, Claude-Alain Pillet, and Lawrence E. Thomas for their collaboration, suggestions, and discussions.

2. Markovian Heat Reservoirs

It is customary to model the interaction of a mechanical system reservoirs by adding suitable random forces (stochastic reservoirs). and it is often done in such a way as to obtain a Markovian dynamics. In general the dynamics of a mechanical system interacting with a Hamiltonian reservoir is not Markovian: there are always memory effects. In certain cases one can obtain a Markovian dynamics by taking a suitable limit (see e.g. [**14, 5, 38**]), but in this section, we show how to obtain a Markovian dynamics by choosing a *particular coupling* with the reservoir. The dynamics of the system is not Markovian, but one can make it Markovian by adding finitely many auxiliary variables. Equations similar to those we derive do appear in [**33**] but, to our best knowledge, their derivation appear first in [**10, 31**]. For simplicity we consider a single particle coupled to one reservoir.

The reservoir is a free phonon gas described by a linear wave equation in $\mathbf{R}^d$. Let $\phi(x) = (\varphi(x), \pi(x))$, $x \in \mathbf{R}^d$, be a pair of real fields, let $\|\phi\|$ be the norm given by $\|\phi\|^2 \equiv \int dx\,(|\nabla\varphi(x)|^2 + |\pi(x)|^2)$, and let us denote $\langle\cdot,\cdot\rangle$ the corresponding scalar product. The phase space of the reservoirs at finite energy is the real Hilbert space of functions $\phi(x)$ such that the energy $H_B(\phi) = \|\phi\|^2/2$ is finite and the equations of motion are

$$\dot\phi(t,x) \,=\, \mathcal{L}\phi(t,x)\,, \quad \mathcal{L} \,=\, \begin{pmatrix} 0 & 1 \\ \Delta & 0 \end{pmatrix}\,. \tag{1}$$

Reservoirs at positive temperature T are described by Gibbs measure at temperature T, ν_T, given (formally) by

$$\nu_T(d\varphi, d\pi) = Z^{-1}\exp\left(-\frac{1}{2T}\int dx\,(|\nabla\varphi(x)|^2 + |\pi(x)|^2)\right)\prod_x d\phi(x)d\pi(x)\,. \tag{2}$$

This expression is formal, but the measure ν_T is simply the product of a Wiener measure times a white noise measure. Its covariance is $T\langle\cdot,\cdot\rangle$. We will construct the stationary states by assuming that, at time $t=0$, the reservoirs initial conditions are distributed according to the Gibbs measure ν_T.

The Hamiltonian of the particle is $H_S(p,q) = p^2/2 + V(q)$, where $(p,q) \in \mathbf{R}^d \times \mathbf{R}^d$, and as the Hamiltonian for the coupled system particle and reservoir we take (dipole approximation)

$$\begin{aligned} H(\phi,p,q) &= \frac{1}{2}\|\phi\|^2 + p^2 + V(q) + q\cdot\int dx\,\nabla\varphi(x)\rho(x) \\ &= H_B(\phi) + H_S(p,q) + q\cdot\langle\phi,\alpha\rangle\,, \end{aligned} \tag{3}$$

where $\rho(x)$ is a real rotation invariant function and $\alpha = (\alpha^{(1)},\cdots,\alpha^{(d)})$ is, in Fourier space, given by $\hat{\alpha}^{(i)}(k) = \big(0, -ik^{(i)}\hat{\rho}(k)/k^2\big)$. Let us introduce the covariance matrix $C^{(ij)}(t) = \langle\exp(\mathcal{L}t)\alpha^{(i)}\,,\,\alpha^{(j)}\rangle$. A simple computation shows that

$$C^{(ij)}(t) = \frac{1}{d}\delta_{ij}\int dk\,|\rho(k)|^2 e^{i|k|(t-s)}\,, \tag{4}$$

and we define a coupling constant λ by putting $\lambda^2 = C^{(ii)}(0) = \frac{1}{d}\int dk|\rho(k)|^2$. The equations of motion of the coupled system are

$$\begin{aligned} \dot{q}(t) &= p(t)\,, \\ \dot{p}(t) &= -\nabla V(q(t)) - \langle\phi,\alpha\rangle\,, \\ \dot{\phi}(t,k) &= \mathcal{L}\left(\phi(t,k) + q(t)\cdot\alpha(k)\right)\,. \end{aligned} \tag{5}$$

With the change of variables $\psi(k) = \phi(k) + q\cdot\alpha(k)$, Eqs. (5) become

$$\begin{aligned} \dot{q}(t) &= p(t)\,, \\ \dot{p}(t) &= -\nabla V_{\text{eff}}(q(t)) - \langle\psi,\alpha\rangle\,, \\ \dot{\psi}(t,k) &= \mathcal{L}\psi(t,k) + p(t)\cdot\alpha(k)\,, \end{aligned} \tag{6}$$

where $V_{\text{eff}}(q) = V(q) - \lambda^2q^2/2$. Integrating the last of Eqs. (6) with initial condition $\psi_0(k)$ one finds

$$\psi(t,k) = e^{\mathcal{L}t}\psi_0(k) + \int_0^t ds\,e^{\mathcal{L}(t-s)}\alpha(k)\cdot p(s)\,, \tag{7}$$

and inserting into the second of Eqs. (6) gives

$$\begin{aligned} \dot{q}(t) &= p(t)\,, \\ \dot{p}(t) &= -\nabla V_{\text{eff}}(q(t)) - \int_0^t dsC(t-s)p(s) - \langle\psi_0, e^{-\mathcal{L}t}\alpha\rangle\,. \end{aligned} \tag{8}$$

Our assumption on the initial condition of the reservoirs imply that the force $\xi(t) = \langle\psi_0, e^{-\mathcal{L}t}\alpha\rangle$ is a d-dimensional stationary Gaussian process with mean 0 and covariance $TC(t-s)$. Note that the covariance itself appears in the deterministic memory term on the r.h.s. of Eq.(8) (fluctuation-dissipation relation).

We choose the coupling function ρ such that

$$|k|^{d-1}|\rho(k)|^2 = P(k^2)^{-1}\,, \tag{9}$$

where P is a polynomial. As a consequence there is a polynomial $p(u)$ which is a real function of iu and has its roots in the lower half plane such that

$$C^{(ii)}(t) \;=\; \int_{-\infty}^{\infty} du\, \frac{1}{|p(u)|^2} e^{iut} \,. \tag{10}$$

Note that this is a Markovian assumption [**6**]: for such couplings $\xi(t)$ is a Markovian Gaussian process: $p(-id/dt)\xi(t) = \dot\omega(t)$, where $\dot\omega(t)$ is a white noise. For simplicity we will take $P(k^2) = C(k^2+\gamma^2)$ and then $\xi(t)$ is an Ornstein-Uehlenbeck process; other polynomials can be treated similarly. This assumption together with the fluctuation-dissipation relation permits, by extending the phase space with one auxiliary variable, to rewrite the integro-differential equations (8) as a Markov process. We have $C^{(ii)}(t) = \lambda^2 e^{-\gamma|t|}$ and introducing the variable r defined by

$$\lambda r(t) \;=\; \int_0^t ds\, C(t-s)p(s) + \xi(t)\,, \tag{11}$$

we obtain from Eqs.(8) the set of Markovian differential equations:

$$\begin{aligned} \dot q(t) &= p(t)\,, \\ \dot p(t) &= -\nabla V_{\text{eff}}(q(t)) - \lambda r(t)\,, \\ dr(t) &= (-\gamma r(t) + \lambda p(t))\, dt + (2T\gamma)^{1/2} d\omega(t)\,. \end{aligned} \tag{12}$$

The dynamics of $(p(t), q(t), r(t))$ is Markovian, and similar equations may be obtained for any polynomial P.

3. Ergodic properties: the chain

Let us consider a chain of n anharmonic oscillators given by the Hamiltonian

$$H_S(p,q) \;=\; \sum_{i=1}^{n} \frac{p_i^2}{2} + V(q_1,\cdots,q_n)\,,$$

$$V(q) \;=\; \sum_{i=1}^{n} U^{(1)}(q_i) + \sum_{i=1}^{n-1} U^{(2)}(q_i - q_{i+1})\,.$$

Our assumptions on the potential $V(q)$ are

H1 Growth at infinity: The potentials $U^{(1)}(x)$ and $U^{(2)}(x)$ are $\mathcal{C}^\infty$ and grow at infinity like $\|x\|^{k_1}$ and $\|x\|^{k_2}$: There exist constants C_i, D_i, $i = 1,2$ such that

$$\lim_{\lambda\to\infty} \lambda^{-k_i} U^{(i)}(\lambda x) \;=\; a^{(i)} \|x\|^{k_i}\,, \tag{13}$$

$$\lim_{\lambda\to\infty} \lambda^{-k_i+1} \nabla U^{(i)}(\lambda x) \;=\; a^{(i)} k_i \|x\|^{k_i-2} x\,, \tag{14}$$

$$\|\partial^2 U^{(i)}(x)\| \;\le\; (C_i + D_i V(x))^{1-\frac{2}{k_i}}\,. \tag{15}$$

where $\|\cdot\|$ in Eq. (15) denotes some matrix-norm.

Moreover we will assume that

$$k_2 \;\ge\; k_1 \;\ge\; 2\,, \tag{16}$$

so that, for large $\|x\|$ the interaction potential $U^{(2)}$ is "stiffer" than the one-body potential $U^{(1)}$.

H2 Non-degeneracy: The coupling potential between nearest neighbors $U^{(2)}$ is non-degenerate in the following sense. For $x \in \mathbf{R}^d$ and $m = 1, 2, \cdots$, let $A^{(m)}(x) : \mathbf{R}^d \to \mathbf{R}^{d^m}$ denote the linear maps given by

$$(A^{(m)}(x)v)_{l_1 l_2 \cdots l_m} = \sum_{l=1}^{d} \frac{\partial^{m+1} U^{(2)}}{\partial x^{(l_1)} \cdots \partial x^{(l_m)} \partial x^{(l)}}(x) v_l \,. \tag{17}$$

We assume that for each $x \in \mathbf{R}^d$ there exists m_0 such that

$$\mathrm{Rank}(A^{(1)}(x), \cdots A^{(m_0)}(x)) = d \,. \tag{18}$$

For example any confining polynomial potential of even degree satisfy assumptions **H1** and **H2**.

We couple the first and n^{th} particle each to one reservoir at temperatures T_1 and T_n respectively. We assume that the couplings to be as in Section 2 so that, by introducing two auxiliary variables r_1 and r_n, we obtain the set of stochastic differential equations equations

$$\begin{aligned}
\dot{q}_1 &= p_1 \,, \\
\dot{p}_1 &= -\nabla_{q_1} V(q) - \lambda r_1 \,, \\
dr_1 &= (-\gamma r_1 + \lambda p_1)\, dt + (2T_1\gamma)^{1/2} d\omega_1 \,, \\
\dot{q}_j &= p_j \,, \qquad\qquad j = 2, \ldots, n-1 \,, \\
\dot{p}_j &= -\nabla_{q_j} V(q) \,, \quad j = 2, \ldots, n-1 \,, \\
\dot{q}_n &= p_n \,, \\
\dot{p}_n &= -\nabla_{q_n} V(q) - \lambda r_n \,, \\
dr_n &= (-\gamma r_n + \lambda p_n)\, dt + (2T_n\gamma)^{1/2} d\omega_n \,.
\end{aligned} \tag{19}$$

The solution $x(t) = (p(t), q(t), r(t))$ of Eq.(19) is a Markov process. We denote T^t as the associated semigroup,

$$T^t f(x) = \mathbf{E}_x[f(x(t)] \,, \tag{20}$$

with generator

$$\begin{aligned}
L = & \sum_{i \in \{1,n\}} \gamma \left(\nabla_{r_i} T \nabla_{r_i} - r_i \nabla_{r_i}\right) + \lambda \left(p_i \nabla_{r_i} - r_i \nabla_{p_i}\right) \\
& + \sum_{i=1}^{n} p_i \nabla_{q_i} - (\nabla_{q_i} V(q)) \nabla_{p_i} \,,
\end{aligned} \tag{21}$$

and $P_t(x, dy)$ as the transition probability of the Markov process $x(t)$. There is a natural energy function which is associated to Eq.(19), given by

$$G(p, q, r) = \frac{r^2}{2} + H(p, q) \,, \tag{22}$$

and a straightforward computation shows that at equilibrium (i.e., if $T_1 = T_n = T$) the Gibbs measure $Z^{-1} \exp\left(-G(p, q, r)/T\right)$ is an invariant measure for the Markov process $x(t)$.

The function

$$W_\theta = \exp(\theta G) \tag{23}$$

will be used repeatedly. We denote as $|\cdot|_\theta$ the weighted total variation norm given by

$$|\pi|_\theta = \sup_{|f|\le W_\theta} \left| \int f d\pi \right| , \tag{24}$$

for any (signed) measure π. We introduce norms $\|\cdot\|_\theta$ and Banach spaces $\mathcal{H}_\theta$ given by

$$\|f\|_\theta = \sup_{x\in X} \frac{|f(x)|}{W_\theta(x)} , \quad \mathcal{H}_\theta = \{ f \,:\, \|f\|_\theta < \infty \} , \tag{25}$$

and write $\|K\|_\theta$ for the norm of an operator $K : \mathcal{H}_\theta \to \mathcal{H}_\theta$.

Our results on the ergodic properties of Eqs. (19) are summarized in

THEOREM 3.1. **: Ergodic properties**

(a) The Markov process $x(t)$ has a unique invariant measure μ. The measure μ is ergodic and mixing and has a $\mathcal{C}^\infty$ everywhere positive density.

(b) For any θ with $0 < \theta < (\max\{T_1, T_n\})^{-1}$ the semigroup $T^t : \mathcal{H}_\theta \to \mathcal{H}_\theta$ is compact for all $t > 0$. In particular the process $x(t)$ converges exponentially fast to its stationary state μ: there exist constants $r = r(\theta) > 1$ and $R = R(\theta) < \infty$ such that

$$|P_t(x,\cdot) - \mu|_\theta \le R r^{-t} W_\theta(x) , \tag{26}$$

for all $x \in X$. Furthermore for all functions f, g with f^2, $g^2 \in \mathcal{H}_\theta$ and all $t > 0$ we have

$$\left| \int g T^t f \, d\mu - \int f \, d\mu \int g \, d\mu \right| \le R r^{-t} \|f^2\|_\theta^{1/2} \|g^2\|_\theta^{1/2} , \tag{27}$$

(exponential decay of correlations in the stationary state).

There are essentially two proofs of Theorem 3.1 which follow quite different strategies. The (chronologically) first one [**11, 31, 32**] is probabilistic and is based on a detailed analysis of the dynamical effects of dissipation and fluctuations. The second proof [**10, 8, 18, 9**] is purely functional-analytic and use global hypoelliptic estimates on the generator L. In our opinion the first approach has the advantage to be a little simpler and also to display better the dynamical mechanisms at play. It singles out the breathers as a (possible) obstacle to the existence of a stationary state. The second approach has the advantage to be a bit more constructive and so it gives more precise information on the location of the spectrum. We sketch the main steps of the proof of Theorem 3.1, following the probabilistic approach taken in [**11, 31, 32**].

Hypoellipticity: The first thing to realize is that the generator L is hypoelliptic. The operator L has the form $L = \sum_{j=1}^M X_j^2 + X_0$ where the X_i are smooth vector fields which satisfy the following Hörmander-type condition: the vector fields $\{X_j\}_{j\ge1}; \{[X_i, X_j]\}_{i,j\ge0}; \{[[X_i, X_j]X_k]\}_{i,j,k\ge0}; \cdots$ span the whole tangent space at every point x. This implies [**19, 20, 29**] that the the transition probabilities have a smooth density.

Control theory and Uniqueness: The *uniqueness* of the invariant measure is obtained with a control-theoretic argument. Using the Support Theorem of [**41**], one study the following control problem: replace in Eqs. (19) the (rough) white noise $\dot{\omega}(t)$ by a smoother (e.g. piecewise smooth) control. The Support Theorem asserts in particular that the support of the transition probabilities $P_t(x, dy)$ is the same as the closure of the set of all points reachable in a time t starting from x with a smooth control. One can show [**11**] that for all t and for all x the transition probabilities have full support. This is achieved done by an explicit construction of the possible controls which drive the system from x to y in a given time span. This controllability property together with the smoothness of the transition probability imply that there is at most an invariant measure.

Liapunov functions, Existence, and Compactness: The *existence* of the invariant measure is the most difficult property to establish. This is in sharp contrast with equilibrium where the invariant measure is given, a priori, by the usual Gibbs Ansatz. Also as we prove the existence of an invariant measure we prove strong ergodic properties which, of course, are also of interest at equilibrium. The idea is to construct a Liapunov function for the Markov process $x(t)$ (for a detailed exposition of the subject see [**28**]). For this problem we proved the following. Fix $t > 0$ and $\theta < (\max\{T_1, T_n\})^{-1}$ and consider the function $W_\theta(x)$ given by Eq. (23). There exist a constant E_0 and functions $\kappa(E)$ and $b(E)$ defined on $[E_0, \infty)$ with $\lim_{E\to\infty} \kappa(E) = 0$such that for $E > E_0$

$$T^t W_\theta(x) \;\leq\; \kappa(E) W_\theta(x) + b(E)\chi_{\{G\leq E\}}(x)\,. \tag{28}$$

This means that, outside the compact set $\{G \leq E\}$, the dynamics is dissipative and since $\kappa(E)$ tends to zero as E tends to infinity, the dissipation at high energies can be made arbitrarily strong. This particular property of the Liapunov function together with the smoothness of the transition probabilities implies that the semigroup T^t is compact on the Banach spaces $\mathcal{H}_\theta$.

One should think of the dynamics as follows: to the conservative Hamiltonian dynamics two forces are added, a dissipative force (the terms $-\gamma r_i$ in (19)) and a random force (the white noises) which are proportional to the temperature. At high energies, i.e., at energies much bigger than the temperatures of the reservoirs, dissipation dominates and there is a strong drift which let the energy of the system decrease and the fluctuating forces are negligible compared to the dissipation. At low energies, on the contrary the fluctuations are not dominated by the dissipation anymore.

Since both dissipation and noise act only at the boundary of the chain, a key ingredient in the analysis is a bound on propagation of energy in anharmonic lattices. Think for example of an initial condition in which the energy is concentrated in one oscillator far away from the boundary. To prove Eq. (28) one must have a lower bound on how much of the energy propagates through the chain to the boundary to get dissipated. For this bound the condition **H2** is crucial. It is well-known [**40, 25, 3**] that in networks of anharmonic oscillators there are breathers which are (Nekhoroshev-stable) time periodic exponentially localized solutions of the Hamiltonian equations of motions. A simple scaling argument shows that the high energy behavior of breathers is very different depending on whether the condition **H2** is satisfied or not. If it is not satisfied, the higher the energy, the more localized the breather tends to be: at high energy we can have states with oscillators oscillating very fast and barely interacting with their neighbors which are essentially at rest. On the contrary, if Condition **H2** is satisfied, then one can show that for any initial condition of sufficiently large energy E, the kinetic energy of the oscillator on the boundary will be at least of order E^{2/k_2} on a time interval of order 1.

To prove (28), in a first step one sets $T_1 = T_n = 0$ in (19) and one obtains a set of deterministic ODE's equations. Using the bound on propagation of energy one shows that for large enough $G(0) = E$ we have

$$G(1) - G(0) \leq -cE^{2/k_2}\,. \tag{29}$$

Note that this corresponds to the physical situation where the reservoirs, at time $t = 0$ are at energy 0. In this case the system simply radiates all its energy into the reservoirs and relax into a state corresponding to a stationary point of the Hamiltonian H. If the temperatures are non-zero, one shows that on a suitable time interval the random solution of (19) do follow closely the deterministic trajectories with very high probability. So for most trajectories, an estimate of the type (29) also holds. To conclude of the proof of (28), one considers the function $W_\theta = \exp(\theta G)$ and uses some stochastic analysis (see [**31**] for details).

4. Heat Flow and Entropy Production

To define the heat flow and the entropy production we write the energy of the chain H as a sum of local energies $H = \sum_{i=1}^{n} H_i$ where

$$\begin{aligned} H_1 &= \frac{p_1^2}{2} + U^{(1)}(q_1) + \frac{1}{2}U^{(2)}(q_1 - q_1)\,, \\ H_i &= \frac{p_i^2}{2} + U^{(1)}(q_i) + \frac{1}{2}\Big(U^{(2)}(q_{i-1} - q_i) + U^{(2)}(q_i - q_{i+1})\Big)\,, \\ H_n &= \frac{p_n^2}{2} + U^{(1)}(q_n) + \frac{1}{2}U^{(2)}(q_n - q_{n-1})\,. \end{aligned} \tag{30}$$

Differentiating with respect to time one finds

$$\frac{d}{dt}T^t H_i = T^t(\Phi_{i-1} - \Phi_i)\,, \tag{31}$$

where

$$\begin{aligned} \Phi_0 &= -\lambda r_1 p_1\,, \\ \Phi_i &= \frac{(p_i + p_{i+1})}{2}\nabla U^{(2)}(q_i - q_{i+1})\,, \\ \Phi_n &= \lambda r_n p_n\,. \end{aligned} \tag{32}$$

It is natural interpret Φ_i, $i = 1, \cdots, n-1$ as the heat flow from the i^{th} to the $(i+1)^{th}$ particle, Φ_0 as the flow from the left reservoir into the chain, and Φ_n as the flow from the chain into the right reservoir. We define corresponding entropy productions by

$$\sigma_i = \left(\frac{1}{T_1} - \frac{1}{T_n}\right)\Phi_i\,. \tag{33}$$

There are other possible definitions of heat flows and corresponding entropy production that one might want to consider. One might, for example, consider the flows at the boundary of the chains, and define $\sigma_b = \Phi_1/T_1 - \Phi_n/T_n$. Also our choice of local energy is somewhat arbitrary, other choices are possible but this does not change the subsequent analysis.

Our results on the heat flow are summarized in

THEOREM 4.1. **: Entropy production**

(a) The expectation of the entropy production σ_j *in the stationary state is independent of* j *and nonnegative*

$$\int \sigma_j d\mu \geq 0\,, \tag{34}$$

and it is positive away from equilibrium

$$\int \sigma_j d\mu = 0 \qquad \text{if and only if} \qquad T_1 = T_n\,. \tag{35}$$

(b) The ergodic averages

$$\frac{1}{t}\int_0^t \sigma_j(x(s)) \tag{36}$$

satisfy the large deviation principle: There exist a neighborhood O *of the interval* $[-\int \sigma_j d\mu, \int \sigma_j d\mu]$ *and a rate function* $e(w)$ *(both independent of* j*) such that for all intervals* $[a, b] \subset O$ *we have*

$$\lim_{t\to\infty} -\frac{1}{t}\log \mathbf{P}_x\{\overline{\sigma}_i{}^t \in [a,b]\} = \inf_{w\in[a,b]} e(w)\,. \tag{37}$$

Moreover the rate function $e(w)$ *satisfy the relation*

$$e(w) - e(-w) = -w\,, \tag{38}$$

i.e., the odd part of e *is linear with slope* $-1/2$.

Let us consider the functions R_j given by

$$R_j = \frac{1}{T_1}\left(\frac{r_1^2}{2} + \sum_{k=1}^{j} H_k(p,q)\right) + \frac{1}{T_n}\left(\sum_{k=j+1}^{n} H_k(p,q) + \frac{r_n^2}{2}\right)\,, \tag{39}$$

so that $\exp(-R_j)$ is a "two-temperatures" Gibbs state. We denote by J the time reversal operator which changes the sign of the momenta of all particles $Jf(p,q,r) = f(-p,q,r)$ and we denote as L^T the formal adjoint of the generator L (the Fokker-Planck operator). The following (formal) operator identities are easily verified

$$e^{R_j} J L^T J e^{-R_j} = L - \sigma_j\,, \tag{40}$$

and also for any constant α

$$e^{-R_j} J (L^T - \alpha\sigma_j) J e^{R_j} = L - (1-\alpha)\sigma_j\,. \tag{41}$$

These identities are the key element to prove both Eqs. (34) and (38). The fact that the entropy production is strictly positive away from equilibrium do require more work [**11**].

Let us sketch the proof of Eqs. (34). We write the positive density $\rho(x)$ of $\mu(dx) = \rho(x)dx$ as

$$\rho = J e^{-R_j} e^{-F_j}\,. \tag{42}$$

Let L^* denote the adjoint of L on $L^2(\mu)$, it is given by $L^* = \rho^{-1} L \rho$ and using Eq. (40) a simple computation shows that

$$\begin{aligned} JL^*J &= e^{F_j}(L-\sigma_j)e^{-F_j} \\ &= L - \sigma_j - (LF_j) - 2\sum_{i\in\{1,n\}} T_i(\nabla_{r_i}F_j)\nabla_{r_i} \\ &\quad + \sum_{i\in\{1,n\}} (T_i|\nabla_{r_i}F_j|^2)\,. \end{aligned} \tag{43}$$

The operator JL^*J is the generator of the time-reversed process and using that $L^*1 = 0$ we find the identity

$$\sigma_i \;=\; \sum_{i\in\{1,n\}} T_i|\nabla_{r_i}F_j|^2 - LF_i\,. \tag{44}$$

The first term is obviously positive while the expectation of the second term in the stationary state vanishes and so we obtain Eq. (34).

Let us turn now to Eq. (38). Let us give first a formal proof, ignoring any technicality (the argument is essentially from [**22**]). To the study of the large deviations the large deviations of $t^{-1}\int_0^t \sigma_i(x(s))ds$ we consider the moment generating functionals

$$\Gamma_x^i(t,\alpha) \;=\; \mathbf{E}_x\left[e^{-\alpha\int_0^t \sigma_i(x(s))\,ds}\right]\,. \tag{45}$$

Formally the Feynman-Kac formula gives $\Gamma_x^i(t,\alpha) = e^{t(L-\alpha\sigma_i)}1(x)$ and the large deviation functional $e(w)$ is given by the Legendre transform of the function

$$e(\alpha) \equiv \lim_{t\to\infty} -\frac{1}{t}\log\Gamma_x^i(t,\alpha)\,. \tag{46}$$

By a Perron-Froebenius argument $e(\alpha)$ is the largest eigenvalue of $L - \alpha\sigma_i$. Since $L-\alpha\sigma_i$ is conjugated to $L^T - (1-\alpha)\sigma_i$ by Eq. (41) and since $L-\alpha\sigma_i$ and $L^T - \alpha\sigma_i$ should have the same spectrum we conclude that $e(\alpha) = e(1-\alpha)$. Taking Legendre transform we obtain Eq. (38).

How do we make this argument rigorous? From the form of the entropy production σ (it is an unbounded function), one sees that $L - \alpha\sigma_i$ is not a relatively bounded perturbation of L. A priori it is not even obvious $L-\alpha\sigma_i$ is the generator of a semigroup, i.e., that the function $\Gamma_x^i(t,\alpha)$ is finite for $\alpha \neq 0$. To make things work we will use the following identity which can be checked easily

$$L - \alpha\sigma_i \;=\; e^{\alpha R_i}\overline{L}_\alpha e^{-\alpha R_i}\,, \tag{47}$$

where

$$\overline{L}_\alpha \;=\; L + \gamma\sum_{i\in\{1,n\}}\left(2\alpha r_i\nabla_{r_i} - (\alpha-\alpha^2)T_i^{-1}r_i^2\right) + 2d\gamma\alpha\,. \tag{48}$$

This shows that all the operators $L-\alpha\sigma_i$ are conjugated to the same operator $\overline{L}_\alpha$. It is not hard to see that $\overline{L}_\alpha$ is relatively bounded perturbation of L. Using the same techniques as the one used in the proof of Theorem 3.1 one can show that $\exp{(t\overline{L}_\alpha)}$ defines a quasibounded compact semigroup on $\mathcal{H}_\theta$ provided that $-\alpha < \theta T_i < 1-\alpha$ and using Eq. (48) this shows that the function $e(\alpha)$ exists and is real analytic provided

$$\alpha \in \left(-\frac{T_{\min}}{T_{\max}-T_{\min}}\,,\, 1+\frac{T_{\min}}{T_{\max}-T_{\min}}\right)\,. \tag{49}$$

Using Gaertner-Ellis Theorem concludes the proof of Theorem 4.1.

REMARK 4.2. **Time reversal and entropy production I.** It is instructive to give a interpretation of Eq. (43) in terms of the path space measure of the process (see [**26**]). At equilibrium ($T_1 = T_n = T$) this is simply detailed balance, $R_i = G$, $JL^*J = L$ or $p_t(Jy, Jx) = p_t(x,y)\exp(-(G(y)-G(x))/T)$. If we are away from equilibrium we can interpret it as follows. Let P_{st} denotes the path space measure of the stationary process starting in the state μ and let θ denote the operator defined by $\theta x(t) = x(-t)$. The path space measure of the (stationary) time reversed process is given by $P_{st}^{rev} = JP_{st} \circ \theta^{-1}$ and its generator is JL^*J. Using the relation (43) and Feynman-Kac formula we find

$$\frac{dP_{st}^{rev}}{dP_{st}}(x(t)) \;=\; e^{-\int_0^t ds\sigma_j(x(s))} \times e^{-(F_j(x(t))-F_j(x(0)))} \,. \tag{50}$$

As pointed out in [**26**], this gives a microscopic definition of the entropy production and relates it directly to the action of time-reversal.

REMARK 4.3. **Time reversal and entropy production II.** If we go back to the original Hamiltonian description of the system, we note that the dynamics and the in ital conditions of the reservoirs are invariant under time reversal: changing t into $-t$, and changing the signs of the momenta p of the crystal and of the fields Π leaves the equations of motion unchanged. Also the initial condition of the reservoirs are distributed according to the Gibbs measure and are invariant under reversal of the velocities in the reservoirs. Consequently we can study the behavior of the system as $t \to -\infty$ simply by changing p into $-p$, π into $-\pi$ and considering $t \to \infty$. If we do this and reduce the dynamics as in the section 2 we obtain a Markov process with a generator given by JLJ (the variables r are left unchanged) and the system relaxes into the stationary state $J\mu$.

Since σ_j is an odd function of p, we have $\int \sigma_j d\mu \le 0$. One might be tempted to draw the conclusion that, in the far distant past, heat was flowing from the cold reservoir into the hot one. This is incorrect since the very definition of the heat flows involves a time-derivative, if we consider $t \to -\infty$ one should change the definition of the flows accordingly.

REMARK 4.4. **Green-Kubo formula.** As noted in [**15, 22**] one can derive the Green-Kubo from the fluctuation theorem. Here the external "field" is the inverse temperature difference $\Delta\beta = (\beta_n - \beta_1)$ and we have $\sigma_j = \Delta\beta\phi_j$. We consider the function $f(a, \Delta\beta)$ given by

$$f(a,\Delta\beta) \equiv \lim_{t\to\infty} -\frac{1}{t}\log \mathbf{E}_\mu\left[e^{-a\int_0^t \phi_i(x(s))\,ds}\right] \,, \tag{51}$$

where $a = \alpha\Delta\beta$ and the second variable in f indicates the dependence of the dynamics of the stationary state μ on $\Delta\beta$. From the compactness properties of the semigroups involved it is easy to see that $f(a, \Delta\beta)$ is a real-analytic function of both variables a and $\Delta\beta$. The relation $e(\alpha) = e(1-\alpha)$ now reads

$$f(a,\Delta\beta) \;=\; f(\Delta\beta - a, \Delta\beta) \,. \tag{52}$$

Differentiating this relation we find

$$\frac{\partial^2 f}{\partial a \partial(\Delta\beta)}(0,0) \;=\; -\frac{\partial^2 f}{\partial a \partial(\Delta\beta)}(0,0) - \frac{\partial^2 f}{\partial a^2}(0,0) \,. \tag{53}$$

We have

$$\frac{\partial f}{\partial a}(0,\Delta\beta) = \int \phi_j d\mu\,, \tag{54}$$

$$\frac{\partial^2 f}{\partial a^2}(0,0) = -\frac{1}{2}\int_0^\infty \left(\int (T_0^t\phi_j)\phi_j d\mu_O\right) ds\,, \tag{55}$$

where T_0^t is the semigroup at equilibrium ($\Delta_\beta = 0$) and μ_0 is the equilibrium measure $Z^{-1}\exp(-\beta G)$. We obtain

$$\frac{\partial}{\partial(\Delta\beta)}\left(\int \phi_j d\mu\right)\bigg|_{\Delta\beta=0} = \frac{1}{2}\int_0^\infty \left(\int (T^t\phi_j)\phi_j d\mu\right) ds\,, \tag{56}$$

and this is the familiar Green-Kubo formula.

5. Langevin equations and other lattice of oscillators

5.1. Hypercubes. The reader may wonder why we are only considering one-dimensional lattice of oscillators. Although it is not difficult to construct Hamiltonian models of higher dimensional lattice of oscillators interacting with reservoirs, the reduction to a tractable set of SDE's is not trivial. In particular it is not easy to prove that reservoir provide enough noise/dissipation to carry the analysis done to prove Theorem 3.1.

If we consider hypercubes of oscillators and stochastic reservoirs given by Langevin equations much can be said. For $i \in \mathbf{Z}^d$, let $|i| = \sup_{1\leq k} \leq |i_k|$ and let Λ be the hypercube $\Lambda = \{i \in \mathbf{Z}^d\,,\ |i| \leq N\}$. The side of the cube N is arbitrary, but finite. On each site of Λ there is an oscillator with coordinates $(p_i, q_i) \in \mathbf{R}^d \times \mathbf{R}^d$ and the Hamiltonian of the system is given by

$$H(p,q) = \sum_{i\in\Lambda}\left(\frac{p_i^2}{2} + U^{(1)}(q_i) + \sum_{j\in\Lambda\,:\,|j-i|=1} U^{(2)}(q_i - q_j)\right)\,. \tag{57}$$

As a model of reservoirs add an Ornstein-Uehlenbeck process to each oscillator on two opposite sides of the hypercube Λ. The equations of motions are

$$\begin{aligned}\dot q_i &= p_i\,,\\ dp_i &= (-\nabla_{q_i}V(q) - \lambda p_i)\,dt + \sqrt{2\lambda T_L}d\omega_i\,, \quad \text{if } i_1 = -N\,,\end{aligned} \tag{58}$$

$$\begin{aligned}\dot q_i &= p_i\,,\\ dp_i &= (-\nabla_{q_i}V(q) - \lambda p_i)\,dt + \sqrt{2\lambda T_R}d\omega_i\,, \quad \text{if } i_1 = N\,,\end{aligned} \tag{59}$$

$$\begin{aligned}\dot q_i &= p_i\,,\\ \dot p_i &= -\nabla_{q_i}V(q)\,, \quad \text{if } i_1 \neq -N, N\,.\end{aligned} \tag{60}$$

We denote by $x(t) = (p(t), q(t))$ the Markov process which solves Eqs. (58)–(60). We have, similarly to Theorem 3.1

Ergodic properties: The Markov process $x(t)$ has a unique invariant measure μ. The measure μ is ergodic and mixing and has a $\mathcal{C}^\infty$ everywhere positive density. The convergence to the stationary state occurs exponentially fast.

We can also prove a result analogous to Theorem 4.1 by considering the heat flow through an hypersurface $\{i_1 = k\}$. We define the energy of the oscillators in the hyperplane $\{i_1 = k\}$ to be

$$H_k(p,q) \;=\; \sum_{i\,:\,i_1=k}\left(\frac{p_i^2}{2}+U^{(1)}(q_i)+\frac{1}{2}\sum_{j\in\Lambda\,:\,j_1=k,|j-i|=1}U^{(2)}(q_i-q_j)\right)\,, \tag{61}$$

then the total heat flow Φ_k between the hypersurfaces $\{i_1 = k\}$ and $\{i_1 = k+1\}$ is given by

$$\Phi_k \;=\; \sum_{i:i_1=k}\frac{p_i+p_{i+e_1}}{2}\nabla U^{(2)}(q_i-q_{i+e_1})\,, \tag{62}$$

where $e_1 = (1,0,\cdots,0)$. The corresponding entropy production is defined by $\sigma_k = (T_R^{-1} - T_L^{-1})\Phi_k$. As in Section (4.1) we have

Positivity of the entropy production: The expectation of the entropy production σ_k in the stationary state is independent of j and nonnegative

$$\int \sigma_k d\mu \;\geq\; 0\,, \tag{63}$$

and it is positive away from equilibrium

$$\int \sigma_k d\mu \;=\; 0 \qquad \text{if and only if} \qquad T_1 = T_n\,. \tag{64}$$

Gallavotti-Cohen fluctuation theorem: The ergodic averages

$$\frac{1}{t}\int_0^t \sigma_k(x(s)) \tag{65}$$

obey the large deviation principle with a rate function $e(w)$ which satisfy the relation

$$e(w) - e(-w) \;=\; -w\,. \tag{66}$$

The techniques used to prove Theorem 3.1 can be used to analyze Eqs. (58)–(60). To see this just think of the set of all oscillators on the hyperplane $i_1 = k$ as one $(2L+1)^{d-1}$-dimensional oscillator Q_k with one-body potential

$$W^{(1)}(Q_j) = \sum_{i\,:\,i_1=k}U^{(1)}(q_i) + \sum_{i,j\,:\,i_1=j_1=k}U^{(2)}(q_i-q_j)\,, \tag{67}$$

and two-body potential

$$W^{(2)}(Q_k - Q_{k-1}) = \sum_{i,j\,:\,i_1=k,j_1=k-1}U^{(2)}(q_i-q_j)\,. \tag{68}$$

Doing this we obtain a "chain" of (high-dimensional) oscillators. The noise and dissipation are slightly different, but this can be analyzed using exactly the same methods.

5.2. General Graphs. A natural problem, considered in [**27, 42**], is the following. Consider an arbitrary graph $G = (V, E)$, at each vertex i of G there is an oscillator with coordinates (p_i, q_i) and energy $p_i^2/2 + U^{(1)}(q_i)$ and for each edge $e \in E$ between i and j the two oscillators interact via a two-body potential $U^{(2)}(q_i - q_j)$. The boundary of the graph is a subset ∂V of the set of vertices V and if $i \in \partial V$, an Ornstein Uehlenbeck modeling the interaction with the reservoir is added to the Hamiltonian equation.

Given such a graph, one might ask under which condition on the graph the analysis done for the chain can be carried over. This is largely an open problem but the following can be said

Quadratic potentials: If the potentials are quadratic, then the SDE's are linear and necessary and sufficient conditions are known for the existence and uniqueness of stationary states. It can be given in purely algebraic terms, see e.g. [**20**].

Nonuniqueness of the stationary state: On the other hand, linear models have (too) many invariants and very simple model have more than one invariant measure, e.g., four harmonic oscillators arranged in a diamond shape with two opposite oscillators connected to heat baths have a one-parameter family of invariant measures [**42, 27**].

Entropy production: The nonnegativity of the entropy production is very easy to establish at the formal level. Let R be the function given by $R = \sum_{i\in\partial V}(T_i)^{-1}p_i^2/2$ where T_i is the temperature of the reservoirs attached to the oscillator i. We have the relation $e^R JL^T je^{-R} = L - \sigma$, where $\sigma = \sum_{i\in\partial V} T_i^{-1}(p_i^2 - T_i)$. The quantity is $(T_i - P_i^2)$ is to be interpreted as the heat flow from the system into the corresponding reservoir at temperature T_i. As in section 4.1 one shows that this relation implies the nonnegativity of the entropy production in the stationary state. Using conservation laws other entropy productions involving heat flows through the bulk of the lattice can be considered too.

Positivity of the entropy production: In [**27**] an interesting condition is given which implies the positivity of the entropy production, provided one assumes the existence of a smooth positive stationary state. As mentioned above, if the elements of a graph are connected to many others, the potential should be "sufficiently" non-linear. The condition is the following: a function f is called n-nondegenerate provided the set

$$\mathcal{U}^n = \{(q_1, \cdots, q_n) \in \mathbf{R}^n : \exists (q_1', \cdots, q_n') \in \mathbf{R}^n : \det(f(q_i' - q_j)) \neq 0\} , \tag{69}$$

is dense in $\mathbf{R}^n$. For example the polynomials of degree r are n-nondegenerate provided $r \geq n - 1$. One can show ([**27**] for details) that if $d^2U^(2)/dq^2$ is n-nondegenerate for n sufficiently large then the entropy production is non-negative. How large n should be depends on the graph, in particular on how many nearest neighbors an oscillator has and if there are many loops in the graph. We conjecture that such a condition should also imply existence and uniqueness of the stationary state.

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