Nonequilibrium statistical mechanics of open classical systems

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We describe the ergodic and thermodynamical properties of chains of anharmonic oscillators coupled, at the boundaries, to heat reservoirs at positive and different temperatures. We discuss existence and uniqueness of stationary states, rate of convergence to stationarity, heat flows and entropy production, Kubo formula and Gallavotti-Cohen fluctuation theorem.

1. Introduction

We report on a series results obtained through various collaborations with J.-P. Eckmann, M. Hairer, C.-A. Pillet and L. E. Thomas [2–5, 18–21]. We study the statistical mechanics of chains of anharmonic oscillators coupled at both ends to heat reservoirs at different temperatures. The reservoirs are modeled by linear wave equations and the model is completely Hamiltonian. Such oscillators chains (with various models of reservoirs) are widely used as simple models to test the validity of Fourier Law (see [1, 15] for reviews and references) which is a fundamental open question in nonequilibrium statistical mechanics.

We consider a chain of n (arbitrary but finite) d-dimensional oscillators with coordinates $q = (q_1, \ldots, q_n) \in \mathbb{R}^{nd}$, and momenta $p = (p_1, \ldots, p_n) \in \mathbb{R}^{nd}$ and with Hamiltonian

$$\begin{aligned} H_C(p,q) &= \sum_{i=1}^{n} \frac{p_i^2}{2} + \sum_{i=1}^{n} U^{(1)}(q_i) + \sum_{i=1}^{n-1} U^{(2)}(q_i - q_{i+1}) \\ &= \sum_{i=1}^{n} \frac{p_i^2}{2} + V(q)\,, \end{aligned} \tag{1}$$

where $U^{(1)}$ and $U^{(2)}$ are $\mathcal{C}^\infty$ confining potentials.

Each of the reservoirs is described by a wave equation in $\mathbb{R}^d$ with Hamiltonian $H_B(\varphi, \pi) = \frac{1}{2}\int_{\mathbb{R}^d} (|\nabla\varphi(x)|^2 + |\pi(x)|^2)\, dx$. One reservoir, denoted by the subscript L, is coupled to the first particle in the chain and another reservoir denoted by the subscript R is coupled to the n^{th} particle. As an interaction between the chain and reservoirs we choose a dipole approximation and the total Hamiltonian of the system is

$$\begin{aligned} H_B(\varphi_L, \pi_L) + q_1 \int_{\mathbb{R}^d} \nabla\varphi_L(x)\rho_L(x)\, dx + H_C(p,q) \\ + q_n \int_{\mathbb{R}^d} \nabla\varphi_R(x)\rho_R(x)\, dx + H_B(\varphi_R, \pi_R)\,. \end{aligned} \tag{2}$$

The Hamiltonian (2) describes the system at finite energy, i.e., at temperature zero. The inverse temperatures of the reservoirs β_L and β_R are introduced by assuming that the initial conditions of the reservoirs are distributed according to Gibbs measures μ_{β_L} and

μ_{β_R}. Formally these measures are given by

$$\text{“}Z^{-1}\exp(-\beta_k H(\varphi_k,\pi_k))\prod_{x\in\mathbb{R}^d} d\varphi_k(x)d\pi_k(x)\text{”}\,. \tag{3}$$

The equation (3) is merely a formal but suggestive expression. The measures μ_{β_k} are constructed as follows: The space of finite energy solutions of a wave equation is the real Hilbert space $\mathcal{H}=\dot{H}_1\times L^2$ with a scalar product denoted by $\langle\cdot\,,\,\cdot\rangle$. We have then $H_B(\varphi,\pi)=\frac{1}{2}\langle(\varphi,\pi)\,,\,(\varphi,\pi)\rangle$. The Gibbs measure μ_{β_k} is, by definition, the Gaussian measure (supported on the space of tempered distributions $\mathcal{S}'\times\mathcal{S}'$) with mean 0 and covariance $\beta_k^{-1}\langle\cdot\,,\,\cdot\rangle$. The existence of this measure follows from Bochner-Minlos Theorem. Almost surely, the initial conditions of the reservoir have infinite energy. For example in dimension $d=1$ one recognizes this measure as the product of a Wiener measure (for the φ) with a white noise measure (for the π).

In the case of one single reservoir, or several reservoirs at the same temperatures one expects and and one can show, under quite general conditions [10], that the system returns to equilibrium: the coupled system converges to the Gibbs state corresponding to the Hamiltonian (2). If the temperatures of the reservoirs are different, the stationary state of the system is not known explicitly any more. Even its mere existence turns out to be a nontrivial mathematical problem which requires a detailed understanding of the dynamics. One also expects this stationary state to have nontrivial transport properties. Under suitable assumptions on the potential in the chain and coupling to the reservoirs we show

(a) Existence and uniqueness of stationary states. They generalize the Gibbs states of equilibrium.
(b) Exponential rate of convergence of suitable initial distributions to the stationary state. This result is new even in equilibrium.
(c) Existence of a positive heat flow through the system if the temperatures of the reservoir are different or, in other words, positivity of entropy production.
(d) "Universal" properties of the entropy production. Its large fluctuations (of large deviations type) satisfy a symmetry known as Gallavotti-Cohen fluctuation theorem. Its small fluctuations (of central limit theorem type) around equilibrium are governed by Kubo formula.

Existence and uniqueness of the stationary state and positivity of entropy production were first obtained in [4,5] for potentials with quadratic growth at infinity and extended to more general polynomial growth in [2]. The exponential rate of convergence was obtained first in [20] and later by another method in [3,11]. The fluctuation theorem [6–8,12,14,17] is proved in [21]. The (exactly solvable) chain with quadratic potentials was considered earlier in [22,23]. Apart from the aforementioned properties, little is known (rigorously) on the properties of the nonequilibrium steady states, in particular virtually nothing is know on the dependence on n of the stationary state (see [1,15] for a review of the numerous numerical results, and [13] for a perturbative approach).

2. Ergodic properties

We describe and comment our technical assumptions.

H1 Polynomial Growth: There exist constants $A_i > 0$, $i = 1, 2$, such that

$$\lim_{\lambda \to \infty} \lambda^{-k_i} U^{(i)}(\lambda x) = A_i \|x\|^{k_i}\,, \tag{4}$$

and similar conditions for the first and second derivatives of $U^{(i)}$. Moreover we have

$$k_2 \geq k_1 \geq 2\,. \tag{5}$$

H2 Non-degeneracy of $U^{(2)}$: For $x \in \mathbb{R}^d$ and $m = 1, 2, \ldots$, let $A^{(m)}(x) : \mathbb{R}^d \to \mathbb{R}^{d^m}$ denote the linear maps given by

$$(A^{(m)}(x)v)_{l_1 l_2 \cdots l_m} = \sum_{l=1}^{d} \frac{\partial^{m+1} U^{(2)}}{\partial x_{l_1} \cdots \partial x_{l_m} \partial x_l}(x) v_l\,. \tag{6}$$

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

$$\mathrm{Rank}(A^{(1)}(x), \ldots, A^{(m_0)}(x)) = d\,. \tag{7}$$

The first part of **H1** is a mild condition of polynomial growth on $U^{(1)}(x)$ and $U^{(2)}(x)$. The condition **H2** is a local non-degeneracy condition which will ensures that energy is transmitted through the chain. In the special case $d = 1$, **H2** reduces to the fact that for any q, there exists $m = m(q) \geq 2$ such that $\frac{d^m U^{(2)}}{dq^m}(q) \neq 0$, i.e., there are neither linear pieces in the potential nor infinitely degenerate points. The second part of **H1**, equation(5), ensures that the two-body potential $U^{(2)}$ grows as fast or faster than the one-body potential $U^{(1)}(x)$ at infinity. This assumption has a dynamical significance. Infinite chains of nonlinear oscillators are known to exhibit breathers, i.e., spatially exponentially localized, time periodic solutions (see e.g. [16]). The condition (5) ensures that these breathers get more and more delocalized as their energy increases. On the contrary, if $k_1 > k_2$, a simple scaling argument shows that, at high energy, the oscillators in the chain behave essentially as uncoupled oscillators (the so-called anticontinuum limit). A crucial ingredient of our dynamical analysis is to show that initial conditions with energy localized far away from the boundaries spread sufficiently in order to interact with the reservoirs and dissipate their energies into them. In the case $k_1 > k_2$ we are unable to have good enough estimates to show even the existence of a stationary state. We expect, in any case, to have a much slower rate of convergence to the stationary state.

H3 Rational coupling: The Fourier transforms $\hat{\rho}_k(w)$, $k \in \{L, R\}$, of the coupling functions ρ_k have the form

$$|\omega|^{d-1} |\hat{\rho}_k(w)|^2 = \frac{1}{P_k(w^2)} \tag{8}$$

where P_k are polynomials.

The assumption **H3** is, in effect a Markovian assumption. With a change of variables one can reduce the dynamics of the chain coupled to the reservoirs at positive temperature to a set of Markovian stochastic differential equations for the variables p, q, and a finite number of auxiliary variables. In the simplest case $P_k(w^2) \propto w^2 + \gamma_k^2$ the equations have the form

$$\begin{aligned}
dq_1 &= p_1\, dt, \\
dp_1 &= (-\nabla_{q_1} V(q) - \lambda_L r_L)\, dt, \\
dr_L &= (-\gamma_L r_L + \lambda_L p_1)\, dt + (2\beta_L^{-1}\gamma_L)^{1/2} dB_L, \\
dq_j &= p_j\, dt, \quad j = 2, \ldots, n-1, \\
dp_j &= -\nabla_{q_j} V(q)\, dt, \quad j = 2, \ldots, n-1, \\
dq_n &= p_n\, dt, \\
dp_n &= (-\nabla_{q_n} V(q) - \lambda_R r_R)\, dt, \\
dr_R &= (-\gamma r_R + \lambda_R p_n)\, dt + (2\beta_R^{-1}\gamma_R)^{1/2} dB_R,
\end{aligned} \tag{9}$$

where r_k, $k \in \{L, R\}$ are auxiliary variables, λ_k are coupling constants given by $\lambda_k^2 = \int |\rho_k(x)|^2\, dx$, and B_k, $k \in \{L, R\}$ are Brownian motions. For more general polynomials one obtains similar equations [20].

One can state all our result in terms of the Markov process which solves equations (9), but we will choose here to state them in terms of the original variables. Consider the Hamiltonian equations of motion for the Hamiltonian (2). We concentrate on the variable of the chain and denote by

$$p_t = p_t(p, q, \Phi)\,, \quad q_t = q_t(p, q, \Phi)\,, \tag{10}$$

the solution with initial conditions (p, q) for the chain and initial conditions $\Phi \equiv (\varphi_L, \pi_L, \varphi_R, \pi_R)$ for the reservoirs. Since the initial condition of the reservoirs Φ is distributed according the Gaussian Gibbs measure $\mu_{\beta_L} \times \mu_{\beta_R}$ on $\Omega = (\mathcal{S}')^4$, we may view the solution equation(10) as a stochastic process

$$(t, \Phi) \in \mathbb{R} \times \Omega \mapsto (p_t, q_t) \in \mathbb{R}^{2nd}. \tag{11}$$

The measure $\mu_{\beta_L} \times \mu_{\beta_R}$ induces naturally a probability distribution on path space which we denote by $\mathbf{P}_{p,q}^{(\beta_L, \beta_R)}$ and we denote by $\mathbf{E}_{p,q}^{(\beta_L, \beta_R)}$ the corresponding expectation, where the subscript (p, q) indicates the initial conditions of the chain.

Theorem 2.1 (Ergodic properties). *If conditions* ***H1***, ***H2***, *and* ***H3*** *are satisfied we have*

(a) ***Ergodicity:*** *There exists a measure π_{β_L, β_R} on $\mathbb{R}^{2nd}$ with a positive smooth density such that*

$$\lim_{t \to \infty} \frac{1}{t} \int_0^t f(p_s, q_s)\, ds = \int f(p, q)\, d\pi_{\beta_L, \beta_R}(p, q)\,, \tag{12}$$

for all initial condition $x = (p, q)$ of the system, for $\mu_{\beta_L} \times \mu_{\beta_R}$ almost all initial conditions of the reservoirs, and for all observables $f \in L^1(\pi_{\beta_L, \beta_R})$.

(b) ***Exponential convergence:*** *Let $\theta < \min\{\beta_L, \beta_R\}$ and let $f(p, q)$ be an observable such that $|f(p, q)| \leq Ce^{\theta H(p,q)}$, then there exist positive constants $C = C_\theta$ and $\alpha = \alpha_\theta$ such that*

$$\left| \mathbf{E}_{p,q}^{(\beta_L, \beta_R)} \left[f(p_t, q_t) \right] - \int f(p, q)\, d\pi_{\beta_L, \beta_R}(p, q) \right| \leq Ce^{-\alpha t} \|f\|_\theta e^{\theta H(p,q)}\,, \tag{13}$$

where $\|f\|_\theta = \sup_{p,q} |f| \exp(-\theta H)$.

Part (a) of Theorem 2.1 tells us that, for almost all initial conditions of the reservoirs, the system will converge to a stationary state, while part (b) shows that this convergence occurs, in average, at a exponential rate.

The proof of Theorem 2.1 can be found in [20] and is based on a detailed analysis of the Markov process given by equation (9). We prove hypoellipticity of the generator to obtains smooth transition probabilities. We use control-theoretic tools and the support theorem of Stroock-Varadhan to show the irreducibility of the Markov process. Finally the central part of the proof consist in establishing dissipation estimates on the dynamics and constructing a Liapunov function for the Markov semigroup. Altogether we show that the Markov semigroup is a compact irreducible semigroup on a suitable function space.

3. Entropy production and its fluctuations

If the reservoirs have unequal temperatures one does expect that in the stationary state, energy is flowing from the hot reservoir through the chain into the cold reservoir (positivity of entropy production). Little is known about the general properties of systems in a nonequilibrium stationary state. The Kubo formula and Onsager reciprocity relations are such properties which are known to hold near equilibrium (i.e., if the temperatures of the reservoirs are close) and this is a result about small fluctuations around equilibrium (of central limit theorem type). In the last few years, a new general relation about nonequilibrium states has been discovered, the so-called Gallavotti-Cohen fluctuation Theorem. It asserts that the large fluctuations of the ergodic average of the entropy production have a certain symmetry. This symmetry can be seen as a generalization of Kubo formula and Onsager reciprocity relations to situations far from equilibrium. It has been discovered in numerical experiments in [6], proved as a theorem for Anosov maps [7,8] (modeling systems with deterministic thermostats), and extended to Markov processes in [12,14,17].

For our model this relation is proved in [21]. The large deviations aspects are nontrivial, due to the noncompactness of the phase space, the unboundedness of the observable of entropy production, and the degeneracy of the coupling (at the boundaries only). Note that the fluctuation theorem is derived entirely within Hamiltonian formalism without a-priori chaoticity or randomness assumptions on the dynamics (see also [9]).

To define the heat flows and the entropy productions we define the energy of the j^{th} oscillators of the chain as

$$H_j = \frac{p_j^2}{2} + U^{(1)}(q_j) + \frac{1}{2}\left(U^{(2)}(q_{j-1} - q_j) + U^{(2)}(q_j - q_{j+1})\right), \tag{14}$$

i.e., its kinetic energy, its potential energy plus half of its interaction energy with its neighbors. This choice is somewhat arbitrary, but other choices lead to exactly the same results.

Differentiating along a trajectory we find that

$$\frac{dH_j}{dt}(p_t, q_t) = F_{j-1}(p_t, q_t) - F_j(p_t, q_t), \tag{15}$$

where

$$F_j(p,q) = \frac{(p_j + p_{j+1})}{2} \nabla U^{(2)}(q_j - q_{j+1}). \tag{16}$$

It is natural to interpret F_j as the heat flow from the j^{th} to the $(j+1)^{\text{th}}$ particle in the chain. We define corresponding entropy productions by

$$\sigma_j = (\beta_R - \beta_L) F_j \,. \tag{17}$$

Our results on the heat flow and entropy production are summarized in

Theorem 3.1 (Entropy production). *If conditions **H1**, **H2**, and **H3** are satisfied we have*

(a) ***Positivity of entropy production:*** *The average of the entropy production σ_j in the stationary state π_{β_L,β_R} is independent of j and nonnegative, $\int \sigma_j d\pi_{\beta_L,\beta_R} \geq 0$ and it is positive away from equilibrium*

$$\int \sigma_j d\pi_{\beta_L,\beta_R} = 0 \quad \textit{if and only if} \quad \beta_L = \beta_R \,. \tag{18}$$

(b) ***Large deviations and fluctuation theorem:*** *The ergodic averages*

$$\overline{\sigma}_j{}^t \equiv \frac{1}{t}\int_0^t \sigma_j(x(s)) \tag{19}$$

satisfy the large deviation principle: There exist a neighborhood O of the interval

$$\left[- \int \sigma_j d\pi_{\beta_L,\beta_R} \,,\, \int \sigma_j d\pi_{\beta_L,\beta_R} \right] \tag{20}$$

and a rate function $e(w)$ (both independent of j) such that for all intervals $[a,b] \subset O$ we have

$$\lim_{t\to\infty} -\frac{1}{t} \log \mathbf{P}_{p,q}^{(\beta_L,\beta_R)}\{\overline{\sigma}_j{}^t \in [a,b]\} = \inf_{w\in[a,b]} e(w) \,. \tag{21}$$

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

$$e(w) - e(-w) = -w \,, \tag{22}$$

i.e., the odd part of e is linear with slope $-1/2$ (Gallavotti-Cohen fluctuation Theorem).

(c) ***Central limit theorem and Kubo formula:*** *Let us put $\beta = (\beta_L + \beta_R)/2$ and $\eta = \beta_R - \beta_L$. The fluctuations of the heat flow at equilibrium satisfy the central limit theorem*

$$\lim_{t\to\infty} \mathbf{P}_x^{\beta,\beta}\left\{ a < \frac{1}{\sqrt{\kappa^2 t}} \int_0^t F_j(p_s, q_s)\, ds < b \right\} = \frac{1}{\sqrt{2\pi}} \int_a^b \exp\left(-\frac{y^2}{2}\right) dy \,. \tag{23}$$

where κ^2 is finite and positive, independent of j, and given by the integrated autocorrelation function

$$\kappa^2 = \int_0^\infty \left(\int F_j(p,q)\, \mathbf{E}_{p,q}^{(\beta,\beta)}[F_j(p_t,q_t)]\, d\pi_{\beta,\beta}(p,q) \right) dt \,. \tag{24}$$

Moreover we have Kubo formula

$$\frac{\partial}{\partial \eta}\left(\int F_j d\pi_{\beta_L,\beta_R} \right)\Bigg|_{\eta=0} = \kappa^2 \,. \tag{25}$$

The central limit theorem follows easily from the strong ergodic properties obtained in Theorem 2.1. The large deviations for σ_i are more difficult, in particular since σ_i is an unbounded observable, not even bounded by the energy. But we use the very intimate link of the entropy production with the dynamics to show that it satisfies a large deviation principle. Note also that all our results on the fluctuations of σ_j are independent of j, the fluctuations are the same wherever the flow is measured and this would remain true even if we would choose different potentials at each lattice site or bond.

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