Open classical systems

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1 Introduction

Open systems are usually understood as a small Hamiltonian system (i.e. with a finite number of degrees of freedom) in contact with one or several large reservoirs. There are several ways to model reservoirs and we will take the point of view that the reservoirs are also Hamiltonian systems themselves. It is a convenient physical and mathematical idealization to separate scales and assume that the reservoirs have infinitely many degrees of freedom. We will also assume that, to start with, the reservoirs are in equilibrium, i.e., the initial states of the reservoirs are distributed according to Gibbs distribution with given temperatures. It is also mathematically convenient to assume that the Gibbs measures of the reservoir have very good ergodic properties. This is, in general, a mathematically difficult problem and we will circumvent it by assuming that our reservoirs have a linear dynamics (i.e the Gibbs measures are Gaussian measures).

Our model of a reservoir will be the classical field theory given by a linear wave equation in $\mathbf{R}^d$

$$\partial_t^2 \varphi_t(x) \;=\; \Delta \varphi_t(x)\,. \tag{1.1}$$

This is a Hamiltonian system for the Hamiltonian

$$H(\varphi, \pi) \;=\; \int_{\mathbf{R}^d} (|\nabla_x \varphi(x)|^2 + |\pi(x)|^2)\,. \tag{1.2}$$

If we consider a single particle in a confining potential with Hamiltonian

$$H(p, q) \;=\; \frac{p^2}{2} + V(q)\,, \tag{1.3}$$

we will take as Hamiltonian of the complete system

$$H(\varphi, \pi) + H(p, q) + q \int_{\mathbf{R}^d} \nabla \varphi(x) \rho(x)\, dx\,, \tag{1.4}$$

which corresponds to a dipole coupling approximation ($\rho(x)$ is a given function which models the coupling of the particle with the field).

If one considers finite-energy solutions for the wave equation, we will say the model is at temperature zero. In this case the physical picture is "radiation damping". The particle energy gets dissipated into the field and relaxes to a stationary point of the Hamiltonian (i.e. $p = 0$, $\nabla V(q) = 0$). This problem is studied in [14] for a slightly different model.

We will say the model is at inverse temperature β if we assume that the initial conditions of the wave equations are distributed according to a Gibbs measure at inverse temperature β. Typical configurations of the field have then infinite energy and thus provide enough energy to let the system "fluctuate". In this case one expects "return to equilibrium", an initial distribution of the system will converge to a stationary state which is given by the Gibbs distribution

$$Z^{-1} e^{-\beta H(p,q)} dpdq \,. \tag{1.5}$$

The property of return to equilibrium is proved [13] under rather general conditions.

If the small system is coupled to more than one reservoir and the reservoirs have different temperatures (and/or chemical potentials), then one can extract an infinite amount of energy or work from the reservoirs and transmit them through the small system from reservoir to reservoir. Doing this, one can maintain the small systems in a stationary (i.e time independent) nonequilibrium states in which energy and/or matter is flowing. Think e.g. of a bar of metal which is heated at one end and cooled at the other. Contrary to the two previous situations where we know a priori the final state of the system, in nonequilibrium situations, in general, we do not. Even the existence of a stationary state turns out to be a nontrivial mathematical problem and requires a quite detailed understanding of the dynamics. In these lectures we will consider a simple, yet physically realistic model of heat conduction through a lattice of anharmonic oscillators.

Our small system will consist of a chain of anharmonic oscillators with Hamiltonian

$$\begin{aligned} H(p,q) &= \sum_{i=1}^{n} \frac{p_i^2}{2} + V(q_1, \cdots, q_n) \,, \\ V(q) &= \sum_{i=1}^{n} U^{(1)}(q_i) + \sum_{i=1}^{n-1} U^{(2)}(q_i - q_{i+1}) \,. \end{aligned} \tag{1.6}$$

where $V(q)$ is a confining potential. The number oscillators, n, will be arbitrary (but finite). In a realistic model, the coupling should occur only at the boundary and we will couple the first particle of the chain to one reservoir at inverse temperature β_1 and the n-th particle to another reservoir at inverse temperature β_n. The Hamiltonian of the complete system is

$$\begin{aligned} H(\varphi_1, \pi_1) + q_1 \int_{\mathbf{R}^d} \nabla\varphi_1(x)\rho_1(x) \ + H(p_1, \cdots, p_n, q_1, \cdots, q_n) \\ +q_n \int_{\mathbf{R}^d} \nabla\varphi_n(x)\rho_n(x) + H(\varphi_n, \pi_n) \,. \end{aligned} \tag{1.7}$$

Our analysis of this model will establish, that under suitable assumptions on the potential energy V and on the coupling functions ρ_i, we have

1. Existence and uniqueness of stationary states which generalize the Gibbs states of equilibrium.

2. Exponential rate of convergence of initial distribution to the stationary distribution. This is a new result even for equilibrium.

3. 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.

4. "Universal" properties of the entropy production. Its (large) fluctuations satisfy a symmetry known as Gallavotti-Cohen fluctuation theorem (large deviation theorem) recently discovered in [8, 11]. Its small fluctuations (of central limit theorem type) are governed by Green-Kubo formula which we prove for this model.

See [24, 25] for results on the linear chain and [6, 7, 21, 4, 22, 23, 12, 5] for results on the nonlinear chain. We follow here mostly [22, 23]

An important ingredient in our approach is the use of rather special coupling functions ρ ("rational couplings"). They will allow us to reduce the dynamics of the coupled system to a Markov process in a suitable enlarged phase space and therefore to take advantage of the numerous analytical tools developed for Markov processes (semigroups, PDE's, control theory, see our lecture on Markov processes in these volumes [20]). Physically these couplings are not unreasonable, but it would be nice to go beyond and prove similar results for more general couplings.

We conclude this introduction by mentioning one outstanding problem in mathematical physics: describe quantitatively the transport properties in large systems. One would like, for example, to establish the dependence of the heat flow on the size of the system (here the number n of oscillators). For heat conduction the relevant macroscopic law is the Fourier law of heat conduction. If we denote by J the stationary value of the heat flow and δT the temperature difference between the reservoirs, one would like to prove for example that for large n

$$J \approx \kappa \frac{\delta T}{n}, \tag{1.8}$$

where the coefficient κ is known as the heat conductivity. A more refined version of this law would to prove that a (local) temperature gradient is established through the system and that the heat flow is proportional to the temperature gradient

$$J \approx -\kappa \nabla T, \tag{1.9}$$

This is a stationary version of the time dependent macroscopic equation

$$c_v \partial_t T(x,t) = -\nabla J(x,t) = \nabla \kappa \nabla T(x,t), \tag{1.10}$$

where c_v is the specific heat of the system. This is just the heat equation! In other words the challenge is to derive the heat equation from a microscopic Hamiltonian system. No mechanical model has been shown to obey Fourier law of heat conduction so far (see [1, 17] for reviews of this problem and references).

2 Derivation of the model

2.1 How to make a heat reservoir

Our reservoir is modeled by a linear wave equation in $\mathbf{R}$ (the restriction to one-dimension is for simplicity, similar considerations apply to higher dimensions),

$$\partial_t^2 \varphi_t(x) = \partial_x^2 \varphi_t(x), \tag{2.1}$$

with $t \in \mathbf{R}$ and $x \in \mathbf{R}$. The equation (2.1) is a second order equation and we rewrite it as a first order equation by introducing a new variable $\pi(x)$

$$\begin{aligned} \partial_t \varphi_t(x) &= \pi_t(x), \\ \partial_t \pi_t(x) &= \partial_x^2 \varphi_t(x). \end{aligned} \tag{2.2}$$

The system (2.2) has an Hamiltonian structure. Let us consider the Hamiltonian function

$$H(\varphi,\pi) \;=\; \int_{\mathbf{R}} (|\partial_x\varphi(x)|^2 + |\pi(x)|^2)\, dx\,. \qquad (2.3)$$

then Eqs. (2.2) are the Hamiltonian equations of motions for the Hamiltonian (2.3). Let us introduce the notation $\phi = (\varphi,\pi)$ and the norm

$$\|\phi\| \;=\; \int_{\mathbf{R}} (|\partial_x(x)|^2 + |\pi|^2)\, dx\,. \qquad (2.4)$$

We have then $H(\phi) = \frac{1}{2}\|\phi\|^2$ and denote $\mathcal{H} = \dot{H}_1(\mathbf{R}) \times L^2(\mathbf{R})$ the corresponding Hilbert space of finite configurations.

In order to study the statistical mechanics of such systems we need to consider the *Gibbs measure* for such systems. We recall that for an Hamiltonian systems with finitely many degrees of freedom with Hamiltonian $H(p,q) = p^2/2 + V(q)$, $p,q \in \mathbf{R}^n$, the Gibbs measure for inverse temperature β is given by

$$\mu_\beta(dpdq) \;=\; Z^{-1} e^{-\beta H(p,q)}\, dpdq\,, \qquad (2.5)$$

where $\beta = 1/T$ is the inverse temperature and $Z = \int \exp(-\beta H(p,q))\, dp\, dq$ is a normalization constant which we assume to be finite. One verifies easily that the probability measure μ_β is invariant under the dynamics, i.e., if (p_t,q_t) is a solution of Hamiltonian equations of motion then

$$\int f(p_t,q_t)\mu_\beta(dpdq) \qquad (2.6)$$

is independent of t. (Use conservation of energy and Liouville theorem)

We now construct Gibbs measures for the linear wave equation Eq. (2.1). If we think of $\{\varphi(x),\pi(x)\}_{x\in\mathbf{R}}$ as the dynamical variables, the Gibbs measure should be, formally, given by

$$\mu_\beta(d\varphi d\pi) \;=\; {}''Z^{-1}\exp(-\beta H(\varphi,\pi)) \prod_{x\in\mathbf{R}} d\varphi(x)d\pi(x)''\,. \qquad (2.7)$$

It turns out that this expression is merely formal: it is a product of three factors which are all infinite, nevertheless the measure can be constructed. We sketch this construction.

We first note that this measure should be a Gaussian measure since H is quadratic in $\phi = (\varphi,\pi)$. A Gaussian measure μ_β on $\mathbf{R}$ with mean 0 and variance β is completely characterized by the fact that its characteristic function (the Fourier transform of the measure) is given by

$$S(\xi) = \int e^{i\langle \xi , x\rangle} \mu_\beta(dx) = e^{-\frac{1}{2\beta}\langle x , x\rangle} . \tag{2.8}$$

is again a Gaussian. Let $\mathcal{H}$ be an infinite dimensional Hilbert space, $\phi \in \mathcal{H}$, $\xi \in \mathcal{H}^* = \mathcal{H}$. Can we construct a measure μ_β on the Hilbert space $\mathcal{H}$, such that

$$S(\xi) = \int e^{i\langle \phi , \xi\rangle} \mu_\beta(d\phi) = e^{-\frac{1}{2\beta}\langle \xi , \xi\rangle} ? \tag{2.9}$$

The answer is **NO**.
Proof: By contradiction. Let $\{e_n\}$ be an orthonormal basis of $\mathcal{H}$. We then have $S(e_n) = e^{-1/2\beta}$. For any $\phi \in \mathcal{H}$, $\langle \phi , e_n\rangle \to 0$ as $n \to \infty$. By dominated convergence we have

$$\lim_{n\to\infty} S(e_n) = 1 \neq e^{-\frac{1}{2\beta}} . \tag{2.10}$$

and this is a contradiction. ∎

All what this says is that we must give up the requirement that the measure μ be supported on the Hilbert space $\mathcal{H}$ (i.e., on finite energy configurations). The Bochner-Minlos Theorem allows us to construct such measures supported on larger spaces of distributions. Let A be the operator on $\mathcal{H}$ given by

$$A = \begin{pmatrix} (1-\partial_x^2 + x^2)^{\frac{1}{2}} & 0 \\ 0 & (1-\partial_x^2 + x^2)^{\frac{1}{2}} \end{pmatrix} . \tag{2.11}$$

We it leave to the reader to verify that A has compact resolvent and that A^{-s} is Hilbert-Schmidt if $s > 1/2$. For $s > 0$ we define Hilbert spaces

$$K_s = \{u \in L^2 ; \|u\|_s \equiv \|A^s u\| < \infty\} , \tag{2.12}$$

and for $s < 0$, $K_s = K_{-s}^*$ where $*$ is the duality in $\mathcal{H}$. We have, for $0 \leq s_1 \leq s_2$,

$$H_{s_2} \subset H_{s_1} \subset L^2 \subset H_{-s_1} \subset H_{-s_2} , \tag{2.13}$$

with dense inclusions. We set

$$\mathcal{S} = \bigcap_s H_s , \quad \mathcal{S}' = \bigcup_s H_s . \tag{2.14}$$

The space $\mathcal{S}'$ is simply a space of tempered distributions.

Theorem 2.1 (Bochner-Minlos Theorem) *There is a one-to-one correspondence between measures on $\mathcal{S}'$ and functions $S : \mathcal{S} \to \mathbf{R}$ which satisfy*

1. *S is continuous.*
2. *$S(0) = 1$.*
3. *S is of positive type, i.e. $\sum_{i,j=1}^{n} S(f_i - f_j)\overline{z}_i z_j \geq 0$, for all $n \geq 1$, for all $f_1, \cdots, f_n \in \mathcal{S}$, and for all $z \in \mathbf{C}^n$.*

The function S is the characteristic function of the measure. The Gaussian Gibbs measures μ_β are then specified by the characteristic function

$$S(\xi) \;=\; \int e^{i\langle \phi\,,\,\xi\rangle} \mu_\beta(d\phi) \;=\; e^{-\frac{1}{2\beta}\langle \xi\,,\,\xi\rangle}\,. \tag{2.15}$$

where $\langle \phi\,,\,\xi\rangle$ denotes now the $\mathcal{S} - \mathcal{S}'$ duality. If we put $\xi = a_1\xi_1 + a_2\xi_2$, the characteristic function allows us to compute the correlation functions (differentiate with respect to a_1, a_2 and compare coefficients):

$$\begin{aligned} \int_{\mathcal{S}'} \langle \phi\,,\,\xi\rangle \mu_\beta(d\phi) &= 0\,, \\ \int_{\mathcal{S}'} \langle \phi\,,\,\xi_1\rangle\,\langle \phi\,,\,\xi_2\rangle \mu_\beta(d\phi) &= \beta^{-1}\langle \xi_1\,,\,\xi_2\rangle\,. \end{aligned} \tag{2.16}$$

We have then

Lemma 2.2 *If $s > \frac{1}{2}$, then*

$$\int \|A^{-s}\phi\|^2\,\mu_\beta(d\phi) \;=\; \beta^{-1}\mathrm{trace}(A^{-2s}) \;<\; \infty\,. \tag{2.17}$$

and thus $\|A^{-s}\phi\|$ is finite μ_β a.s.

Proof: Let λ_j denote the eigenvalues of A and e_j the orthonormal basis of eigenvectors of A. We have $A^{-s}\phi = \sum_j \lambda_j^{-s} e_j \langle \phi\,,\,e_j\rangle$ and thus

$$\int \|A^{-s}\phi\|^2\,\mu_\beta(d\phi) \;=\; \sum_j \lambda_j^{-2s} \int (\langle \phi\,,\,e_j\rangle)^2 \mu_\beta(d\phi) \;=\; \beta^{-1}\sum_j \lambda_j^{-2s}\,. \tag{2.18}$$

∎

As a consequence we see that for a typical element $\phi = (\varphi, \pi)$ in the support of μ_β, φ has $\frac{1}{2} - \epsilon$ derivatives for all $\epsilon > 0$ and π has $-\frac{1}{2} - \epsilon$ derivatives. Let us compute now the correlations

$$\int \pi(x_1)\pi(x_2)\mu_\beta(d\phi) \quad \text{and} \int \varphi(x_1)\varphi(x_2)\mu_\beta(d\phi)\,. \tag{2.19}$$

These expressions have to be interpreted in the distribution sense. Our computations are formal but can be easily justified. If we choose $\xi_1 = (0, \delta(x - x_1))$ and $\xi_2 = (0, \delta(x - x_2))$ we obtain from Eq. (2.16)

$$\int \pi(x_1)\pi(x_2)\mu_\beta(d\phi) \;=\; \beta^{-1}\delta(x_1 - x_2)\,, \tag{2.20}$$

i.e., if we think of x as "time" then $\pi(x)$ is a white noise process. On the other hand if we choose $\xi_1 = (\theta(x-t), 0)$ and $\xi_2 = (\theta(x-s), 0)$ and use that $\partial_x\theta(x) = \delta(x)$ we obtain from Eq. (2.16)

$$\begin{aligned}
\int (\varphi(x_1) - \varphi(x_2))^2\mu_\beta(d\phi) &= \int_{x_1}^{x_2}\int_{x_1}^{x_2}\int \partial_x\varphi(t)\partial_x\varphi(s)\,\mu_\beta(d\phi)\,dt\,ds \\
&= \beta^{-1}\int_{x_1}^{x_2}\int_{x_1}^{x_2}\delta(t-s)\,dt\,ds \\
&= \beta^{-1}|x_2 - x_1|\,.
\end{aligned} \tag{2.21}$$

i.e., if we think of x as "time" then $\varphi(x)$ is a Brownian motion. Note that if we combine this computation with Kolmogorov Continuity Theorem we obtain that the paths of Brownian motion are almost surely Hölder continuous with exponents $\alpha < 1/2$ and almost never Hölder continuous with exponents $\alpha \geq 1/2$.

If we consider the wave equation in $\mathbf{R}^d$, then one obtains similar results (random fields indexed by $\mathbf{R}^d$ instead of "stochastic processes").

2.2 Markovian Gaussian stochastic processes

In this section we describe a few facts on Gaussian stochastic process, in particular we describe a situation when Gaussian stochastic processes are Markovian (see [3]).

Let us consider a one dimensional Gaussian stochastic process x_t. Recall that Gaussian means that for all k and all $t_1 < \cdots < t_k$, the random variable $Z = (x_{t_1}, \cdots, x_{t_k})$ is a normal random variable. Let us assume that

x_t has mean 0, $\mathbf{E}[x_t] = 0$, for all t. Then the Gaussian process is uniquely determined by the expectations

$$\mathbf{E}[x_t x_s]\,. \tag{2.22}$$

which are called the covariance of x_t. If x_t is stationary, then (2.22) depends only on $|t-s|$:

$$C(t-s) \;=\; \mathbf{E}[x_t x_s]\,. \tag{2.23}$$

Note that $C(t-s)$ is positive definite. If C is a continuous function then a special case of Bochner-Minlos theorem (with $\mathcal{S}' = \mathbf{R}$) implies that

$$C(t) \;=\; \int_{\mathbf{R}} e^{ikt} d\Delta(k)\,, \tag{2.24}$$

where $\Delta(k)$ is an odd nondecreasing function with $\lim_{k\to\infty}\Delta(k) < \infty$. If we assume that $\Delta(k)$ has no singular part, then $d\Delta(k) = \Delta'(k)dk$ and the function $\Delta'(k)$ is called the *spectral function* of the Gaussian process x_t. Note that

$$\Delta'(k) \geq 0\,, \tag{2.25}$$

since Δ is nondecreasing and that

$$\overline{\Delta'(k)} \;=\; \Delta'(-k)\,, \tag{2.26}$$

since $C(t)$ is real. We will consider here only the special case when $(\Delta')^{-1}$ is a polynomial. By the conditions (2.25) and (2.26) there is a polynomial

$$p(k) \;=\; \sum_m c_m(-ik)^m\,, \tag{2.27}$$

with real coefficients c_m and root in the upper half plane such that

$$\Delta'(k) = \frac{1}{|p(k)|^2}\,. \tag{2.28}$$

Under these conditions we have

Proposition 2.3 *If $p(k) = \sum_m^M c_m(-ik)^m$ is a polynomial with real coefficients and roots in upper half plane then the Gaussian process with spectral density $|p(k)|^{-2}$ is the solution of the stochastic differential equation*

$$\left(p\left(-i\frac{d}{dt}\right)x_t\right)\,dt \;=\; dB_t \tag{2.29}$$

Proof: The proof follows from the following representation of x_t: let us define a kernel $k(t)$ by

$$k(t) = \frac{1}{\sqrt{2\pi}} \int_{\mathbf{R}} e^{ikt} \frac{1}{p(k)} dk \,. \tag{2.30}$$

Since the zeros of p are in the upper half-plane, we have $k(t) = 0$ if $t < 0$. We claim that x_t can be represented as the stochastic integral

$$x_t = \int_{-\infty}^{\infty} k(t-t')dB_{t'} = \int_{-\infty}^{t} k(t-t')dB_{t'} \tag{2.31}$$

It suffices to compute the variance, we have

$$\begin{aligned}
\mathbf{E}[x_t x_s] &= \frac{1}{2\pi}\int_{\mathbf{R}}\int_{\mathbf{R}} k(t-t')k(s-s')\mathbf{E}[dB_{t'}dB_{s'}] \\
&= \frac{1}{2\pi}\int_{\mathbf{R}}\int_{\mathbf{R}} k(t-t')k(s-s')\delta(t'-s')\, dt'\, ds' \\
&= \frac{1}{2\pi}\int_{\mathbf{R}} k(t-s')k(s-s')\, ds' \\
&= \frac{1}{2\pi}\int_{\mathbf{R}}\int_{\mathbf{R}}\int_{\mathbf{R}} e^{ik(t-s')}e^{ik'(s-s')}\frac{1}{p(k)p(k')}\, ds'\, dk\, dk' \\
&= \int_{\mathbf{R}}\int_{\mathbf{R}} e^{ikt}e^{ik's}\frac{1}{p(k)p(k')}\delta(k+k')\, dk\, dk' \\
&= \int_{\mathbf{R}} e^{i(t-s)k}\frac{1}{p(k)p(-k)} dk
\end{aligned} \tag{2.32}$$

and this proves the claim. From Eq. (2.31) we obtain

$$\begin{aligned}
p\left(-i\frac{d}{dt}\right) x_t &= \int_{-\infty}^{t}\int_{\mathbf{R}} p\left(-i\frac{d}{dt}\right) e^{ik(t-t')}\frac{1}{p(k)}\, dk\, dB_{t'} \\
&= \int_{-\infty}^{t}\int_{\mathbf{R}} e^{ik(t-t')}\, dk\, dB_{t'} = \frac{dB}{dt}\,.
\end{aligned} \tag{2.33}$$

and this concludes the proof of the proposition. ∎

For example let us take

$$\Delta'(k) = \frac{\gamma}{\pi}\frac{1}{k^2+\gamma^2} \tag{2.34}$$

and so $p(k) \propto (ik+\gamma)$ Then

$$C(t) = \frac{\gamma}{\pi}\int e^{ikt}\frac{1}{k^2+\gamma^2}dk = e^{-\gamma|t|}\,, \tag{2.35}$$

and

$$
\begin{aligned}
k(t) &= \sqrt{2\gamma}e^{-\gamma t}\,, \quad t \geq 0\,. \\
x(t) &= \sqrt{2\gamma}\int_{-\infty}^{t} e^{-\gamma(t-t')}dB_{t'}
\end{aligned}
\tag{2.36}
$$

and we obtain

$$
dx_t \;=\; -\gamma x_t + \sqrt{2\gamma}dB_t\,. \tag{2.37}
$$

This is the Ornstein-Uhlenbeck process.

It is good exercise to compute the covariances $C(t)$ and derive the corresponding stochastic differential equations for the spectral densities with $p(k) \propto (ik+iu+\gamma)(ik-iu+\gamma)$ and $p(k) \propto (ik+\gamma)^2$.

2.3 How to make a Markovian reservoir

We derive effective equations for the small system. In spirit we are close to [9], although we are deriving different equations. Let us consider first a model of one single particle with Hamiltonian $H_S(p,q) = p^2/2 + V(q)$, where $(p,q) \in \mathbf{R} \times \mathbf{R}$, coupled to a single reservoir. The total Hamiltonian is, using the notation (2.4)

$$
\begin{aligned}
H(\phi,p,q) &= \frac{1}{2}\|\phi\|^2 + p^2 + V(q) + q\int \partial_x\varphi(x)\rho(x)\,dx \\
&= H_B(\phi) + H_S(p,q) + q\langle \phi\,,\,\alpha\rangle\,,
\end{aligned}
\tag{2.38}
$$

where, in Fourier space, $\hat{\alpha}(k) = (-ik\hat{\rho}(k)/k^2, 0)$. Let $\mathcal{L}$ be the linear operator given by

$$
\mathcal{L} \;=\; \begin{pmatrix} 0 & 1 \\ \partial_x^2 & 0 \end{pmatrix}. \tag{2.39}
$$

In Fourier space the semigroup $e^{t\mathcal{L}}$ is given by

$$
e^{t\mathcal{L}} \;=\; \begin{pmatrix} \cos(kt) & k^{-1}\sin(kt) \\ -k\sin(kt) & \cos(kt) \end{pmatrix}. \tag{2.40}
$$

Let us introduce the covariance function $C(t) = \langle \exp(\mathcal{L}t)\alpha\,,\,\alpha\rangle$. We have

$$
C(t) \;=\; \int k^2\frac{ik}{k^2}\overline{\hat{\rho}(k)}\cos(kt)\frac{-ik}{k^2}\hat{\rho}(k)\,dk \;=\; \int |\hat{\rho}(k)|^2 e^{ikt}\,dk\,, \tag{2.41}
$$

and thus $C(t)$ is the covariance function of a Gaussian process with spectral density $|\rho(k)|^2$. We also define a coupling constant λ by setting

$$\lambda^2 = C(0) = \int dk|\rho(k)|^2 \,. \tag{2.42}$$

The equations of motion of the coupled system particle and reservoir are

$$\begin{aligned} \dot{q}_t &= p_t \,, \\ \dot{p}_t &= -\partial_q V(q_t) - \langle \phi, \alpha \rangle \,, \\ \dot{\phi}_t(k) &= \mathcal{L}\left(\phi_t(k) + q_t\alpha(k)\right) \,. \end{aligned} \tag{2.43}$$

Integrating the last equation of (2.43) we have

$$\phi_t(k) = e^{\mathcal{L}t}\phi_0(k) + \int_0^t e^{\mathcal{L}(t-s)}\mathcal{L}\alpha(k)q_s \, ds \,. \tag{2.44}$$

Inserting into the second equation of (2.43) we obtain

$$\begin{aligned} \dot{q}_t &= p_t \,, \\ \dot{p}_t &= -\partial_q V(q_t) - \int_0^t D(t-s)q_s \, ds - \langle \phi_0, e^{-\mathcal{L}t}\alpha \rangle \,. \end{aligned} \tag{2.45}$$

where

$$D(t) = \langle e^{\mathcal{L}t}\mathcal{L}\alpha \,, \, \alpha \rangle = \dot{C}(t) \,. \tag{2.46}$$

Let us assume that the initial conditions of the reservoir ϕ_0 are distributed according to the Gibbs measure μ_β defined in Section 2.1. Then

$$y_t = \langle \psi_0 e^{-\mathcal{L}t}\alpha \rangle \,, \tag{2.47}$$

is a Gaussian process with covariance

$$\mathbf{E}[y_t y_s] = \int \langle \phi_0, e^{-\mathcal{L}t}\alpha \rangle \langle \phi_0, e^{-\mathcal{L}s}\alpha \rangle \mu_\beta(d\phi) = \beta^{-1}C(t-s) \,. \tag{2.48}$$

The equation (2.45) is a random integro-differential equation, since it contains memory terms both deterministic and random. The relation between the kernel D in the deterministic memory term and the covariance of the random term goes under the general name of Fluctuation-Dissipation Theorem. The solution of (2.45) is a random process. Note that the randomness in this equation comes from our choice on initial conditions of the reservoir. Let us choose the coupling function ρ, as in Section 2.2, such that

$$|\rho(k)|^2 = \frac{1}{|p(k)|^2}\,, \tag{2.49}$$

where p is a real polynomial in ik with roots in the lower half-plane. For simplicity we choose $p(k) \propto (ik + \gamma)$ This assumption together with the fluctuation-dissipation relation permits, by extending the phase space with one auxiliary variable, to rewrite the integro-differential equations (2.45) as a Markov process. We have then $C(t) = \lambda^2 e^{-\gamma|t|}$. It is convenient to introduce the variable r which is defined defined by

$$\lambda r_t = \lambda^2 q_t + \int_0^t D(t-s) q_s\, ds + y_t\,, \tag{2.50}$$

and we obtain from Eqs.(2.45) the set of Markovian differential equations:

$$\begin{aligned} dq_t &= dp_t\, dt\,, \\ dp_t &= (-\partial_q V_{\text{eff}}(q_t) - \lambda r_t)\,, \\ dr_t &= (-\gamma r_t + \lambda p_t)\, dt + \sqrt{2\beta^{-1}\gamma}\, dB_t\,. \end{aligned} \tag{2.51}$$

where $V_{\text{eff}}(q) = V(q) - \lambda^2 q^2/2$. The potential V is renormalized by the coupling to the reservoir. This is an artifact of the dipole approximation we have been using. Namely if we start with a translation invariant coupling of the form

$$\int \phi(x)\rho(x-q)\, dx\,, \tag{2.52}$$

the dipole expansion leads to terms of the form

$$q \int \partial_x \phi(x)\rho(x)\, dx + \frac{q^2}{2} \int |\rho(x)|^2\, dx\,, \tag{2.53}$$

and the second term exactly compensates the normalization of the potential. We will ignore this renormalization in the sequel.

If one chooses other polynomials, similar equations can be derived. One should add one auxiliary variable for each pole of the polynomial $p(k)$. It is a good exercise to derive the SDE's for a particle coupled to a wave equation if we choose $p(k) \propto (ik + iu - \gamma)(ik - iu - \gamma)$ or $p(k) \propto (ik - \gamma)^2$.

One can recover the Langevin equation,

$$\begin{aligned} dq_t &= dp_t\, dt\,, \\ dp_t &= (-\partial V(q_t)\, dt - \kappa p_t)\, dt + \sqrt{2\beta^{-1}\kappa}\, dB_t\,. \end{aligned}$$

but only in a suitable limit. Formally one would obtain these equations if $C(t-s) \propto \delta(t-s)$ (this corresponds to choosing $\rho(k) = 1$ which is not square integrable). But then the coupling constant $\lambda^2 = C(0)$ becomes infinite. Rather one should consider a suitable sequence of covariance which tends to a delta function and simultaneously rescale the coupling constant.

3 Ergodic properties: the chain

We consider here a model of non-equilibrium statistical mechanics: a one-dimensional "crystal" coupled at each end to reservoirs at different temperatures.

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

$$\begin{aligned} H_S(p,q) &= \sum_{i=1}^{n} \frac{p_i^2}{2} + V(q_1, \cdots, q_n)\,, \\ V(q) &= \sum_{i=1}^{n} U^{(1)}(q_i) + \sum_{i=1}^{n-1} U^{(2)}(q_i - q_{i+1})\,. \end{aligned}$$

where $(p_i, q_i) \in \mathbf{R} \times \mathbf{R}$. 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

$$\lim_{\lambda\to\infty} \lambda^{-k_i} U^{(i)}(\lambda x) = a^{(i)} |x|^{k_i}\,, \tag{3.1}$$

$$\lim_{\lambda\to\infty} \lambda^{-k_i+1} \partial_x U^{(i)}(\lambda x) = a^{(i)} k_i |x|^{k_i-1}\,, \tag{3.2}$$

$$|\partial_x^2 U^{(i)}(x)| \le (C_i + D_i U^{(i)}(x))^{1-\frac{2}{k_i}}\,. \tag{3.3}$$

Moreover we will assume that

$$k_2 \ge k_1 \ge 2\,, \tag{3.4}$$

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 any $q \in \mathbf{R}$, there exists $m = m(q) \geq 2$ such that $\partial^m U^{(2)}(q) \neq 0$. This means that $U^{(2)}$ has no flat pieces nor infinitely degenerate critical points. Note that we require this condition for $U^{(2)}$ only and not for $U^{(1)}$.

For example if $U^{(1)}$ and $U^{(2)}$ are polynomials of even degree, with a positive coefficients for the monomial of highest degree and $\deg U^{(2)} \geq \deg U^{(1)} \geq 2$, then both conditions **H1** and **H2** are satisfied.

We couple the first and the n^{th} particle to reservoirs at inverse temperatures β_1 and β_n, respectively. We assume that the couplings to be as in Section 2.3 so that, by introducing two auxiliary variables r_1 and r_n, we obtain the set of stochastic differential equations equations

$$\begin{aligned}
dq_{1t} &= dp_{1t}\, dt\,, \\
dp_{1t} &= (-\partial_{q_1} V(q_t) - \lambda r_{1t}) dt\,, \\
dr_{1t} &= (-\gamma r_{1t} + \lambda p_{1t})\, dt + (2\beta_1^{-1}\gamma)^{1/2} dB_{1t}\,, \\
dq_{jt} &= dp_{jt}\, dt\,, \qquad\qquad j = 2, \ldots, n-1\,, \\
dp_{jt} &= -\partial_{q_j} V(q_t)\, dt\,, \qquad j = 2, \ldots, n-1\,, \\
dq_{nt} &= p_{nt}\, dt\,, \\
dp_{nt} &= (-\partial_{q_{nt}} V(q_t) - \lambda r_{nt})\, dt\,, \\
dr_{nt} &= (-\gamma r_{nt} + \lambda p_{nt})\, dt + (2\beta_n^{-1}\gamma)^{1/2} dB_{nt}\,.
\end{aligned} \tag{3.5}$$

It will be useful to introduce the following notation. We define the linear maps $\Lambda : \mathbf{R}^n \to \mathbf{R}^2$ by $\Lambda(x_1, \ldots, x_n) = (\lambda x_1, \lambda x_n)$ and $T : \mathbf{R}^2 \to \mathbf{R}^2$ by $T(x, y) = (\beta_1^{-1} x, \beta_n^{-1} y)$. We can rewrite Eq.(3.5) in the compact form

$$\begin{aligned}
dq_t &= p_t\, dt\,, \\
dp_t &= (-\nabla_q V(q_t) - \Lambda^* r)\, dt\,, \\
dr_t &= (-\gamma r_t + \Lambda p_t)\, dt + (2\gamma T)^{1/2} dB_t\,.
\end{aligned} \tag{3.6}$$

where $B = (B_1, B_n)$ is a two dimensional Brownian motion. The solution $x_t = (p_t, q_t, r_t) \in \mathbf{R}^{2n+2}$ of Eq.(3.6) is a Markov process. We denote T_t the associated semigroup and $P_t(x, dy)$ the transition probabilities

$$T_t f(x) = \mathbf{E}_x[f(x_t)] = \int_{\mathbf{R}^n} P_t(x, dy) f(y)\,. \tag{3.7}$$

The generator of T_t is given by

$$L = \gamma\left(\nabla_r T \nabla_r - r\nabla_r\right) + \left(\Lambda p \nabla_r - r\Lambda\nabla_p\right) + \left(p\nabla_q - (\nabla_q V(q))\nabla_p\right) , \quad (3.8)$$

and the adjoint of L (Fokker-Planck operator) is given by

$$L^* = \gamma\left(\nabla_r T \nabla_r + \nabla_r r\right) - \left(\Lambda p \nabla_r - r\Lambda\nabla_p\right) - \left(p\nabla_q - (\nabla_q V(q))\nabla_p\right) . \quad (3.9)$$

There is a natural energy function which is associated to Eq.(3.6), given by

$$G(p,q,r) = \frac{r^2}{2} + H(p,q) . \quad (3.10)$$

Since we assumed that $H(p,q)$ is a smooth function, we have local solutions for the SDE (3.6). A straightforward computation shows that we have

$$LG(p,q,r) = \gamma(\mathrm{tr}(T) - r^2) \le \gamma\mathrm{tr}(T) . \quad (3.11)$$

Therefore we obtain global existence for the solutions of (3.6) (see Theorem 5.9 in [20]). Also a straightforward computation shows that in the special case of equilibrium, i.e., if $\beta_1 = \beta_n = \beta$ we have

$$L^* e^{-\beta G(p,q,r)} = 0 , \quad (3.12)$$

and therefore $Z^{-1}e^{-\beta G(p,q,r)}$ is, in that special case, the density of a stationary distribution for the Markov process $x(t)$. In the sequel we will refer to G as the energy of the system.

We are going to construct a Liapunov function (see Section 8 of [20]) for this system and it is quite natural to try functions of the energy G: let us denote

$$W_\theta = \exp(\theta G) . \quad (3.13)$$

A computation shows that

$$LW_\theta = \gamma\theta W_\theta \left(\mathrm{Tr}(T) - r(1-\theta T)r\right) \quad (3.14)$$

This not quite a Liapunov function, but nearly so. The r.h.s. of Eq. (3.14) is negative provided $\theta/\beta_i < 1$ which we will always assume in the sequel and provided r is not too close to 0. Our proof is based on the following idea: at times r will be small, this corresponds to the situation where there is no dissipation of energy into the reservoir. But we will show that over small time interval, if we start the system at sufficiently large energy E, then with very large probability r^2 will be of order E^α where $\alpha = 2/k_2$ is related to the growth exponent of the interaction energy in the chain (this where we use that $k_2 \geq k_1$). So if we integrate the equation of a small time interval $[0,t]$ we will show that if $G(x) > E$ and E is large enough

$$T_t W_\theta(x) \leq \kappa(E) W_\theta(x) \tag{3.15}$$

where $\kappa(E) \sim \exp(-E^\alpha)$.

We denote as $|\cdot|_\theta$ the weighted total variation norm given by

$$\|\pi\|_\theta = \sup_{|f|\leq W_\theta} \left| \int f d\pi \right| , \tag{3.16}$$

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

$$\|f\|_\theta = \sup_{x\in X} \frac{|f(x)|}{W_\theta(x)} , \quad \mathcal{H}_\theta = \{f : \|f\|_\theta < \infty\} , \tag{3.17}$$

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. (3.6) are summarized in

Theorem 3.1 : Ergodic properties *Let us assume condition* **H1** *and* **H2**.

(a) The Markov process $x(t)$ has a unique stationary distribution μ and μ has a $\mathcal{C}^\infty$ everywhere positive density.

(b) For any θ with $0 < \theta < \beta_{\min} = \min(\beta_1, \beta_n)$ 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 $\gamma = \gamma(\theta) > 0$ and $R = R(\theta) < \infty$ such that

$$|P_t(x,\cdot) - \mu|_\theta \leq Re^{-\gamma t} W_\theta(x) , \tag{3.18}$$

for all $x \in X$ or equivalently

$$\|T_t - \mu\|_\theta \leq Re^{-\gamma t} . \tag{3.19}$$

(c) The Markov process x_t is ergodic: For any $f \in L^1(\mu)$

$$\lim_{t\to\infty} \frac{1}{t} \int_0^t f(x_s)\, ds = \int f(x)\mu(dx) , \tag{3.20}$$

for all initial condition x and for almost all realizations of the noise B_t. The Markov process is exponentially mixing: for all functions f, g with f^2, $g^2 \in \mathcal{H}_\theta$ and all $t > 0$ we have

$$\left|\int g T_t f \, d\mu - \int f \, d\mu \int g \, d\mu\right| \le R e^{-\gamma t} \|f^2\|_\theta^{1/2} \|g^2\|_\theta^{1/2} . \tag{3.21}$$

With the tools we have developed in our lecture on Markov process citeRB, in order to prove Theorem 3.1 it will suffice to prove the following properties:

1. **Strong-Feller property**. The transition probabilities have a density $p_t(x, y)$ which is $\mathcal{C}^\infty$ in (t, x, y).

2. **Irreducibility**. For all $t > 0$, and all x supp $P_t(x, \cdot) = X$.

3. **Liapunov function**. For any $t > 0$, $\theta < \beta_{\min}$, and $E > 0$ there exists functions $\kappa(E) = \kappa(E, \theta, t)$ and $b(E) = b(E, \theta, t)$ with $\lim_{E\to\infty} \kappa(E) = 0$ such that

$$T_t W_\theta(x) \le \kappa(E) W_\theta(x) + b(E) \mathbf{1}_{G \le E}(x) . \tag{3.22}$$

3.1 Irreducibility

Using the results of Section 6 in [20] we consider the control system

$$\begin{aligned} \dot{q}_t &= p_t , \\ \dot{p}_t &= -\nabla_q V(q_t) - \Lambda^* r_t , \\ \dot{r}_t &= -\gamma r_t + \Lambda p_t + u_t . \end{aligned} \tag{3.23}$$

where $t \mapsto u_t \in \mathbf{R}^2$ is a piecewise smooth control. One shows that for this system the set of accessible points from x in time t

$$\overline{A_t(x)} = \mathbf{R}^{2n+2} , \tag{3.24}$$

for any $x \in \mathbf{R}^{2n+2}$ and any $t > 0$.

We will illustrate here how this can be done sketching the proof by for the simpler problem of two oscillators coupled to a single reservoir and by assuming that $\partial_q U^{(2)}(q)$ is a diffeomorphism. Our assumption **H2** only ensures that the map $\partial_q U^{(2)}(q)$ is surjective and that we can find a piecewise smooth right inverse. This is enough to generalize the following argument, but one has to be careful if the initial or final points are one of the points where the right inverse of $\partial_q U^{(2)}(q)$ is not smooth. Let us consider the control system

$$\begin{aligned} \dot{r}_t &= -\gamma r_t + \lambda p_{1t} + u_t \,, \\ \ddot{q}_{1t} &= -\partial_{q_1} U^{(1)}(q_{1t}) - \partial_{q_1} U^{(2)}(q_{1t} - q_{2t}) - \lambda r_t \,, \\ \ddot{q}_{2t} &= -\partial_{q_2} U^{(1)}(q_{2t}) - \partial_{q_2} U^{(2)}(q_{1t} - q_{2t}) \,. \end{aligned} \tag{3.25}$$

and let us choose arbitrary initial and final conditions

$$\begin{aligned} x_0 &= (q_{10}, p_{10}, q_{20}, p_{20}, r_0) \\ x_1 &= (q_{1t}, p_{1t}, q_{2t}, p_{2t}, r_t) \ . \end{aligned} \tag{3.26}$$

Since the map $\partial_q U^{(2)}(q)$ is a diffeomorphism we first rewrite Eq. (3.25) as

$$\begin{aligned} u_t &= f_1(r_t, \dot{r}_t, \dot{q}_{1t}) \,, \\ r_t &= f_2(q_{1t}, q_{2t}, \ddot{q}_{1t}) \,, \\ q_{1t} &= f_3(q_{2t}, \ddot{q}_{2t}) \,, \end{aligned} \tag{3.27}$$

for some smooth function f_i. Then there exists a function F such that

$$u_t = F(q_{2t}, \dot{q}_{2t}, \cdots, q_{2t}^{(5)}) \,. \tag{3.28}$$

On the other hand by differentiating repeatedly the equation of motion we find function smooth function g_k such that

$$q_{2t}^{(k)} = g_k(q_{1t}, \dot{q}_{1t}, q_{2t}, \dot{q}_{2t}, r_t) \,. \tag{3.29}$$

for $k = 0, 1, 2, 3, 4$. Let us choose now any curve q_{2t} which satisfies the boundary conditions

$$\begin{aligned} q_{20}^{(k)} &= g_k(q_{10}, \dot{q}_{10}, q_{20}, \dot{q}_{20}, r_0) \,, \\ q_{2t}^{(k)} &= g_k(q_{1t}, \dot{q}_{1t}, q_{2t}, \dot{q}_{2t}, r_t) \,. \end{aligned} \tag{3.30}$$

We then define the desired control u_t by

$$u_t = F(q_{2t}, \dot{q}_{2t}, \cdots, q_{2t}^{(5)}) \,. \tag{3.31}$$

which drives the system from x_0 to x_1 in time t. Since x_0 and x_1, and t are arbitrary this proves (3.24).

3.2 Strong Feller Property

We apply Hörmander's Theorem (see Section 7 of [20]) to show that the transition probabilities have a smooth density.

The generator of the Markov process $x(t)$ can be written in the form

$$L \;=\; \sum_{i=1}^{2} X_i^2 + X_0 \,. \tag{3.32}$$

with $X_1 = \partial_{r_1}$ $X_2 = \partial_{r_n}$ and

$$x_0 \;=\; -\gamma r \nabla_r + (\Lambda p \nabla_r - r \Lambda \nabla_p) + (p \nabla_q - (\nabla_q V(q)) \nabla_p) \;, \tag{3.33}$$

Let us verify that Hörmander condition is satisfied.

The vector fields X_i, $i = 1, 2$ are, up to a constant, ∂_{r_i}, $i = 1, n$. We have

$$\begin{aligned} [\partial_{r_1} \,, X_0] &= -\gamma \partial_{r_1} - \lambda \partial_{p_1} \,, \\ [\partial_{p_1} \,, X_0] &= \lambda \partial_{r_1} + \partial_{q_1} \,, \end{aligned}$$

and so we can express the vector fields ∂_{p_1} and ∂_{q_1} as linear combinations of X_1, $[X_1, X_0]$, $[[X_1, X_0] X_0]$. Furthermore

$$[\partial_{q_1} \,, X_0] \;=\; (\partial^2 U^{(1)}(q_1) + \partial^2 U^{(1)}(q_1 - q_2)) \partial_{q_1} - \partial^2 U^{(2)}(q_1 - q_2) \partial_{p_2} \,. \tag{3.34}$$

If $U^{(2)}$ is strictly convex, $\partial^2 U^{(2)}(q_1 - q_2)$ is positive and this gives ∂_{p_2} as a linear combination X_1, $[X_1, X_0]$, $[[X_1, X_0] X_0]$, and $[[[X_1, X_0] X_0] X_0]$. In general case we use Condition **H2**: for any q, there exists $m > 2$ such that $\partial^m U^{(2)}(q) \neq 0$ and we consider the commutators

$$\begin{aligned} &\Big[\partial_{q_1} \,, \Big[\cdots \,, \Big[\partial_{q_1} \,, \partial^2 U^{(2)}(q_1 - q_2) \partial_{p_2}\Big]\Big]\Big] \\ &\quad = \partial^m U^{(2)}(q_1 - q_2) \partial_{p_2} \,. \end{aligned}$$

and therefore we can express, at a given point q, ∂_{p_2} as a linear combination of commutators.

Proceeding by induction, we obtain, see Corollary 7.2 of [20]

Proposition 3.2 *If Condition* **H2** *is satisfied then the Lie algebra*

$$\{X_i\}_{i=1}^2 \,, \quad \{[X_i, X_i]\}_{i,j=0}^2 \,, \quad \{[[X_i, X_j], X_k]\}_{i,j,k=0}^2 \,, \quad \cdots \tag{3.35}$$

has rank $\mathbf{R}^{2n+2}$ at every point x. The transition probabilities $P_t(x, y)$ have a density $p_t(x, y)$ which is $\mathcal{C}^\infty$ in (t, x, y).

3.3 Liapunov Function

We first consider the question of energy dissipation for the following deterministic equations

$$
\begin{aligned}
\dot{q}_t &= p_t\,, \\
\dot{p}_t &= -\nabla_q V(q_t) - \Lambda^* r_t\,, \\
\dot{r}_t &= -\gamma r_t + \Lambda p_t\,,
\end{aligned}
\tag{3.36}
$$

obtained from Eq.(3.6) by setting $\beta_1 = \beta_n = \infty$. This corresponds to an initial condition 0 for the reservoirs. A simple computation shows that the energy $G(p,q,r)$ is non-increasing along the flow $x_t = (p_t, q_t, r_t)$ given by Eq.(3.36):

$$
\frac{d}{dt} G(p_t, q_t, r_t) \;=\; -\gamma r_t^2 \;\leq\; 0\,. \tag{3.37}
$$

We now show by a scaling argument that for any initial condition with sufficiently high energy, after a small time, a substantial amount of energy is dissipated.

At high energy, the two-body interaction $U^{(2)}$ in the potential dominates the term $U^{(1)}$ since $k_2 \geq k_1$ and so for an initial condition with energy $G(x) = E$, the natural time scale – essentially the period of a single one-dimensional oscillator in the potential $|q|^{k_2}$ – is $E^{1/k_2 - 1/2}$. We scale a solution of Eq.(3.36) with initial energy E as follows

$$
\begin{aligned}
\tilde{p}_t &= E^{-\frac{1}{2}} p_{E^{\frac{1}{k_2}-\frac{1}{2}} t}\,, \\
\tilde{q}_t &= E^{-\frac{1}{k_2}} q_{E^{\frac{1}{k_2}-\frac{1}{2}} t}\,, \\
\tilde{r}_t &= E^{-\frac{1}{k_2}} r_{E^{\frac{1}{k_2}-\frac{1}{2}} t}\,.
\end{aligned}
\tag{3.38}
$$

Accordingly the energy scales as $G(p,q,r) = E\tilde{G}_E(\tilde{p},\tilde{q},\tilde{r})$, where

$$
\begin{aligned}
\tilde{G}_E(\tilde{p},\tilde{q},\tilde{r}) &= E^{\frac{2}{k_2}-1}\frac{\tilde{r}^2}{2} + \frac{\tilde{p}^2}{2} + \tilde{V}_E(\tilde{q})\,, \\
\tilde{V}_E(\tilde{q}) &= \sum_{i=1}^{n} \tilde{U}^{(1)}(\tilde{q}_i) + \sum_{i=1}^{n-1} \tilde{U}^{(2)}(\tilde{q}_i - \tilde{q}_{i+1})\,, \\
\tilde{U}^{(i)}(\tilde{x}) &= E^{-1}\tilde{U}^{(i)}(E^{\frac{1}{k_2}} x)\,, \quad i = 1, 2\,.
\end{aligned}
$$

The equations of motion for the rescaled variables are

$$\begin{aligned}
\dot{\tilde{q}}_t &= \tilde{p}_t\,, \\
\dot{\tilde{p}}_t &= -\nabla_{\tilde{q}}\tilde{V}_E(\tilde{q}_t) - E^{\frac{2}{k_2}-1}\Lambda^* r_t\,, \\
\dot{\tilde{r}}_t &= -E^{\frac{1}{k_2}-\frac{1}{2}}\gamma\tilde{r}_t + \Lambda\tilde{p}_t\,.
\end{aligned} \tag{3.39}$$

By assumption **H1**, as $E \to \infty$ the rescaled energy becomes

$$\begin{aligned}
\tilde{G}_\infty(\tilde{p},\tilde{q},\tilde{r}) &\equiv \lim_{E\to\infty} \tilde{G}_E(\tilde{p},\tilde{q},\tilde{r}) \\
&= \begin{cases} \tilde{p}^2/2 + \tilde{V}_\infty(\tilde{q}) & k_1 = k_2 > 2 \text{ or } k_2 > k_1 \geq 2 \\ \tilde{r}^2/2 + \tilde{p}^2/2 + \tilde{V}_\infty(\tilde{q}) & k_1 = k_2 = 2 \end{cases}\,,
\end{aligned}$$

where

$$V_\infty(\tilde{q}) = \begin{cases} \sum a^{(1)}|\tilde{q}_i|^{k_2} + \sum a^{(2)}|\tilde{q}_i - \tilde{q}_{i+1}|^{k_2} & k_1 = k_2 \geq 2 \\ \sum a^{(2)}|\tilde{q}_i - \tilde{q}_{i+1}|^{k_2} & k_2 > k_1 \geq 2 \end{cases}\,. \tag{3.40}$$

The equations of motion scale in this limit to

$$\begin{aligned}
\dot{\tilde{q}}_t &= \tilde{p}_t\,, \\
\dot{\tilde{p}}_t &= -\nabla_{\tilde{q}}\tilde{V}_\infty(\tilde{q}_t)\,, \\
\dot{\tilde{r}}_t &= \Lambda\tilde{p}_t\,,
\end{aligned} \tag{3.41}$$

in the case $k_2 > 2$, while they scale to

$$\begin{aligned}
\dot{\tilde{q}}_t &= \tilde{p}_t\,, \\
\dot{\tilde{p}}_t &= -\nabla_{\tilde{q}}\tilde{V}_\infty(\tilde{q}_t) - \Lambda^*\tilde{r}_t\,, \\
\dot{\tilde{r}}_t &= -\gamma\tilde{r}_t + \Lambda\tilde{p}_t\,,
\end{aligned} \tag{3.42}$$

in the case $k_1 = k_2 = 2$.

Remark 3.3 Had we supposed, instead of **H1**, that $k_1 > k_2$, then the natural time scale at high energy would be $E^{1/k_1-1/2}$. Scaling the variables (with k_2 replaced by k_1) would yield the limiting Hamiltonian $\tilde{p}^2/2 + \sum a^{(1)}|\tilde{q}_i|^{k_1}$, i.e., the Hamiltonian of n *uncoupled* oscillators. So in this case, at high energy, essentially no energy is transmitted through the chain. While this does not necessary preclude the existence of an invariant measure, we expect in this case the convergence to a stationary state to be much slower. In any case even the existence of the stationary state in this case remains an open problem.

Theorem 3.4 *Given $\tau > 0$ there are constants $c > 0$ and $E_0 < \infty$ such that for any x with $G(x) = E > E_0$ and any solution $x(t)$ of Eq.(3.36) with $x(0) = x$ we have the estimate, for $t_E = E^{1/k_2 - 1/2}\tau$,*

$$G(x_{t_E}) - E \leq -cE^{\frac{3}{k_2} - \frac{1}{2}}. \tag{3.43}$$

Remark 3.5 In view of Eqs. (3.43) and (3.37), this shows that r is at least typically $O(E^{1/k_2})$ on the time interval $[0, E^{1/k_2-1/2}\tau]$.

Proof: Given a solution of Eq.(3.36) with initial condition x of energy $G(x) = E$, we use the scaling given by Eq.(3.38) and we obtain

$$G(x(t_E)) - E = -\gamma \int_0^{t_E} dt\, r_t^2 = -\gamma E^{\frac{3}{k_2} - \frac{1}{2}} \int_0^{\tau} dt\, \tilde{r}_t^2 , \tag{3.44}$$

where $\tilde{r}_t$ is the solution of Eq.(3.39) with initial condition $\tilde{x}$ of (rescaled) energy $\tilde{G}_E(\tilde{x}) = 1$. By Assumption **H2** we may choose E_0 so large that for $E > E_0$ the critical points of $\tilde{G}_E$ are contained in, say, the set $\{\tilde{G}_E \leq 1/2\}$.

For a fixed E and x with $G(x) = E$, we show that there is a constant $c_{x,E} > 0$ such that

$$\int_0^{\tau} dt\, \tilde{r}_t^2 \geq c_{\tilde{x},E} . \tag{3.45}$$

The proof is by contradiction. Suppose that $\int_0^{\tau} dt\, \tilde{r}_t^2 = 0$, then we have $\tilde{r}_t = 0$, for all $t \in [0, \tau]$. From the third equation in (3.39) we conclude that $\tilde{p}_{1t} = \tilde{p}_{nt} = 0$ for all $t \in [0, \tau]$, and so from the first equation in (3.39) we see that $\tilde{q}_{1t}$ and $\tilde{q}_{nt}$ are constant on $[0, \tau]$. The second equation in (3.39) gives then

$$0 = \dot{\tilde{p}}_1(t) = -\partial_{q_1} \tilde{V}(\tilde{q}_t) = -\partial_{q_1} \tilde{U}^{(1)}(\tilde{q}_{1t}) - \partial_{q_1} \tilde{U}^{(2)}(\tilde{q}_{1t} - \tilde{q}_{2t}) , \tag{3.46}$$

together with a similar equation for $\dot{\tilde{p}}_n$. By our assumption **H1** the map $\nabla \tilde{U}^{(2)}$ has a right inverse g which is piecewise smooth thus we obtain

$$\tilde{q}_{2t} = \tilde{q}_{1t} - g(\tilde{U}^{(1)}(\tilde{q}_{1t})) . \tag{3.47}$$

Since $\tilde{q}_1$ is constant, this implies that $\tilde{q}_2$ is also constant on $[0, \tau]$. Similarly we see that $\tilde{q}_{n-1}$ is constant on $[0, \tau]$. Using again the first equation in (3.39) we obtain now $\tilde{p}_{2t} = \tilde{p}_{n-1t} = 0$ for all $t \in [0, \tau]$. Inductively one concludes that $\tilde{r}_t = 0$ implies $\tilde{p}_t = 0$ and $\nabla_{\tilde{q}} \tilde{V} = 0$ and thus the initial condition $\tilde{x}$ is a critical point of $\tilde{G}_E$. This contradicts our assumption and Eq. (3.45) follows.

Now for given E, the energy surface $\tilde{G}_E$ is compact. Using the continuity of the solutions of O.D.E with respect to initial conditions we conclude that there is a constant $c_E > 0$ such that

$$\inf_{\tilde{x}\in\{\tilde{G}_E=1\}} \int_0^\tau dt\, \tilde{r}_t^2 \geq c_E \,. \tag{3.48}$$

Finally we investigate the dependence on E of c_E. We note that for $E = \infty$, $\tilde{G}_\infty$ has a well-defined limit given by Eq.(3.40) and the rescaled equations of motion, in the limit $E \to \infty$, are given by Eqs. (3.41) in the case $k_2 > 2$ and by Eq. (3.42) in the case $k_1 = k_2 = 2$. Except in the case $k_1 = k_2 = 2$ the energy surface $\{\tilde{G}_\infty = 1\}$ is *not* compact. However, in the case $k_1 = k_2 > 2$, the Hamiltonian $\tilde{G}_\infty$ and the equation of motion are invariant under the translation $r \mapsto r + a$, for any $a \in \mathbf{R}^2$. And in the case $k_2 > k_1 > 2$ the Hamiltonian $\tilde{G}_\infty$ and the equation of motion are invariant under the translation $r \mapsto r + a$ $q \mapsto q + b$, for any $a \in \mathbf{R}^2$ and $b \in \mathbf{R}^n$. The quotient of the energy surface $\{\tilde{G}_\infty = 1\}$ by these translation, is compact.

Note that for a given $\tilde{x} \in \{\tilde{G}_\infty = 1\}$ a similar argument as above show that $\int_0^\tau dt(\tilde{r} + a)^2 > 0$, for any $a > 0$ and since this integral clearly goes to ∞ as $a \to \infty$ there exists a constant $c_\infty > 0$ such that

$$\inf_{\tilde{x}\in\{\tilde{G}_\infty=1\}} \int_0^\tau \tilde{r}_t^2\, dt > c_\infty \,. \tag{3.49}$$

Using again that the solution of O.D.E depends smoothly on its parameters, we obtain

$$\inf_{E>E_0} \inf_{\tilde{x}\in\{\tilde{G}_E=1\}} \int_0^\tau dt\, \tilde{r}_t^2 > c \,. \tag{3.50}$$

This estimate, together with Eq. (3.44) gives the conclusion of Theorem 3.4. ∎

Next we show, that at sufficiently high energies, the overwhelming majority of the random paths $x_t = x_t(\omega)$ solving Eqs.(3.6) follows very closely the deterministic paths x_t^{det} solving Eqs.(3.36). As a consequence, for most random paths the same amount of energy is dissipated into the reservoirs as for the corresponding deterministic ones. We need the following *a priori* "no-runaway" bound on the growth of $G(x_t)$.

Lemma 3.6 *Let $\theta \leq (\max\{T_1, T_n\})^{-1}$. Then $\mathbf{E}_x[\exp(\theta G(x_t))]$ satisfies the bound*

$$\mathbf{E}_x[\exp(\theta G(x_t))] \leq \exp(\gamma \mathrm{Tr}(T)\theta t) \exp(\theta G(x)) \,. \tag{3.51}$$

Moreover for any x with $G(x) = E$ and any $\delta > 0$ we have the estimate

$$\mathbf{P}_x \left\{ \sup_{0 \le s \le t} G(x_s)) \ge (1+\delta)E \right\} \le \exp\left(\gamma \mathrm{Tr}(T)\theta t\right) \exp\left(-\delta\theta E\right). \tag{3.52}$$

Remark 3.7 The lemma shows that for E sufficiently large, with very high probability, $G(x_t) = O(E)$ if $G(x) = E$. The assumption on θ here arises naturally in the proof, where we need $(1 - \theta T) \ge 0$, cf. Eq. (3.53).

Proof: For $\theta \le (\max\{T_1, T_n\})^{-1}$ we have the bound (the generator L is given by Eq. (3.8))

$$\begin{aligned} L \exp\left(\theta G(x)\right) &= \gamma\theta \exp\left(\theta G(x)\right) \left(\mathrm{Tr}(T) - r(1-\theta T) r\right) \\ &\le \gamma\theta \mathrm{Tr}(T) \exp\left(\theta G(x)\right), \end{aligned} \tag{3.53}$$

Then we apply Theorem 5.4 of [20]. ∎

We have the following "tracking" estimates to the effect that the random path closely follows the deterministic one at least up to time t_E for a set of paths which have nearly full measure. We set $\Delta x_t \equiv x_t(\omega) - x_t^{\mathrm{det}} = (\Delta r_t, \Delta p_t, \Delta q_t)$ with both $x_t(\omega)$ and x_t^{det} having initial condition x. Consider the event

$$S(x, E, t) = \{x.(\omega)\,;\, G(x) = E \text{ and } \sup_{0 \le s \le t} G(x_s) < 2E\}. \tag{3.54}$$

By Lemma 3.6, $\mathbf{P}\{S(x, E, t)\} \ge 1 - \exp\left(\gamma\theta \mathrm{Tr}(T)t - \theta E\right)$.

Proposition 3.8 *There exist constants $E_0 < \infty$ and $c > 0$ such that for paths $x_t(\omega) \in S(x, E, t_E)$ with $t_E = E^{1/k_2 - 1/2}\tau$ and $E > E_0$ we have*

$$\sup_{0 \le t \le t_E} \begin{pmatrix} \|\Delta q_t\| \\ \|\Delta p_t\| \\ \|\Delta r_t\| \end{pmatrix} \le c \sup_{0 \le t \le t_E} \|\sqrt{2\gamma T} B_t(\omega)\| \begin{pmatrix} E^{\frac{2}{k_2}-1} \\ E^{\frac{1}{k_2}-\frac{1}{2}} \\ 1 \end{pmatrix}. \tag{3.55}$$

Proof: We write differential equations for Δx_t again assuming both the random and deterministic paths start at the same point x with energy $G(x) = E$. These equations can be written in the somewhat symbolic form:

$$\begin{aligned} d\Delta q_t &= \Delta p_t dt\,, \\ d\Delta p_t &= \left(O(E^{1-2/k_2})\Delta q_t - \Lambda^* \Delta r_t\right) dt\,, \\ d\Delta r_t &= \left(-\gamma \Delta r_t + \Lambda \Delta p_t\right) dt + \sqrt{2\gamma T} dB_t \end{aligned} \tag{3.56}$$

The $O(E^{1-2/k_2})$ coefficient refers to the difference between forces, $-\nabla_q V(\cdot)$ evaluated at $x_t(\omega)$ and $x_t^{\rm det}$; we have that $G(x_t) \leq 2E$, so that $\nabla_q V(q_t(\omega)) - \nabla_q V(q_t^{\rm det}) = O(\partial^2 V)\Delta q_t = O(E^{1-2/k_2})\Delta q_t$. For later purposes we pick a constant c' so large that

$$\rho = \rho(x) = c' E^{1-\frac{2}{k_2}} \geq \sup_i \sum_j \sup_{\{q: V(q) \leq 2E\}} \left| \frac{\partial^2 V(q)}{\partial q_i \partial q_j} \right| \tag{3.57}$$

for all sufficiently large E.

In order to estimate the solutions of Eqs. (3.56), we consider the 3×3 matrix which bounds the coefficients in this system, and which is given by

$$M = \begin{pmatrix} 0 & 1 & 0 \\ \rho & 0 & \lambda \\ 0 & \lambda & \gamma \end{pmatrix} \tag{3.58}$$

We have the following estimate on powers of M; For $\Delta X^{(0)} = (0,0,1)^T$, we set $\Delta X^{(m)} \equiv M^m \Delta X^{(0)}$. For $\alpha = \max(1, \gamma + \lambda)$, we obtain $\Delta X^{(1)} \leq \alpha(0,1,1)^T$, $\Delta X^{(2)} \leq \alpha^2(1,1,1)^T$, and, for $m \geq 3$,

$$\Delta X^{(m)} \equiv \begin{pmatrix} u^{(m)} \\ v^{(m)} \\ w^{(m)} \end{pmatrix} \leq \alpha^m 2^{m-2} \begin{pmatrix} \rho^{\frac{m-2}{2}} \\ \rho^{\frac{m-1}{2}} \\ \rho^{\frac{m-2}{2}} \end{pmatrix},$$

where the inequalities are componentwise. From this we obtain the bound

$$e^{tM} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \leq \begin{pmatrix} \frac{1}{2}(\alpha t)^2 e^{\sqrt{\rho} 2\alpha t} \\ \alpha t e^{\sqrt{\rho} 2\alpha t} \\ 1 + \alpha t + \frac{1}{2}(\alpha t)^2 e^{\sqrt{\rho} 2\alpha t} \end{pmatrix}. \tag{3.59}$$

If $0 \leq t \leq t_E$ we have $\sqrt{\rho} t < \sqrt{c'}$. Then the exponentials in the above equation are bounded, and

$$e^{tM} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \leq c \begin{pmatrix} 1/\rho \\ 1/\sqrt{\rho} \\ 1 \end{pmatrix}, \tag{3.60}$$

for some constant c.

Returning now to the original differential equation system Eq.(3.56), we write this equation in the usual integral equation form:

$$\begin{pmatrix} \Delta q_t \\ \Delta p_t \\ \Delta r_t \end{pmatrix} = \int_0^t \begin{pmatrix} \Delta p_s \\ -\nabla_q V(q_s(\omega))\, ds + \nabla_q V(q_s^{\mathrm{det}}) - \Gamma^* \Delta r_s \\ -\gamma \Delta r_s + \Lambda \Delta p_s \end{pmatrix} ds + \begin{pmatrix} 0 \\ 0 \\ \sqrt{2\gamma T} B_t \end{pmatrix} . \tag{3.61}$$

From this we obtain the bound

$$\begin{pmatrix} \|\Delta q_t\| \\ \|\Delta p_t\| \\ \|\Delta r_t\| \end{pmatrix} \leq \int_0^t M \begin{pmatrix} \|\Delta q_t\| \\ \|\Delta p_t\| \\ \|\Delta r_t\| \end{pmatrix} ds + \begin{pmatrix} 0 \\ 0 \\ B_{\max} \end{pmatrix} , \tag{3.62}$$

where M is given by Eq.(3.58), and $B_{\max} = \sup_{t \leq t_E} \|\sqrt{2\gamma T} B_t\|$. Note that the solution of the integral equation

$$\Delta X_t = \int_0^t ds\, M \Delta X_s + \begin{pmatrix} 0 \\ 0 \\ B_{\max} \end{pmatrix} , \tag{3.63}$$

is $\Delta X_t = \exp(tM)(0, 0, B_{\max})^T$. We can solve both Eq. (3.61) and Eq. (3.63) by iteration. Let Δx_{ms}, ΔX_{ms} denote the respective m^{th} iterates (with $\Delta x_{0s} = (0, 0, \sqrt{2\gamma T} B_s)^T$, and $\Delta X_{0s} = (0, 0, B_{\max})^T$, $0 \leq s \leq t_E$). The ΔX_m's are monotone increasing in m. Then it is easy to see that

$$\begin{pmatrix} \|\Delta q_{mt}\| \\ \|\Delta p_{mt}\| \\ \|\Delta r_{mt}\| \end{pmatrix} \leq \Delta X_{mt} \leq \Delta X_t , \tag{3.64}$$

for each iterate. By Eqs.(3.59), (3.60), and the definition of ρ the conclusion Eq. (3.55) follows. ∎

As a consequence of Theorem 3.4 and Proposition 3.8 we obtain

Corollary 3.9 *Let $\Omega(E) = E^{\alpha}$ with $\alpha < 1/k_2$ and assume that B_t is such that $\sup_{0 \leq t \leq t_E} \|\sqrt{2\gamma T} B_t\| \leq \Omega(E)$ and $x_{\cdot}(\omega) \in S(x, E, t_E)$. Then there are constants $c > 0$ and $E_0 < \infty$ such that all paths $x_t(\omega)$ with initial condition x with $G(x) = E > E_0$ satisfy the bound*

$$\int_0^{t_E} r_s^2 ds \geq c E^{\frac{3}{k_2} - \frac{1}{2}} . \tag{3.65}$$

Remark 3.10 For large energy E, paths *not* satisfying the hypotheses of the corollary have measure bounded by

$$\begin{aligned}
&\mathbf{P}_x \left\{ \sup_{0\le s\le t_E} \|\sqrt{2\gamma T}B_s\| > \Omega(E) \right\} + \mathbf{P}\left\{ S(x,E,t_E)^C \right\} \\
&\le \frac{a}{2}\exp\left(-\frac{\Omega(E)^2}{b\gamma T_{\max}t_E}\right) + \exp\left(\theta(\gamma \mathrm{Tr}(T)t_E - E)\right) \\
&\le a\exp\left(-\frac{\Omega(E)^2}{b\gamma T_{\max}t_E}\right), \qquad (3.66)
\end{aligned}$$

where a and b are constants which depend only on the dimension of ω. Here we have used the reflection principle to estimate the first probability and Eq. (3.52) and the definition of S to estimate the second probability. For E large enough, the second term is small relative to the first.

Proof: It is convenient to introduce the L^2-norm on functions on $[0,t]$, $\|f\|_t \equiv \left(\int_0^t \|f_s\|^2 ds\right)^{1/2}$. By Theorem 3.4, there are constants E_1 and c_1 such that for $E > E_1$ the deterministic paths x_s^{det} satisfy the bound

$$\|r^{\mathrm{det}}\|_{t_E}^2 \;=\; \int_0^{t_E} (r_s^{\mathrm{det}})^2 ds \ge c_1 E^{\frac{3}{k_2}-\frac{1}{2}}\,. \qquad (3.67)$$

By Proposition 3.8, there are constants E_2 and c_2 such that $\|\Delta r_s\| \le c_2\Omega(E)$, uniformly in s, $0 \le s \le t_E$, and uniformly in x with $G(x) > E_2$. So we have

$$\|r\|_{t_E} \ge \|r^{\mathrm{det}}\|_{t_E} - \|\Delta r\|_{t_E} \ge \left(c_1 E^{\frac{3}{k_2}-\frac{1}{2}}\right)^{1/2} - c_2\Omega(E)\left(E^{\frac{1}{k_2}-\frac{1}{2}}\right)^{1/2}. \qquad (3.68)$$

But the last term is $O(E^{\alpha-1/4+1/2k_2})$, which is of lower order than the first since $\alpha < 1/k_2$, so the corollary follows, for an appropriate constant c and E sufficiently large. ∎

With these estimates we now prove the existence of a Liapunov function.

Theorem 3.11 *Let $t > 0$ and $\theta < \beta_{\min}$. Then there are functions $\kappa(E) = \kappa(E,t,\theta) < 1$ and $b(E) = b(E,t,\theta) < \infty$ such that*

$$T_t W_\theta(x) \;\le\; \kappa(E)W_\theta(x) + b(E)\mathbf{1}_{\{G\le E\}}(x)\,. \qquad (3.69)$$

The function $\kappa(E)$ satisfies the bound

$$\kappa(E) \;\le\; A\exp(-BE^{2/k_2})\,, \qquad (3.70)$$

for some constants A and B.

Proof: For any compact set U and for any t, $T^t \exp(\theta G)(x)$ is a bounded function on U, uniformly on $[0,t]$. So, in order to prove Eq.(3.69), we only have to prove that there exist a compact set U and $\kappa < 1$ such that

$$\sup_{x \in U^{\mathrm{C}}} \mathbf{E}_x \left[\exp\left(\theta(G(x_t) - G(x))\right)\right] \le \kappa < 1 \,. \tag{3.71}$$

Using Ito's Formula to compute $G(x_t) - G(x)$ in terms of a stochastic integral we obtain

$$\begin{aligned} &\mathbf{E}_x \left[\exp\left(\theta(G(x_t) - G(x))\right)\right] \\ &= \exp(\theta\gamma \mathrm{tr}(T)t) \mathbf{E}_x \left[\exp\left(-\theta \int_0^t \gamma r_s^2 \, ds + \theta \int_0^t \sqrt{2\gamma T} r_s dB_s\right)\right] . \end{aligned} \tag{3.72}$$

For any $\theta < \beta_{\min}$, we choose $p > 1$ such that $\theta p < \beta_{\min}$. Using Hölder inequality we obtain,

$$\begin{aligned} &\mathbf{E}_x \left[\exp\left(-\theta \int_0^t \gamma r_s^2 \, ds + \theta \int_0^t \sqrt{2\gamma T} r_s dB_s\right)\right] \\ &= \mathbf{E}_x \left[\exp\left(-\theta \int_0^t \gamma r_s^2 \, ds + \frac{p\theta^2}{2} \int_0^t (\sqrt{2\gamma T} r_s)^2 \, ds\right) \times \right. \\ &\qquad \left. \times \exp\left(-\frac{p\theta^2}{2} \int_0^t (\sqrt{2\gamma T} r_s)^2 \, ds + \theta \int_0^t \sqrt{2\gamma T} r_s dB_s\right)\right] \\ &\le \mathbf{E}_x \left[\exp\left(-q\theta \int_0^t \gamma r_s^2 \, ds + \frac{qp\theta^2}{2} \int_0^t (\sqrt{2\gamma T} r_s)^2 \, ds\right)\right]^{1/q} \times \\ &\quad \times \mathbf{E}_x \left[\exp\left(-\frac{p^2\theta^2}{2} \int_0^t (\sqrt{2\gamma T} r_s)^2 \, ds + \theta p \int_0^t \sqrt{2\gamma T} r_s dB_s\right)\right]^{1/p} \\ &= \mathbf{E}_x \left[\exp\left(-q\theta \int_0^t \gamma r_s^2 \, ds + \frac{qp\theta^2}{2} \int_0^t (\sqrt{2\gamma T} r_s)^2 \, ds\right)\right]^{1/q} . \end{aligned}$$

Here, in the next to last line, we have used Girsanov theorem and so the second expectation is equal to 1. Finally we obtain the bound

$$\begin{aligned} &\mathbf{E}_x \left[\exp\left(\theta(G(x_t) - G(x))\right)\right] \\ &\le \exp(\theta\gamma \mathrm{tr}(T)t) \mathbf{E}_x \left[\exp\left(-q\theta(1 - p\theta T_{\max}) \int_0^t \gamma r_s^2 \, ds\right)\right]^{1/q} . \end{aligned} \tag{3.73}$$

In order to proceed we need to distinguish two cases according if $3/k_2 - 1/2 > 0$ or $3/k_2 - 1/2 \le 0$ (see Corollary 3.9). In the first case we let E_0

be defined by $t = E_0^{1/k_2-1/2}\tau$. For $E > E_0$ we break the expectation Eq. (3.73) into two parts according to whether the paths satisfy the hypotheses of Corollary 3.9 or not. For the first part we use Corollary 3.9 and that $\int_0^t r_s^2 ds \geq \int_0^{t_E} r_s^2 \geq cE^{3/k_2-1/2}$; for the second part we use estimate (3.66) in Remark 3.10 on the probability of unlikely paths together with the fact that the exponential under the expectation in Eq. (3.73) is bounded by 1. We obtain for all x with $G(x) = E > E_0$ the bound

$$\begin{aligned} \mathbf{E}_x \left[\exp\left(\theta(G(x_t) - G(x))\right)\right] &\leq \exp\left(\theta\gamma \operatorname{tr}(T) t_{E_0}\right) \times \\ &\times \left[\exp\left(-q\theta(1-p\theta T_{\max})cE^{\frac{3}{k_2}-\frac{1}{2}}\right) + a\exp\left(-\frac{\Omega(E)^2\theta_0}{b\gamma t_E}\right)\right]^{1/q} \end{aligned} \tag{3.74}$$

Choosing the set $U = \{x\,;\, G(x) \leq E_1\}$ with E_1 large enough we can make the term in Eq. (3.74) as small as we want.

If $3/k_2 - 1/2 \leq 0$, for a given t and a given x with $G(x) = E$ we split the time interval $[0,t]$ into $E^{1/2-1/k_2}$ pieces $[t_j, t_{j+1}]$, each one of size of order $E^{1/k_2-1/2}t$. For the "good" paths, i.e., for the paths x_t which satisfy the hypotheses of Corollary 3.9 on each time interval $[t_j, t_{j+1}]$, the tracking estimates of Proposition 3.8 imply that $G(x_t) = O(E)$ for t in each interval. Applying Corollary 3.9 and using that $G(x_{t_j}) = O(E)$ we conclude that $\int_0^t r_s^2\, ds$ is at least of order $E^{3/k_2-1/2} \times E^{1/2-1/k_2} = E^{2/k_2}$. The probability of the remaining paths can be estimated, using Eq. (3.66), not to exceed

$$1 - \left(1 - a\exp\left(-\frac{\Omega_{\max}^2\theta_0}{b\gamma t_E}\right)\right)^{E^{\frac{1}{2}-\frac{1}{k_2}}} . \tag{3.75}$$

The remainder of the argument is essentially as above, Eq. (3.74) and this concludes the proof of Theorem 3.11. ∎

4 Heat Flow and Entropy Production

In this section we study some thermodynamical properties of the stationary distribution. Most interesting is the case where the temperatures of the two reservoirs are different, we expect then to have heat (i.e., energy) flowing through the system from the hot reservoir into the cold one. Very little is known about the 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). In the recent years a new general fact about nonequilibrium has been discovered, the so-called Gallavotti-Cohen fluctuation Theorem. It asserts that the fluctuation of the ergodic mean of the entropy production has 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 [8]. As a theorem it has been proved for Anosov maps [11], these deterministic systems are used to model nonequilibrium systems with reservoirs described by non-Hamiltonian deterministic forces (the so-called Gaussian thermostat). The fluctuation theorem has been formulated and extended to Markov process in [15, 16, 18] and proved for simple systems like Markov chains with a finite state space or non-degenerate diffusions.

We will prove this fluctuation theorem for our model. Both the degeneracy of the Markov process and the non-compactness of the phase space are the technical difficulties which have to be overcome. Our model is the first model which is completely derived from first principles (it is Hamiltonian to start with) and for which the fluctuation theorem can be proved.

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

$$\begin{aligned} H_1 &= \frac{p_1^2}{2} + U^{(1)}(q_1) + \frac{1}{2}U^{(2)}(q_1 - q_1)\,, \\ H_i &= \frac{p_i^2}{2} + U^{(1)}(q_i) + \frac{1}{2}\left(U^{(2)}(q_{i-1} - q_i) + U^{(2)}(q_i - q_{i+1})\right)\,, \\ H_n &= \frac{p_n^2}{2} + U^{(1)}(q_n) + \frac{1}{2}U^{(2)}(q_n - q_{n-1})\,. \end{aligned} \tag{4.1}$$

Using Ito's Formula one finds

$$dH_i(x_t) \;=\; (\Phi_{i-1}(x_t) - \Phi_i(x_t))\, dt\,, \tag{4.2}$$

where

$$\begin{aligned} \Phi_0 &= -\lambda r_1 p_1\,, \\ \Phi_i &= \frac{(p_i + p_{i+1})}{2}\partial_q U^{(2)}(q_i - q_{i+1})\,, \\ \Phi_n &= \lambda r_n p_n\,. \end{aligned} \tag{4.3}$$

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

$$\sigma_i \;=\; (\beta_n - \beta_1)\Phi_i\,. \tag{4.4}$$

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 $\sigma_b = \beta_1\Phi_0 - \beta_n\Phi_n$. 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) **Positivity of entropy production.** *The expectation of the entropy production σ_j in the stationary state is independent of j and nonnegative*

$$\int \sigma_j d\mu \;\geq\; 0\,, \tag{4.5}$$

and it is positive away from equilibrium

$$\int \sigma_j d\mu \;=\; 0 \qquad \text{if and only if} \qquad \beta_1 = \beta_n\,. \tag{4.6}$$

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

$$\overline{\sigma}_j^{\,t} \equiv \frac{1}{t}\int_0^t \sigma_j(x_s) \tag{4.7}$$

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 are independent of j) such that for all intervals $[a,b] \subset O$ we have

$$\lim_{t\to\infty} -\frac{1}{t}\log \mathbf{P}_x\{\overline{\sigma}_j^{\,t} \in [a,b]\} \;=\; \inf_{w\in[a,b]} e(w)\,. \tag{4.8}$$

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

$$e(w) - e(-w) \;=\; -w\,, \tag{4.9}$$

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

(c) **Kubo formula and central limit theorem.** *Let us introduce the parameters $\beta = (\beta_1 + \beta_n)/2$ and $\eta = \beta_n - \beta_1$. We have*

$$\frac{\partial}{\partial \eta} \left(\int \phi_j d\mu \right) \Big|_{\eta=0} = \int_0^\infty \left(\int (T_t^{\mathrm{eq}} \phi_j) \phi_j d\mu^{\mathrm{eq}} \right) ds \,, \tag{4.10}$$

where μ^{eq} is the Gibbs stationary distribution at equilibrum (see Eq. (3.12)) and T_t^{eq} is the semigroup at equilibrium. Moreover, if we consider the fluctuations of the heat flow at equilibrium, they satisfy a central limit theorem

$$\mathbf{P}_x \left\{ a \,<\, \frac{1}{\sqrt{\kappa^2 t}} \int_0^t \Phi_j(x_s)\, ds \,<\, b \right\} \longrightarrow \frac{1}{\sqrt{2\pi}} \int_a^b \exp(-\frac{y^2}{2})\, dy \tag{4.11}$$

as $t \to \infty$, the constant κ^2 is positive, independent of j, and is given by

$$\kappa^2 = \int_0^\infty \left(\int \Phi_j(x) T_s^{\mathrm{eq}} \Phi_j(x) \mu(dx) \right) ds \,. \tag{4.12}$$

Loosely speaking the fluctuation theorem has the following interpretation,

$$\frac{\mathbf{P}_x \left\{ \overline{\sigma}_j{}^t \approx a \right\}}{\mathbf{P}_x \left\{ \overline{\sigma}_j{}^t \approx -a \right\}} \approx e^{ta} \,, \tag{4.13}$$

in other words this gives a bound on the probability to observe a fluctuation of the entropy production which would give rise to a energy flow from the cold reservoir to the hot reservoir (i.e., a "violation" of the second law of thermodynamics). As we will see the Kubo formula is a consequence of the fluctuation theorem and thus we can also view the fluctuation theorem as a generalization of Kubo formula to large fields. We will elaborate on this interpretation later.

4.1 Positivity of entropy production

Let us consider the functions R_j given by

$$R_j = \beta_1 \left(\frac{r_1^2}{2} + \sum_{k=1}^{j} H_k(p,q) \right) + \beta_n \left(\sum_{k=j+1}^{n} H_k(p,q) + \frac{r_n^2}{2} \right) \,, \tag{4.14}$$

so that $\exp(-R_j)$ is a kind of "two-temperatures" Gibbs state. We also denote by J the time reversal operator which changes the sign of the momenta of all particles $Jf(p,q,r) = f(-p,q,r)$.

The following identities can be regarded as operator identities on $\mathcal{C}^\infty$ functions. That the left and right side of Eq. (4.16) actually generate semigroups for some non trivial domain of α is a non trivial result which we will discuss later.

Lemma 4.2 *Let us consider e^{R_i} and e^{-R_i} as multiplication operators. Then we have the operator identities*

$$e^{R_i} J L^* J e^{-R_i} \;=\; L - \sigma_i \,, \tag{4.15}$$

and also for any constant α

$$e^{R_i} J (L^* - \alpha\sigma_i) J e^{-R_i} \;=\; L - (1-\alpha)\sigma_i \,. \tag{4.16}$$

Proof: We write the generator L as $L = L_0 + L_1$ with

$$\begin{aligned} L_0 &= \gamma\left(\nabla_r T \nabla_r - r\nabla_r\right) & (4.17)\\ L_1 &= (\Lambda p \nabla_r - r\Lambda\nabla_p) + (p\nabla_q - (\nabla_q V(q))\nabla_p)\;. & (4.18) \end{aligned}$$

Since L_1 is a first order differential operator we have

$$e^{-R_i} L_1 e^{R_i} \;=\; L_1 + L_1 R_i \;=\; L_1 + \sigma_i \,. \tag{4.19}$$

Using that $\nabla_r R_i = T^{-1} r$ we obtain

$$\begin{aligned} e^{-R_i} L_0 e^{R_i} &= e^{-R_i}\gamma(\nabla_r - T^{-1}r)T\nabla_r e^{R_i} \\ &= \gamma\nabla_r T(\nabla_r + T^{-1}r) \;=\; L_0^* \,. \end{aligned}$$

This gives

$$e^{-R_i} L e^{R_i} \;=\; L_0^* + L_1 + \sigma_i \;=\; JL^*J + \sigma_i \,, \tag{4.20}$$

which is Eq. (4.15). Since $J\sigma_i J = -\sigma_i$, Eq. (4.16) follows immediately from Eq. (4.15). ■

Proof of Theorem 4.1 (a): We write the positive density $\rho(x)$ of $\mu(dx) = \rho(x)dx$ as

$$\rho = J e^{-R_j} e^{-F_j} \,. \tag{4.21}$$

Let $L^\dagger$ denote the adjoint of L on $L^2(\mu)$, it is given by $L^\dagger = \rho^{-1} L^* \rho$ and using Eq. (4.15) a simple computation shows that

$$\begin{aligned} JL^dagger &= e^{F_j}(L - \sigma_j)e^{-F_j} \\ &= L - \sigma_j - (LF_j) - 2(T\nabla_r F_j)\nabla_r + |T^{1/2}\nabla_r F_j|^2)\,. & (4.22) \end{aligned}$$

It is easy to see that the operator $JL^\dagger J$ satisfies $JL^\dagger J1 = 0$ and so applying the Eq. (4.22) to the constant function we find

$$\sigma_j \;=\; |T^{1/2}\nabla F_j|^2 - LF_i\,. \tag{4.23}$$

The first term is obviously positive while the expectation of the second term in the stationary state vanishes and so we obtain Eq. (4.5).

In order to prove positivity of the entropy production, we will make a proof by contradiction. Let us suppose that $\beta_1 \neq \beta_n$ and that $\int \sigma_i(x)\mu(dx) = 0$. Since all σ_i have the same stationary value, it is enough to consider one of them and we choose $\sigma_0 = (\beta_1 - \beta_n)\lambda p_1 r_1$. The assumption implies that $\int |T^{1/2}\nabla_r F_0|^2 \mu(dx) = 0$. Since ρ is positive, this means that $\nabla_r F_0 = 0$, and therefore F_0 does not depend on the r variables. From Eq. (4.23) we obtain

$$\sigma_0 \;=\; -LF_0\,. \tag{4.24}$$

Using the definition of L and σ_0 and the fact that F_0 does not depend on r, we obtain the equation

$$0 \;=\; (p\cdot\nabla_q\varphi - (\nabla_q V)\cdot\nabla_p)\,F_0 + \lambda r_1\partial_{p_1}F_0 + \lambda r_n\partial_{p_n}F_0 \;=\; (\beta_n - \beta_1)\lambda r_1 p_1\,.$$

Since F_0 does not depend on r we get the sytem of equations

$$\begin{aligned} (p\nabla_q - (\nabla_q V)\nabla_p)F_0 &= 0\,, \\ \partial_{p_1}F_0 &= (\beta_n - \beta_1)p_1\,, \\ \partial_{p_n}F_0 &= 0\,. \end{aligned} \tag{4.25}$$

We will show that this system of linear equations has no solution unless $\beta_1 = \beta_n$. To see this we consider the system of equations

$$\begin{aligned} (p\nabla_q - (\nabla_q V)\nabla_p)F_0 &= 0\,, \\ \partial_{p_1}F_0 &= (\beta_n - \beta_1)p_1\,. \end{aligned} \tag{4.26}$$

This system has a solution which is given by $(\beta_n - \beta_1)H(q,p)$. We claim that this the unique solution (up to an additive constant) of Eq. (4.26). If this holds true, then the only solution of Eq. (4.25) is given by $(\beta_n - \beta_1)H(q,p)$ and this is incompatible with the third equation in (4.25) when $\beta_1 \neq \beta_n$.

Since Eq. (4.26) is a linear inhomogeneous equation, it is enough to show that the only solutions of the homogeneous equation

$$\begin{aligned} (p\nabla_q - (\nabla_q V)\nabla_p)F_0 &= 0\,, \\ \partial_{p_1}F_0 &= 0\,. \end{aligned} \tag{4.27}$$

are the constant functions. Since $\partial_{p_1} F_0 = 0$, F_0 does not depend on p_1, we conclude that the first equation in (4.27) reads

$$p_1 \partial_{q_1} F_0 + f_1(q_1, \ldots, q_n, p_2, \ldots p_n) = 0 \,, \tag{4.28}$$

where f_1 does not depend on the variable p_1. Thus we see that $\partial_{q_1} F_0 = 0$ and therefore F_0 does not depend on the variable q_1 either. By the first equation in (4.27) we now get

$$(\partial_{q_1} U^{(2)}(q_1 - q_2))\partial_{p_2} F_0 + f_2(q_2, \ldots, q_n, p_2, \ldots, p_n) = 0 \,, \tag{4.29}$$

where f_2 does not depend on p_1 and q_1. By condition **H2** we see that $\partial_{p_2}\varphi = 0$ and hence f does not depend on p_2. Iterating the above procedure we find that the only solutions of (4.27) are the constant functions.

As a consequence, the stationary state $\mu = \mu_{\beta_1, \beta_n}$ sustains a non-vanishing heat flow in the direction from the hotter to the colder reservoir. Of course if $\beta_1 = \beta_n$ the heat flow vanishes since Φ_j is an odd function of p and the density of the stationary distribution is even in p. ∎

4.2 Fluctuation theorem

Let us consider now the part (b) of Theorem 4.1. Let us first give an outline of the proof. To study the large deviations of $t^{-1} \int_0^t \sigma_i(x_s) ds$ one considers moment generating function

$$\Gamma_x^j(t, \alpha) = \mathbf{E}_x \left[e^{-\alpha \int_0^t \sigma_j(x_s)\, ds} \right] . \tag{4.30}$$

A formal application of Feynman-Kac formula gives

$$\frac{d}{dt} \mathbf{E}_x \left[e^{-\alpha \int_0^t \sigma_j(x_s)\, ds} f(x_t) \right] = (L - \alpha \sigma_j) \left[e^{-\alpha \int_0^t \sigma_j(x_s)\, ds} f(x_t) \right] , \tag{4.31}$$

but since is σ_j is not a bounded function, it is not clear that the expectation $\Gamma_x^j(t, \alpha)$ is even well defined. We will show below that there exists a neighborhood O of the interval $[0, 1]$ such that $\Gamma_x^j(t, \alpha)$ is well defined if $\alpha \in O$. We denote then $T_t^{(\alpha)}$ the semigroup with generator $(L - \alpha \sigma_j)$. We then have

$$\Gamma_x^j(t, \alpha) = \mathbf{E}_x \left[e^{-\alpha \int_0^t \sigma_j(x_s)\, ds} \right] = T_t^{(\alpha)} 1(x) \tag{4.32}$$

Next one shows that the following limit

$$e(\alpha) \equiv \lim_{t\to\infty} -\frac{1}{t}\log\Gamma_x^j(t,\alpha)\,, \tag{4.33}$$

exists, is independent of x and j, and is a $\mathcal{C}^1$ function of α. We will do this by a Perron-Frobenius like argument and identify $\exp(-te(\alpha))$ as the (real) eigenvalue of $T_t^{(\alpha)}$ with biggest modulus (on a suitable function space).

Then a standard and general argument of the theory of large deviations [2] (the Gärtner-Ellis Theorem) gives a large deviation principle for the ergodic average $t^{-1}\int_0^t \sigma_i(x_s)ds$ with a large deviation functional $e(w)$ which is given by the Legendre transform of the function $e(\alpha)$.

Formally, from Eq. (4.16) we see that $T_t^{(\alpha)}$ is conjugated to $(T_t^{(1-\alpha)})^*$, but since $T_t^{(\alpha)}$ has the same spectrum as $(T_t^{(\alpha)})^*$ we conclude that

$$e(\alpha) \,=\, e(1-\alpha)\,. \tag{4.34}$$

Taking now a Legendre transform we have

$$\begin{aligned} I(w) \;&=\; \sup_\alpha\{e(\alpha)-\alpha w\} \,=\, \sup_\alpha\{e(1-\alpha)-\alpha w\} \\ &=\; \sup_\beta\{e(\beta)-(1-\beta)w\} \,=\, I(-w)-w\,. \end{aligned}$$

and this gives the part (b) of Theorem 4.1.

Let us explain how to make this argument rigorous, by making yet another conjugation.

Lemma 4.3 *We have the identity*

$$L-\alpha\sigma_j \,=\, e^{\alpha R_j}\overline{L}_\alpha e^{-\alpha R_j}\,, \tag{4.35}$$

where

$$\overline{L}_\alpha \,=\, \tilde{L}_\alpha - \Big((\alpha-\alpha^2)\gamma r T^{-1} r - \alpha\mathrm{tr}(\gamma I)\Big) \tag{4.36}$$

and

$$\tilde{L}_\alpha \,=\, L + 2\alpha\gamma r\nabla_r\,. \tag{4.37}$$

Proof: As in Lemma 4.2 we write the generator L as $L = L_0 + L_1$, see Eqs.(4.18) and (4.17). Since L_1 is a first order differential operator we have

$$e^{-\alpha R_j}L_1 e^{\alpha R_j} \,=\, L_1 + \alpha(L_1 R_j) \,=\, L_1 + \alpha\sigma_j\,. \tag{4.38}$$

Using that $\nabla_r R_j = T^{-1}r$ is independent of j we find that

$$
\begin{aligned}
e^{-\alpha R_j} L_0 e^{\alpha R_j} &= \gamma \Big((\nabla_r + \alpha T^{-1}r) T (\nabla_r + \alpha T^{-1}r) - r(\nabla_r + \alpha T^{-1}r) \Big) \\
&= L_0 + \alpha\gamma(r\nabla_r + \nabla_r r) + (\alpha^2 - \alpha)\gamma r T^{-1} r \\
&= L_0 + 2\alpha\gamma r\nabla_r + (\alpha^2 - \alpha)\gamma r T^{-1} r + \alpha \mathrm{tr}\gamma I \,. \qquad (4.39)
\end{aligned}
$$

Combining Eqs. (4.38) and (4.39) gives the desired result. ∎

The point of this computation is that it shows that $L - \alpha\sigma_i$ is conjugated to the operator $\overline{L}_\alpha$ which is independent of i. Furthermore $\overline{L}_\alpha$ has the form L plus terms which are quadratic in r and ∇_r. Combining Feynman-Kac and Girsanov formulas we can analyze the spectral properties of this operator by the same methods as the operator L. The basic identity here is as in Section 3.3.

$$
\begin{aligned}
&\overline{L}_\alpha \exp\theta G(x) = \\
&= \exp\theta G(x)\gamma\Big[\mathrm{tr}(\theta T + \alpha I) + r(\theta^2 T - (1-2\alpha)\theta - \alpha(1-\alpha)T^{-1})r\Big] \\
&\le C\exp\theta G(x)\,, \qquad (4.40)
\end{aligned}
$$

provided α and T_i, $i = 1, n$ satisfy the inequality

$$
\theta^2 T_i - (1-2\alpha)\theta - \alpha(1-\alpha)T_i^{-1} \le 0\,, \qquad (4.41)
$$

or

$$
-\alpha < \theta T_i < 1 - \alpha\,. \qquad (4.42)
$$

In particular we see that the semigroup $\overline{T}_t^{(\alpha)}$ defined by

$$
\overline{T}_t^{(\alpha)} = e^{-\alpha R_j} T_t^{(\alpha)} e^{\alpha R_j} \qquad (4.43)
$$

and with generator $\overline{L}_\alpha$ is well defined on the Banach space $\mathcal{H}_\theta$ if $-\alpha < \theta T_i < 1 - \alpha$. Furthermore it has the following properties

1. **Strong-Feller property**. The semigroup $\overline{T}_t^{(\alpha)}$ has a kernel $p_t^{(\alpha)}(x, y)$ which is $\mathcal{C}^\infty$ in (t, x, y).

2. **Irreducibility**. For all $t > 0$, and all nonnegative f, $\overline{T}_t^{(\alpha)} f$ is positive.

3. **Liapunov function**. For any $t > 0$ and θ such that $-\alpha < \theta T_i < 1-\alpha$, there exists functions $\kappa(E) = \kappa(E, \theta, t)$ and $b(E) = b(E, \theta, t)$ with $\lim_{E\to\infty} \kappa(E) = 0$ such that

$$\overline{T}_t^{(\alpha)} W_\theta(x) \;\leq\; \kappa(E) W_\theta(x) + b(E) \mathbf{1}_{G\leq E}(x)\,. \tag{4.44}$$

These properties are proved exactly as in for the operator L, using in addition Girsanov and Feynman-Kac formula (see [22] for details).

As a consequence, by Theorem 8.9 of [20], we obtain that on $\mathcal{H}_\theta$, with $-\alpha < \theta T_i < 1-\alpha$ the semigroup $\overline{T}_t^{(\alpha)}$ is a compact semigroup, it has exactly one eigenvalue with maximal modulus which, in addition is real. In particular $\overline{T}_t^{(\alpha)}$ has a spectral gap. We then obtain

Theorem 4.4 *If*

$$\alpha \in \left(-\frac{\beta_{\max}}{\beta_{\min} - \beta_{\max}} \,,\, 1 + \frac{\beta_{\max}}{\beta_{\min} - \beta_{\max}} \right)\,, \tag{4.45}$$

then

$$e(\alpha) \;=\; \lim_{t\to\infty} -\frac{1}{t} \log \Gamma_x^j(t, \alpha) \tag{4.46}$$

exists, is finite and independent both of j and x.

Proof: The semigroup $\overline{T}_t^{(\alpha)}$ is well defined on$\mathcal{H}_\theta$ if

$$-\alpha < \theta T_i < 1 - \alpha\,. \tag{4.47}$$

A simple computation shows that for given α, β_1, and β_n the set of θ we can choose is non-empty provided if

$$\alpha \in \left(-\frac{\beta_{\max}}{\beta_{\min} - \beta_{\max}} \,,\, 1 + \frac{\beta_{\max}}{\beta_{\min} - \beta_{\max}} \right)\,, \tag{4.48}$$

Using the definition of R_i, Eq. (4.14), $e^{-\alpha R_i} \in \mathcal{H}_\theta$ since $-\alpha + \theta T_i < 0$. Using now Lemma 2.7, we see that $\Gamma_x^i(t, \alpha)$ exists and is given by

$$\Gamma_x^i(t, \alpha) \;=\; T_t^{(\alpha)} 1(x) \;=\; e^{\alpha R_i} \overline{T}_t^{(\alpha)} e^{-\alpha R_i}(x)\,. \tag{4.49}$$

From the spectral properties of $\overline{T}_t^{(\alpha)}$ we infer the existence of a one-dimensional projector P_α such that

1. $P_\alpha f > 0$ if $f \geq 0$

2. We have
$$\overline{T}_t^{(\alpha)} \;=\; e^{-te(\alpha)} P_\alpha + \overline{T}_t^{(\alpha)} (1 - P_\alpha)\,, \tag{4.50}$$
and there exists a constants $d(\alpha) > e(\alpha)$ and C such that
$$\|\overline{T}_t^{(\alpha)} (1 - P_\alpha)\| \;\leq\; C e^{-td(\alpha)}\,, \tag{4.51}$$
or, in other words,
$$|\overline{T}_t^{(\alpha)} (1 - P_\alpha) g| \;\leq\; C e^{-td(\alpha)} \|g\|_\theta W_\theta(x)\,. \tag{4.52}$$

From Lemma 4.3 and Eq. (4.52) we obtain, for all x, that

$$\begin{aligned}
&\lim_{t\to\infty} -\frac{1}{t} \log \Gamma_x^j(t,\alpha) \\
&= \lim_{t\to\infty} -\frac{1}{t} \log e^{\alpha R_j} \overline{T}_t^{(\alpha)} e^{-\alpha R_j}(x) \\
&= \lim_{t\to\infty} -\frac{1}{t} \log e^{\alpha R_j} e^{-te(\alpha) R_j} \left(P_\alpha e^{-\alpha R_j} + e^{te(\alpha)} \overline{T}_t^{(\alpha)} (1 - P_\alpha) e^{-\alpha R_j}(x) \right) \\
&= \lim_{t\to\infty} -\frac{1}{t} \left(\alpha R_j(x) - te(\alpha) + \right. \\
&\qquad\qquad \left. \log \left(P_\alpha e^{-\alpha R_i}(x) + e^{te(\alpha)} \overline{T}_t^{(\alpha)} (1 - P_\alpha) e^{-\alpha R_i}(x) \right) \right) \\
&= e(\alpha)\,.
\end{aligned}$$

This concludes the proof of Theorem 4.4. ∎

It is straightforward now to obtain the symmetry of the Gallavotti-Cohen fluctuation theorem

Theorem 4.5 *If*
$$\alpha \in \left(-\frac{T_{\min}}{T_{\max} - T_{\min}}\,,\, 1 + \frac{T_{\min}}{T_{\max} - T_{\min}} \right)\,, \tag{4.53}$$
then
$$e(\alpha) = e(1 - \alpha)\,. \tag{4.54}$$

Proof: Let us consider the dual semigroup $(\overline{T}_t^{(\alpha)})^*$ acting on $\mathcal{H}_\theta^*$. Since $\overline{T}_t^{(\alpha)}$ has a smooth kernel, $(\overline{T}_t^{(\alpha)})^*\nu$ is a measure with a smooth density, and we denote by $(\overline{T}_t^{(\alpha)})^*$ its action on densities

$$(\overline{T}_t^{(\alpha)})^*\nu(dx) \;=\; \left((\overline{T}_t^{(\alpha)})^*\rho(x)\right)\,dx\,. \tag{4.55}$$

Combining Lemmas 4.2 and 4.3 we have

$$\begin{aligned}
\overline{L}_\alpha &= e^{-\alpha R_j}(L-\alpha\sigma_j)e^{\alpha R_j} \\
&= e^{-(1-\alpha)R_j}J(L-(1-\alpha)\sigma_j)^*Je^{(1-\alpha)R_j} \\
&= J\left(e^{(1-\alpha)R_j}(L-(1-\alpha)\sigma_j)e^{-(1-\alpha)R_j}\right)^*J \\
&= J\overline{L}_{1-\alpha}{}^*J
\end{aligned} \tag{4.56}$$

or

$$\overline{T}_t^{(\alpha)} \;=\; J(\overline{T}_t^{(1-\alpha)})^*J\,. \tag{4.57}$$

The spectral radius formula concludes the proof of Theorem 4.5. ∎

Combining this fact with the formal argument given above, we obtain the proof of part (b) of Theorem 4.1.

4.3 Kubo Formula and Central Limit Theorem

One can derive the Kubo formula of linear response theory from the fluctuation theorem. Here the external "field" driving the system out of equilibrium is the inverse temperature difference $\eta = (\beta_n - \beta_1)$ and we have $\sigma_j = \eta\phi_j$. Instead of the function $e(\alpha)$, we consider a the function $f(a,\eta)$ given by

$$f(a,\eta) \equiv \lim_{t\to\infty} -\frac{1}{t}\log \mathbf{E}_\mu\left[e^{-a\int_0^t \phi_i(x(s))\,ds}\right]\,, \tag{4.58}$$

where $a = \alpha\eta$ and the second variable in f indicates the dependence of the dynamics and of the stationary state μ on η. From our compactness results for the semigroup, one can show that $f(a,\eta)$ is a real-analytic function of both variables a and F. The relation $e(\alpha) = e(1-\alpha)$ now reads

$$f(a,\eta) \;=\; f(\eta - a,\eta)\,. \tag{4.59}$$

Differentiating this relation one finds

$$\frac{\partial^2 f}{\partial a \partial \eta}(0,0) \;=\; -\frac{\partial^2 f}{\partial a \partial \eta}(0,0) - \frac{\partial^2 f}{\partial a^2}(0,0)\,. \tag{4.60}$$

and thus

$$\frac{\partial^2 f}{\partial a \partial \eta}(0,0) \;=\; -\frac{1}{2}\frac{\partial^2 f}{\partial a^2}(0,0)\,. \tag{4.61}$$

This relation is indeed Kubo formula, although in a disguised form. Differentiating and using the stationarity we find

$$\frac{\partial f}{\partial a}(0,\eta) \quad = \quad \mathbf{E}_\mu\left[\frac{1}{t}\int_0^t \phi_j(x_s)ds\right] \;=\; \int \phi_j d\mu\,, \tag{4.62}$$

and therefore

$$\frac{\partial^2 f}{\partial a \partial \eta}(0,0) \;=\; \frac{\partial}{\partial \eta}\left(\int \phi_j d\mu\right)\Big|_{\Delta\beta=0} \tag{4.63}$$

is the derivative of the heat flow at equilibrium. On the other hand

$$\begin{aligned}&\frac{\partial^2 f}{\partial a^2}(0,\eta)\\ &= \lim_{t\to\infty}\mathbf{E}_\mu\left[\frac{1}{t}\int_0^t \phi_j(x_s)ds\right]^2 - \mathbf{E}_\mu\left[\frac{1}{t}\int_0^t \phi_j(x_s)ds\int_0^t \phi_j(x_u)du\right]\end{aligned} \tag{4.64}$$

At equilibrium, $\eta = 0$, the first term vanishes since there is no heat flow at equilibrium. For the second term, we obtain, using stationarity, and changing variables

$$\begin{aligned}&\frac{1}{t}\int_0^t ds\int_0^t du\mathbf{E}_\mu\left[\phi_j(x_s)\phi_j(x_u)\right]\\ &= 2\frac{1}{t}\int_0^t ds\int_s^t du\mathbf{E}_\mu\left[\phi_j(x_s)\phi_j(x_u)\right]\\ &= 2\frac{1}{t}\int_0^t ds\int_s^t du\mathbf{E}_\mu\left[\phi_j(x_0)\phi_j(x_{u-s})\right]\\ &= 2\frac{1}{t}\int_0^t ds\int_0^{t-s} du\mathbf{E}_\mu\left[\phi_j(x_0)\phi_j(x_u)\right]\\ &= 2\frac{1}{t}\int_0^t ds\int_0^{s} du\mathbf{E}_\mu\left[\phi_j(x_0)\phi_j(x_u)\right]\end{aligned} \tag{4.65}$$

By Theorem 3.1 we obtain

$$\mathbf{E}_\mu\left[\phi_j(x_0)\phi_j(x_u)\right] \;=\; \int \phi_j(x)T_u\phi_j(x)\mu(dx) \;\leq\; Ce^{-u\gamma}\|\phi_j^2\|_{W\infty} \tag{4.66}$$

and thus it is an integrable function of u. We then obtain

$$\begin{aligned}\frac{\partial^2 f}{\partial a^2}(0,0) &= \lim_{t\to\infty} 2\frac{1}{t}\int_0^t ds \int_0^s du \mathbf{E}_\mu \left[\phi_j(x_0)\phi_j(x_u)\right] \\ &= 2\int_0^\infty ds \int \phi_j(x) T_u \phi_j(x)\mu(dx)\,, \end{aligned} \tag{4.67}$$

is the integral of the flow autocorrelation function. Combining Eqs. (4.61), (4.63), and (4.67) we obtain

$$\frac{\partial}{\partial \eta}\left(\int \phi_j d\mu\right)\Big|_{\eta=0} = \int_0^\infty \left(\int (T_t\phi_j)\phi_j d\mu\right) ds\,, \tag{4.68}$$

and this is the familiar Kubo formula. Note that this formula involves only the equilibrium dynamics and the equilibrium stationary distribution.

The appearance of an autocorrelation function is not fortuitous and can be interpreted in terms of the central limit theorem. With the strong ergodic properties we have established in Theorem 3.1, one can prove [19] a central limit theorem for any function f such that $f^2 \in \mathcal{H}_\theta$ (see the condition for exponential mixing in Theorem 3.1). For any such function we have that

$$\mathbf{P}_x\left\{a < \frac{1}{\sqrt{\kappa^2 t}}\int_0^t \left(f(x_t) - \int f(x)\mu(dx)\right) ds < b\right\} \longrightarrow \frac{1}{\sqrt{2\pi}}\int_a^b e^{-\frac{y^2}{2}}\, dy \tag{4.69}$$

provided the variance

$$\kappa^2 = \int_0^\infty \left(\int g(x)T_t g(x)\mu(dx) - (\int g(x)\mu(dx))^2\right) \tag{4.70}$$

does not vanish. In our case $f = \phi_j$, it follows from (4.68) and from the positivity of entropy production that κ^2 is positive.

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