Fluctuations of the Entropy Production in Anharmonic Chains

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Abstract

We prove the Gallavotti-Cohen fluctuation theorem for a model of heat conduction through a chain of anharmonic oscillators coupled to two Hamiltonian reservoirs at different temperatures.

1 Introduction

The Gallavotti-Cohen fluctuation theorem refers to a symmetry in the fluctuations of the entropy production in nonequilibrium statistical mechanics. It was first discovered in numerical experiments of Evans, Cohen and Morris [8] and then discussed in [9] in the context of *thermostated systems*. As a mathematical theorem it was proved for Anosov dynamical systems [9, 10]. Soon thereafter the fluctuation theorem was discussed in the context of *stochastic dynamical systems* first by Kurchan [17] and then, more systematically by Lebowitz and Spohn, and Maes [22, 18]. In particular, Maes discovered a general formulation of the fluctuation theorem in the context of space-time Gibbs measures which covers both Markovian stochastic dynamics and chaotic deterministic dynamics (via a Markov partition). As a mathematical theorem the fluctuation theorem is proven for quite general stochastic models with *finite* state space, such as lattices gases in a finite box. Relations for the free energy related to the fluctuation theorem have been also discussed in [15, 2].

Among the consequences of the fluctuation theorem is the *non-negativity* of entropy production although the proof of its *positivity* is more difficult and is so far proved only in particular examples [7, 20]. We also note that in the related context of open systems, classical and quantum, the production of entropy is discussed at a general level in [27, 13, 24]. Again the non-negativity of entropy production is relatively easy to establish, while the strict positivity has been established only in particular models [7, 14].

In this paper we consider an *open system* consisting of a finite (but of arbitrary size) chain of anharmonic oscillators coupled at its ends only to reservoirs of free

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phonons at positive and different temperatures [6, 7, 5, 25, 26]. In particular our model is completely Hamiltonian and its phase space is not compact.

In order to establish the fluctuation theorem, two ingredients are needed: one needs to prove a *large deviation theorem* for the ergodic average of the entropy production and establish a *symmetry* of the large deviation functional. The second part is usually relatively straightforward to establish, at a formal level, since it follows from a symmetry of the generator of the dynamics. This formal derivation for models related to ours can be found in [22] and [19].

The first part, proving the existence of the large deviation functional, involves technical difficulties, in particular if the phase space of the model is *not compact*. In this case large deviation theorems are established provided the system satisfies very strong ergodic properties (such as hypercontractivity) see e.g. [3, 4, 29]. In addition the entropy production is in general an *unbounded* observable while standard results of large deviations apply only to bounded observables.

In this paper we show how to treat these difficulties in the model at hand. The techniques we use are based on the construction of Liapunov functions for certain Feynman-Kac semigroups and Perron-Frobenius-like theorem in Banach spaces. We heavily rely on the strong ergodic properties of our model established in [6, 7, 5] and especially in [26].

The Hamiltonian of the model, as in [6], has the form

$$H \;=\; H_B + H_S + H_I \,. \tag{1}$$

The two reservoirs of free phonons are described by wave equations in $\mathbf{R}^d$ with Hamiltonian

$$\begin{aligned} H_B &= H(\varphi_L, \pi_L) + H(\varphi_R, \pi_R)\,, \\ H(\varphi, \pi) &= \frac{1}{2}\int dx\,(|\nabla\varphi(x)|^2 + |\pi(x)|^2)\,, \end{aligned}$$

where L and R stand for the "left" and "right" reservoirs, respectively. The Hamiltonian describing the chain of length n is given by

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

where $(p_i, q_i) \in \mathbf{R}^d \times \mathbf{R}^d$ are the coordinates and momenta of the i^{th} particle of the chain. The phase space of the chain is $\mathbf{R}^{2dn}$. The interaction between the chain and the reservoirs occurs at the boundaries only and is of dipole-type

$$H_I \;=\; q_1 \cdot \int dx\, \nabla\varphi_L(x)\rho_L(x) + q_n \cdot \int dx\, \nabla\varphi_R(x)\rho_R(x)\,,$$

where ρ_L and ρ_R are coupling functions ("charge densities").

Our assumptions on the anharmonic lattice described by $H_S(p,q)$ are the following:

- **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 A_i, B_i, and C_i, $i=1,2$ such that

  $$\begin{aligned} \lim_{\lambda\to\infty} \lambda^{-k_i} U^{(i)}(\lambda x) &= A_i \|x\|^{k_i}\,, \\ \lim_{\lambda\to\infty} \lambda^{-k_i+1} \nabla U^{(i)}(\lambda x) &= A_i k_i \|x\|^{k_i-2} x\,, \\ \|\partial^2 U^{(i)}(x)\| &\leq (B_i + C_i V(x))^{1-\frac{2}{k_i}}\,. \end{aligned}$$

  Moreover we will assume that

  $$k_2 \geq k_1 \geq 2\,,$$

  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: For $x \in \mathbf{R}^d$ and $m = 1, 2, \cdots$, let $A^{(m)}(x) : \mathbf{R}^d \to \mathbf{R}^{d^m}$ denote the linear maps given by

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

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

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

- **H3 Rationality of the coupling**: Let $\hat{\rho}_i$ denote the Fourier transform of ρ_i. We assume that

  $$|\hat{\rho}_i(k)|^2 = \frac{1}{Q_i(k^2)}\,,$$

  where Q_i, $i \in \{L, R\}$ are polynomials with real coefficients and no roots on the real axis.

We introduce now the temperatures of the reservoirs by choosing initial conditions for the reservoirs. The Hamiltonian of a reservoir is quadratic in $\Psi \equiv (\phi, \pi)$, $H = \langle \Psi, \Psi \rangle / 2$, and therefore the Gibbs measure at temperature T, $d\mu_T(\Psi)$ is the Gaussian measure with covariance $T\langle \cdot\,, \cdot \rangle$. To construct nonequilibrium steady states we assume that

- The initial conditions $\Psi_L = (\phi_L, \pi_L)$ and $\Psi_R = (\phi_R, \pi_R)$ of the reservoirs are distributed according the gaussian Gibbs measures $d\mu_{T_L}$ and $d\mu_{T_R}$ respectively.

In order to define the heat flow through the bulk of the crystal we consider the energy of the i^{th} oscillator which we take to be

$$H_i = \frac{p_i^2}{2} + U^{(1)}(q_i) + \frac{1}{2}\left(U^{(2)}(q_{i-1} - q_i) + U^{(2)}(q_i - q_{i+1})\right) . \tag{2}$$

Differentiating H_i with respect to time, one finds that

$$\frac{dH_i}{dt} = \Phi_{i-1} - \Phi_i ,$$

where

$$\Phi_i = \frac{(p_i + p_{i+1})}{2} \nabla U^{(2)}(q_i - q_{i+1}) \tag{3}$$

is the heat flow from the i^{th} to the $(i+1)^{th}$ particle. We define a corresponding entropy production by

$$\sigma_i = \left(\frac{1}{T_R} - \frac{1}{T_L}\right) \Phi_i ,$$

where T_R and T_L are the temperatures of the reservoirs.

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 Φ_L, Φ_R at the boundary of the chains, and define $\sigma_b = -\Phi_L/T_L - \Phi_R/T_R$, or one might take other quantities as local energies. But using conservation laws it is easy to see that all these heat flows have the same average in the steady state. Moreover we will show that all the entropy productions have the same large deviations functionals: the exponential part of their fluctuations are identical.

We denote $(p(t), q(t)) = (p(t, p_0, q_0, \Psi_L, \Psi_R), q(t, p_0, q_0, \Psi_L, \Psi_R))$ as the Hamiltonian flow generated by the Hamiltonian (1), and consider the ergodic average

$$\overline{\sigma}_i{}^t \equiv \frac{1}{t}\int_0^t \sigma_i(p(s), q(s))\, ds .$$

The quantity $\sigma_i(p(s), q(s))$ depends on both the initial conditions of the chain and of the reservoirs which, by assumption, are distributed according to thermal equilibrium. By the ergodic theorem proven in [26] there exists a measure $d\nu$ on $\mathbf{R}^{2dn}$ such that

$$\lim_{t\to\infty} \overline{\sigma}_i{}^t = \int \sigma_i \, d\nu .$$

for all (p_0, q_0) and $d\mu_{T_L}$ and $d\mu_{T_R}$ almost surely. Moreover $\int \sigma_i \, d\nu \equiv \langle\sigma\rangle_\nu$ is independent of i and as shown in [7]

$$\langle\sigma\rangle_\nu \geq 0 \text{ and } \langle\sigma\rangle_\nu = 0 \text{ if and only if } T_L = T_R .$$

Given a set $A \subset \mathbf{R}$, we say that the fluctuations of σ_i in A satisfy the large deviation principle with large deviation functional $I(w)$ provided

$$\inf_{w \in \mathrm{Int(A)}} I(w) \;\leq\; \liminf_{t \to \infty} -\frac{1}{t} \log \mathbf{P}\{\overline{\sigma}_i{}^t \in A\} \;\leq\;$$
$$\limsup_{t \to \infty} -\frac{1}{t} \log \mathbf{P}\{\overline{\sigma}_i{}^t \in A\} \;\leq\; \inf_{w \in \mathrm{Clos(A)}} I(w)\,.$$

The study of large deviations for σ_i is based on the moment generating functionals $e_i(\alpha)$ given by

$$e_i(\alpha) \;=\; \lim_{t \to \infty} -\frac{1}{t} \log \int d\mu_{T_L} d\mu_{T_R} e^{-\alpha \int_0^t \sigma_i(p(s),q(s))\, ds}\,.$$

The main technical result of this paper is

Theorem 1.1 *If*

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

$e(\alpha) \;\equiv\; e_i(\alpha)$ *is finite and independent of* i *and the initial conditions* (p_0, q_0). *Moreover* $e(\alpha)$ *satisfies the relation*

$$e(\alpha) = e(1 - \alpha)\,.$$

As an application of the Gärtner-Ellis Theorem, see [4], Theorem 2.3.6, we obtain the Gallavotti-Cohen fluctuation theorem.

Theorem 1.2 *There is a neighborhood* O *of the interval* $[-\langle \sigma \rangle_\nu\,, \langle \sigma \rangle_\nu]$ *such that for* $A \subset O$ *the fluctuations of* σ_i *in* A *satisfy the large deviation principle with a large deviation functional* $I(w)$ *obeying*

$$I(w) - I(-w) \;=\; -w\,,$$

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

Theorem 1.2 provides information on the ratio of the probabilities of observing the entropy production to be w and $-w$: roughly speaking we have

$$\frac{\mathbf{P}\{\overline{\sigma}_i{}^t \in (w - \epsilon, w + \epsilon)\}}{\mathbf{P}\{\overline{\sigma}_i{}^t \in (-w - \epsilon, -w + \epsilon)\}} \sim e^{wt}\,.$$

2 Fluctuations of the entropy production

2.1 Exponential mixing and compactness

As shown in [6, 26], under condition **H3** the dynamics of the complete system can be reduced to a Markov process on the extended phase space consisting of the phase space of the chain $\mathbf{R}^{2dn}$ and of a finite number of auxiliary variables which we denote as r. In the simplest case which we consider here, (corresponding to $\hat{\rho}(k) \sim (k^2+\gamma^2)^{-1}$), $r=(r_1,r_n) \in \mathbf{R}^{2d}$ and the resulting equations of motion take the form

$$\begin{aligned}
\dot{q} &= p\,, \\
\dot{p} &= -\nabla_q V - \Lambda^T r\,, \\
dr &= (-\gamma r + \Lambda p)\,dt + (2\gamma T)^{1/2} d\omega\,. \qquad (4)
\end{aligned}$$

Here $p=(p_1,\cdots,p_n)$ and $q=(q_1,\cdots,q_n)$ denote the momenta and positions of the particle, $r=(r_1,r_n)$ are the auxiliary variables and ω is a standard $2d$-dimensional Wiener process. The linear map $\Lambda : \mathbf{R}^{dn} \to \mathbf{R}^{2d}$ is given by $\Lambda(p_1,\ldots,p_n) = (\lambda p_1, \lambda p_n)$ and $T : \mathbf{R}^{2d} \to \mathbf{R}^{2d}$ by $T(x,y) = (T_1 x, T_n y)$. Here $T_1 \equiv T_L$ and $T_n \equiv T_R$ are the temperatures of the reservoirs attached to the first and n^{th} particles respectively, γ is the constant appearing in $\hat{\rho}$ and λ is a coupling constant equal to $\|\rho\|_{L^2}$.

The solution of Eq. (4), $x(t) = (p(t),q(t),r(t))$ with $x \in X = \mathbf{R}^{2d(n+1)}$ is a Markov process. We denote T^t as the corresponding semigroup

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

with generator

$$L \,=\, \gamma\,(\nabla_r T \nabla_r - r\nabla_r) + (\Lambda p \nabla_r - r\Lambda\nabla_p) + (p\nabla_q - (\nabla_q V(q))\nabla_p)\;, \qquad (5)$$

and we denote $P_t(x,dy)$ as the transition probability of the Markov process $x(t)$. In [26] we proved that the Markov process $x(t)$ has smooth transition probabilities, in particular it is *strong Feller*, and that it is (small-time) *irreducible*: For any $t>0$, any $x \in X$ and any open set $A \subset X$ we have $P_t(x,A) > 0$.

There is a natural energy function associated to Eq.(4), given by

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

which we employ throughout our discussion. In [26] we have constructed a *Liapunov function* for $x(t)$ from G: Let $t>0$ and $0<\theta<\max(T_1,T_n)^{-1}$. Then there exists E_0 such that for all $E>E_0$ there exist functions $\kappa=\kappa(E)<1$ and $b=b(E)<\infty$ such that

$$T^t e^{\theta G}(x) \,\le\, \kappa(E) e^{\theta G}(x) + b(E)\mathbf{1}_{\{G\le E\}}(x)\,. \qquad (6)$$

Moreover $\kappa(E)$ can be made arbitrarily small by choosing E sufficiently large, in fact there exist positive constants $c_1 = c_1(\theta,t)$ and $c_2 = c_2(\theta,t)$ such that

$$\kappa(E) \le c_1 e^{-c_2 E^{2/k_2}}\,. \qquad (7)$$

By results of [21] it is also shown in [26] that the convergence to the unique stationary state, denoted by μ, occurs exponentially fast: Let $\mathcal{H}_{\infty,\theta}$ denote the Banach space $\{f\,;\,\|f\|_{\infty,\theta} \equiv \sup_x |f(x)|e^{-\theta G(x)} < \infty\}$. Then there exist constants $r > 1$ and $R < \infty$

$$|T^t f(x) - \int f d\mu| \leq R r^{-t} \|f\|_{\infty,\theta} e^{\theta G(x)}\,, \tag{8}$$

which means that T^t, acting on $\mathcal{H}_{\infty,\theta}$ has a spectral gap. The methods of [21] are probabilistic and rely on a nice probabilistic construction called splitting as well as coupling arguments and renewal theory.

Under the condition given here, by taking advantage of the fact that the constant κ in the Liapunov bound (6) can be made arbitrarily small (this is not assumed in [21]), we can prove stronger ergodic properties and also give a direct analytical proof of Eq. (8).

Besides the Banach space $\mathcal{H}_{\infty,\theta}$ defined above we also consider the Banach space $\mathcal{H}^0_{\infty,\theta} = \{f, |f|e^{-\theta G} \in C_0(X)\}$ with norm $\|\cdot\|_{\infty,\theta}$ ($C_0(X)$ denotes the set of continuous functions which vanish at infinity). Furthermore for $1 \leq p < \infty$ we consider the family of Banach spaces $\mathcal{H}_{p,\theta} = L^p(X, e^{-p\theta G(x)}dx)$ and denote $\|\cdot\|_{p,\theta}$ the corresponding norms.

Theorem 2.1 *If $0 < \theta T_i < 1$, the semigroup T^t extends to a strongly continuous quasi-bounded semigroup on $\mathcal{H}_{p,\theta}$, for $1 \leq p < \infty$ and on $\mathcal{H}^0_{\infty,\theta}$. For any $t > 0$, T^t is compact on $\mathcal{H}_{p,\theta}$, for $1 < p \leq \infty$ and on $\mathcal{H}^0_{\infty,\theta}$.*

As an immediate consequence of the spectral properties of positive semigroups [11] and the irreducibility of $x(t)$ we have

Corollary 2.2 *The Markov process $x(t)$ has a unique invariant measure $d\mu$ and Eq. (8) holds.*

Proof: : Since T^t is a Markovian, compact, and irreducible semigroup the eigenvalue 1 is simple with the constant as the eigenfunction. This shows that the Markov process $x(t)$ has a unique invariant measure. Moreover by the cyclicity properties of the spectrum of a positive semigroup [11], and by the compactness of T^t, there are no other eigenvalues of modulus 1. Eq. (8) follows immediately. ■

Proof of Theorem 2.1 In [26], Lemma 3.6, we showed that for some constant C $T^t e^{\theta G} \leq e^{ct} e^{\theta G}$ provided $\theta T_i < 1$ (see also Lemma 2.9 below). Therefore for f C^∞ with compact support we have, using Ito's and Girsanov's formulas

$$\begin{aligned} e^{-\theta G} T^t e^{\theta G} f(x) &= \mathbf{E}_x \left[e^{\theta(G(x(t))-G(x))} f(x) \right] \\ &= \mathbf{E}_x \left[e^{\theta \int_0^t \gamma(\mathrm{Tr}(T)-r^2)\, ds + \theta \int_0^t \sqrt{2\gamma T} r\, d\omega(s)} f(x(t)) \right] \\ &= \mathbf{E}_x \left[e^{\gamma\theta \mathrm{Tr}(T) + \gamma \tilde{r}(\theta^2 T - \theta)\tilde{r}} f(\tilde{x}(t)) \right] \,, \end{aligned}$$

where $\tilde{x}$ is the process with generator

$$\tilde{L}_\theta \;=\; L + 2\gamma\theta r T\nabla_r\,.$$

A computation shows that $\tilde{L}_\theta^T 1 = \gamma \mathrm{Tr}(1-2\theta T)$. Standard arguments show then that the semigroup associated with the process $\tilde{x}$ extends to a quasi-bounded and strongly continuous semigroup on $L^p(dx)$, $1 \le p < \infty$ and on $C_0(X)$. Using the assumption that $\theta T_i < 1$ and Feynman-Kac formula we see that $e^{-\theta G}T^t e^{\theta G}$ extends too to a quasi-bounded and strongly continuous semigroup on $L^p(dx)$, $1 \le p < \infty$ and on $C_0(X)$. This implies immediately that T^t extends to a strongly continuous semigroup on $\mathcal{H}_{p,\theta}$, $1 \le p < \infty$ and $\mathcal{H}^0_{\infty,\theta}$. The computation above also shows that T^t extends to a quasi-bounded semigroup on $\mathcal{H}_{\infty,\theta}$.

We first prove the compactness of T^t for $\mathcal{H}_{\infty,\theta}$. If $f \in \mathcal{H}_{\infty,\theta}$ then $|f(x)| \le \|f\|_{\infty,\theta} e^{\theta G(x)}$ and by (6) and (7) we obtain

$$\begin{aligned}
|\mathbf{1}_{G\ge E} T^t f(x)| &\le e^{\theta G(x)} \sup_{\{y: G(y)\ge E\}} \frac{|T^t f(y)|}{e^{\theta G(y)}} \\
&\le e^{\theta G(x)} \|f\|_{\infty,\theta} \sup_{\{y: G(y)\ge E\}} \frac{T^t e^{(\theta G(y))}}{e^{\theta G(y)}} \\
&\le \kappa(E) e^{\theta G(x)} \|f\|_{\infty,\theta}\,. \qquad (9)
\end{aligned}$$

From the bounds (9) and (7) we conclude that the operator $\mathbf{1}_{\{G\ge E\}}T^t$ converges uniformly to 0 in $\mathcal{H}_{\infty,\theta}$ as $E \to \infty$. The semigroup T^t has a C^∞ kernel since it is generated by a hypoelliptic operator see [26], Proposition 4.1, so, by the Arzela-Ascoli theorem $\mathbf{1}_{\{G\le E\}}T^{t/2}\mathbf{1}_{\{G\le E\}}$ is compact, for any E. Therefore we obtain

$$T^t \,=\, \lim_{E\to\infty} \mathbf{1}_{\{G\le E\}} T^{t/2} \mathbf{1}_{\{G\le E\}} T^{t/2}\,,$$

where the limit is in the norm sense from (9) above, i.e., T^t is the uniform limit of compact operators, hence is compact.

The compactness of T^t for $\mathcal{H}^0_{\infty,\theta}$ follows from the same argument. In fact by Eq.(7), for any $t > 0$, $T^t\mathcal{H}_{\infty,\theta} \subset \mathcal{H}^0_{\infty,\theta}$.

To prove the compactness of T^t on $\mathcal{H}_{p\theta}$, $1 < p < \infty$, we note that

$$\begin{aligned}
|T^t f(x)| &= |\mathbf{E}_x[f(x(t))]| \\
&= |\mathbf{E}_x[e^{\frac{\theta}{q}G(x(t))} e^{-\frac{\theta}{q}G(x(t))} f(x(t))]| \\
&\le \Big(\mathbf{E}_x[e^{\theta G(x(t))}]\Big)^{1/q} \Big(\mathbf{E}_x[e^{-\frac{p\theta}{q}G(x(t))} f^p(x(t))]\Big)^{1/p}\,.
\end{aligned}$$

Thus using the bound (7) and the fact that T^t is quasi-bounded on $\mathcal{H}_{1,\theta}$ we obtain

$$\|\mathbf{1}_{G\ge E} T^t f\|^p_{\theta,p} \;\le \int_{\{x: G(x)\ge E\}} \mathbf{E}_x[e^{\theta G(x(t))}]^{\frac{p}{q}}\; \mathbf{E}_x[e^{-\frac{p\theta}{q}G(x(t))} f^p(x(t))] e^{-p\theta G(x)} dx$$

$$
\begin{aligned}
&\le \sup_{\{x:G(x)\ge E\}} \left(\frac{\mathbf{E}_x[e^{\theta G(x(t))}]}{e^{\theta G(x)}}\right)^{\frac{p}{q}} \|T^t(e^{-\frac{p\theta}{q}G} f^p)\|_{1,\theta} \\
&\le \kappa(E)^{\frac{p}{q}} e^{ct} \|e^{-\frac{p\theta}{p}G} f^p\|_{1,\theta} \\
&= \kappa(E)^{\frac{p}{q}} e^{ct} \|f\|^p_{\theta,p} \,.
\end{aligned}
$$

As in the case $p=\infty$, we conclude from the bound (7) that the operator $\mathbf{1}_{G\ge E}T^t$ converges uniformly to 0 in $\mathcal{H}_{p,\theta}$ as $E\to\infty$. Using that the kernel of $\mathbf{1}_{\{G\le E\}}T^t\mathbf{1}_{\{G\le E\}}$ is bounded, we conclude that T^t is compact on $\mathcal{H}_{p,\theta}$ for $1<p<\infty$. ∎

2.2 Heat flow and generating functionals

In order to define the heat flows we note that we have

$$
\frac{d}{dt}T^tH \;=\; LT^tH \;=\; T^t(-r\Lambda p) \;=\; T^t(-\lambda r_1 p_1 - \lambda r_n p_n)\,.
$$

Hence we identify $\Phi_0 \equiv -\lambda r_1 p_1$ as the observable describing the heat flow from the left reservoir into the chain and $\Phi_n \equiv \lambda r_n p_n$ as the heat flow from the chain into the right reservoir. As in the introduction we define the energy H_i of the i^{th} oscillators by Eq.(2), for $i\le 2\le n-1$, and

$$
\begin{aligned}
H_1 &= \frac{p_1^2}{2} + U^{(1)}(q_1) + \frac{1}{2}U^{(2)}(q_1-q_2)\,, \\
H_n &= \frac{p_n^2}{2} + U^{(1)}(q_n) + \frac{1}{2}U^{(2)}(q_{n-1}-q_n)\,.
\end{aligned}
$$

With the heat flows Φ_i, $i=1,\cdots,n$, defined as in Eq. (3) we have

$$
LH_i \;=\; \Phi_{i-1} - \Phi_i\,, \quad i=1,\cdots,n\,.
$$

and we define the entropy productions σ_i, $i=0,\cdots,n$ by

$$
\sigma_i \;=\; \left(\frac{1}{T_1} - \frac{1}{T_n}\right)\Phi_i \quad i=0,\cdots,n\,.
$$

We now provide several identities involving the generator of the dynamics and the entropy production, which will play a crucial role in our subsequent analysis.

Lemma 2.3 *Let the function R_i, $i=0,\cdots,n$ be given by*

$$
R_i \;=\; \frac{1}{T_1}\left(\frac{r_1^2}{2} + \sum_{k=1}^{i} H_i(p,q)\right) + \frac{1}{T_n}\left(\sum_{k=i+1}^{n} H_i(p,q) + \frac{r_n^2}{2}\right)\,. \tag{10}
$$

Then we have

$$
\sigma_i = rT^{-1}r - \mathrm{Tr}(I) + LR_i\,. \tag{11}
$$

Proof: This is a straightforward computation. ■

Remark 2.4 This shows that, up to a derivative, all the entropy productions are equal to the quantity $rT^{-1}r - \mathrm{Tr}\gamma I$ which is independent of i and involves only the r-variables.

Let L^T be the formal adjoint of the operator L given by Eq. (5)

$$L^T \,=\, \gamma\left(\nabla_r T \nabla_r + r\nabla_r\right) - \left(\Lambda p \nabla_r - r\Lambda\nabla_p\right) - \left(p\nabla_q - (\nabla_q V(q))\nabla_p\right) \,, \tag{12}$$

and let J be 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. (14) actually generate semigroups for some non trivial domain of α is a non trivial result which we will discuss in Section 2.3.

Lemma 2.5 *We have the operator identities*

$$e^{R_i} J L^T J e^{-R_i} \,=\, L - \sigma_i \,, \tag{13}$$

and also for any constant α

$$e^{-R_i} J (L^T - \alpha\sigma_i) J e^{R_i} \,=\, L - (1-\alpha)\sigma_i \,. \tag{14}$$

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

$$\begin{aligned} L_0 &= \gamma\left(\nabla_r T \nabla_r - r\nabla_r\right) && (15)\\ L_1 &= \left(\Lambda p \nabla_r - r\Lambda\nabla_p\right) + \left(p\nabla_q - (\nabla_q V(q))\nabla_p\right) \,. && (16)\end{aligned}$$

Since L_1 is a first order differential operator we have

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

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

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

This gives

$$e^{-R_i} L e^{R_i} \,=\, L_0^T + L_1 + \sigma_i \,=\, J L^T J + \sigma_i \,,$$

which is Eq. (13). Since $J\sigma_i J = -\sigma_i$, Eq. (14) follows immediately from Eq. (13).

Remark 2.6 In the equilibrium situation, i.e., for $T_1 = T_n = T$, Eq. (14) is

$$e^{G/T} J L^T J e^{-G/T} \,=\, L \,,$$

which is simply *detailed balance*. Eq. (14) can be interpreted in path space in the following manner [18]: Let Π denote the time-reversal in path space on the time interval $[0,t]$: $\Pi(p(s),q(s),r(s)) = (-p(t-s),q(t-s),r(t-s))$ and let dP denote the measure on $\mathcal{C}([0,t],X)$ induced by $x(t)$. Then Eq. (14) implies that

$$\frac{dP\circ\Pi}{dP} \;=\; e^{R_i(x(t))-R_i(x(0))-\int_0^t \sigma_i(x(s))\,ds}\,.$$

This formula exhibits the fact that the lack of microscopic reversibility is intimately related to the entropy production.

We now turn to the study of the large deviations. As shown in [26] the Markov process $x(t)$ is ergodic. In order to study the large deviations of $t^{-1}\int_0^t \sigma_i(x(s))ds$ we consider the moment generating functionals

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

Formally the Feynman-Kac formula gives $\Gamma_x^i(t,\alpha) = e^{t(L-\alpha\sigma_i)}1(x)$, but since σ_i is not bounded, nor even relatively bounded by L, it is not obvious that $\Gamma_x^i(t,\alpha)$ exists for $\alpha\neq 0$. Our goal is to prove that $\Gamma_x^i(t,\alpha)$ exists and that the limit

$$e(\alpha)\equiv\lim_{t\to\infty}-\frac{1}{t}\log\Gamma_x^i(t,\alpha) \tag{17}$$

exists and is finite in a neighborhood of the interval $[0,1]$, and is independent of i and of the initial condition x.

The technical difficulty in proving the existence of the limit (17) lies in the fact that the functions σ_i are *unbounded*. Standard large deviation theorems for Markov processes (see e.g. [3, 4, 29]) are proven usually under strong ergodic properties for bounded functions and are not directly applicable. Large deviations for unbounded functions are considered in [1] for discrete time countable state space Markov chains under conditions which amount in our case to $\sigma = o(G)$. In our case this is clearly not satisfied since, in general σ is *not* bounded by G.

But the σ_i are very special observables, in particular they are intimately linked with the dynamics as shown by the identities Eqs.(13) and (14). The next lemma displays another identity which will be important in our analysis.

Lemma 2.7 *We have the identity*

$$L-\alpha\sigma_i \;=\; e^{\alpha R_i}\overline{L}_\alpha e^{-\alpha R_i}\,, \tag{18}$$

where

$$\overline{L}_\alpha \;=\; \tilde{L}_\alpha - \big((\alpha-\alpha^2)\gamma r T^{-1} r - \alpha\mathrm{Tr}(\gamma I)\big) \tag{19}$$

and

$$\tilde{L}_\alpha \;=\; L + 2\alpha\gamma r\nabla_r\,. \tag{20}$$

Proof: As in Lemma 2.5 we write the generator L as $L = L_0 + L_1$, see Eqs.(16) and (15). Since L_1 is a first order differential operator we have

$$e^{-\alpha R_i} L_1 e^{\alpha R_i} \;=\; L_1 + \alpha(L_1 R_i) \;=\; L_1 + \alpha\sigma_i\,. \tag{21}$$

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

$$\begin{aligned} e^{-\alpha R_i} L_0 e^{\alpha R_i} &= \gamma\left((\nabla_r + \alpha T^{-1} r) T (\nabla_r + \alpha T^{-1} r) - r(\nabla_r + \alpha T^{-1} r)\right) \\ &= L_0 + \alpha\gamma(r\nabla_r + \nabla_r r) + (\alpha^2 - \alpha)\gamma r T^{-1} r \\ &= L_0 + 2\alpha\gamma r\nabla_r + (\alpha^2 - \alpha)\gamma r T^{-1} r + \alpha \mathrm{Tr}\gamma I\,. \end{aligned} \tag{22}$$

Combining Eqs. (21) and (22) gives the desired result. ■

Remark 2.8 The identity (18) shows that all operators $L - \alpha\sigma_i$ are conjugate to the same operator $\overline{L}_\alpha$. This will be the key element to prove that $e(\alpha)$ is independent of i. Furthermore it can be seen from Eqs. (19) and (20) that $\overline{L}_\alpha$ has the form of L plus a perturbation which is a quadratic form in r and ∇_r. Such a perturbation is indeed nicer than $\alpha\sigma_i$. Also it should be noted that $\tilde{L}_\alpha$ has very much the same form as the operator L: they differ only by the coefficient in front of the term $r\nabla_r$. This fact will allow us to use several results on L obtained in [26].

2.3 Liapunov Function for Feynman-Kac Semigroups

At this point we begin the study of $\overline{L}_\alpha$ as the generator of a semigroup.

Proposition 2.9 *If θ and α satisfy the condition*

$$-\alpha < \theta T_i < 1 - \alpha\,, \tag{23}$$

then there exists a constant $C = C(\alpha, \theta)$ such that $e^{t\overline{L}_\alpha} e^{\theta G}(x) \leq e^{Ct} e^{\theta G}(x)$.

Proof: We note first that $\tilde{L}_\alpha$, defined in Eq. (19), for all $\alpha \in \mathbf{R}$, is the generator of a Markov process which we denote as $\tilde{x}(t)$. Indeed we have that

$$\tilde{L}_\alpha G(x) \;=\; \mathrm{Tr}(\gamma T) - (1 + 2\alpha) r^2 \;\leq\; C_1 + C_2 G(x)$$

Since G grows at infinity, G is a Liapunov function for $\tilde{x}(t)$ and a standard argument [16] shows that the Markov process $\tilde{x}(t)$ is non-explosive. Furthermore we have the bound

$$\begin{aligned} &\overline{L}_\alpha \exp\theta G(x) \;= \\ &= \exp\theta G(x)\gamma\left[\mathrm{Tr}(\theta T + \alpha I) + r(\theta^2 T - (1 - 2\alpha)\theta - \alpha(1-\alpha) T^{-1}) r\right] \\ &\leq C \exp\theta G(x)\,, \end{aligned} \tag{24}$$

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

$$\theta^2 T_i - (1-2\alpha)\theta - \alpha(1-\alpha)T_i^{-1} \leq 0\,,$$

or

$$-\alpha < \theta T_i < 1-\alpha\,.$$

We denote σ_R as the exit time from the set $\{G(x) < R\}$, i.e., $\sigma_R = \inf\{t \geq 0, G(\tilde{x}(t)) \geq R\}$. If the initial condition x satisfies $G(x) = E < R$, we denote by $\tilde{x}_R(t)$ the process which is stopped when it exits $\{G(x) < R\}$, i.e., $\tilde{x}_R(t) = \tilde{x}(t)$ for $t < \sigma_R$ and $\tilde{x}_R(t) = x(\sigma_R)$ for $t \geq \sigma_R$. Finally we set $\sigma_R(t) = \min\{\sigma_R, t\}$.

By Eq. (24), the function $W(t,x) = e^{-Ct}e^{\theta G(x)}$ satisfies the inequality $(\partial_t + \overline{L}_\alpha)W(t,x) \leq 0$ and applying Ito's formula with stopping time to the function $W(t,x)$ we obtain

$$\mathbf{E}_x \left[e^{-\int_0^{\sigma_R(t)} \left((\alpha-\alpha^2)\gamma\tilde{r}T^{-1}\tilde{r} - \alpha \mathrm{Tr}(\gamma I)\right)\, ds} e^{\theta G(\tilde{x}(\sigma_R(t)))} e^{-C\sigma_R(t)} \right] - e^{\theta G(x)} \leq 0\,,$$

and thus

$$\mathbf{E}_x \left[e^{-\int_0^{\sigma_R(t)} \left((\alpha-\alpha^2)\gamma\tilde{r}T^{-1}\tilde{r} - \alpha \mathrm{Tr}(\gamma I)\right)\, ds} e^{\theta G(\tilde{x}(\sigma_R(t)))} \right] \leq e^{Ct} e^{\theta G(x)}\,.$$

Since the Markov process $\tilde{x}(t)$ is non-explosive $G(\tilde{x}_R(t)) \to G(\tilde{x}(t))$ almost surely as $R \to \infty$, so by the Fatou lemma we have

$$e^{t\overline{L}_\alpha} e^{\theta G}(x) \leq e^{Ct} e^{\theta G}(x)\,.$$

This concludes the proof of Lemma 2.9. ■

The next three theorems are all consequences of the fact that $\tilde{L}_\alpha$ is the generator of a Markov process which is similar to the process generated by L: Indeed L and $\tilde{L}_\alpha$ differ only by the coefficient in front of the $r\nabla_r$ term. Therefore repeating the proofs of [26] we obtain

Theorem 2.10 *The semigroup* $e^{t\overline{L}_\alpha}$ *has a smooth kernel* $q_\alpha(t,x,y)$ *which belongs to* $\mathcal{C}^\infty((0,\infty)\times X \times X)$.

Proof: The operator $\tilde{L}_\alpha$ satisfies the same Hörmander-type condition that L proven in [26], Proposition 4.1.The result follows then from [12] or [23]. ■

Theorem 2.11 *The semigroup* $e^{t\overline{L}_\alpha}$ *is positivity improving for all* $t > 0$.

Proof: The semigroup $e^{t\tilde{L}_\alpha}$ is shown to be irreducible exactly as e^{tL}, see [7, 26] using explicit computation and the Support Theorem of [28]. The statement follows then from the Feynman-Kac formula. ■

As is apparent from the form of $\overline{L}_\alpha$ we will need estimates on the observable r^2 in the sequel. Such estimates were also crucial in [26] for the construction of a Liapunov function.

Theorem 2.12 *Let $0 \leq \alpha < 1/k_2$ and let $t_E = E^{1/k_2 - 1/2}$. There exists a set of paths*

$$S(x,E,t_E) \subset \{ f \in \mathcal{C}([0,t_E],X)\,;\, f(0) = x, G(x) = E \}\,,$$

and constants $E_0 < \infty$ and $A, B, C > 0$ such that for $E > E_0$

$$\mathbf{P}\left\{\tilde{x} \in S(x,E,t_E)\right\} \,\geq\, 1 - Ae^{-BE^{2\alpha+1/2-1/k_2}}\,,$$

and

$$\int_0^{t_E} \tilde{r}^2(s)\,ds \,\geq\, CE^{3/k_2-1/2}\,, \qquad \text{if} \qquad \tilde{x} \in S(x,E,t_E)\,. \tag{25}$$

Proof: The proof is exactly as in [26]. One first sets $T_1 = T_n = 0$ in the equations of motion and then, by a scaling argument, Theorem 3.3 of [26], one shows that the deterministic trajectory satisfies the estimate (25). Then one shows, see Proposition 3.7 and Corollary 3.8 of [26], that the overwhelming majority of the random trajectories follows very closely the deterministic ones. We refer the reader to [26] for further details. ■

Remark 2.13 For large energy E, paths satisfying the bound (25) have a very high probability. From Eq. (25) we obtain that, on a time interval of order 1,

$$\int_0^t \tilde{r}^2(s) \geq CE^{2/k_2}\,,$$

for an overwhelming majority of the paths.

Theorem 2.14 *Let $t > 0$ be fixed and suppose that α and θ satisfy the condition Eq.(23). There exist a constant E_0 and functions $\kappa(E)$ and $b(E)$ such that for $E > E_0$*

$$e^{t\overline{L}_\alpha} e^{\theta G}(x) \,\leq\, \kappa(E) e^{\theta G(x)} + b(E)\mathbf{1}_{\{G \leq E\}}(x)\,. \tag{26}$$

Moreover there exist constants c_1 and c_2 such that

$$\kappa(E) \leq c_1 e^{-c_2 E^{2/k_2}}\,.$$

Proof: By Proposition 2.9 the function $e^{t\overline{L}_\alpha} e^{\theta G}(x)$ is bounded on any compact set. Therefore to show (26) it suffices to show that

$$\sup_{\{x\,:\,G(x)>E\}} \mathbf{E}_x \left[e^{-\int_0^t \left(\alpha(1-\alpha)\gamma\tilde{r}T^{-1}\tilde{r} - \alpha\mathrm{Tr}(\gamma I)\right)ds} e^{\theta(G(\tilde{x}(t)) - G(\tilde{x}))} \right] \,\leq\, \kappa(E)\,.$$

Using Ito's formula we have

$$G(\tilde{x}(t)) - G(x) \,=\, \int_0^t \gamma(\mathrm{Tr}(T) - \tilde{r}^2)\,ds + \int_0^t \sqrt{2\gamma T}\tilde{r}\,d\omega(s)\,,$$

and thus we obtain

$$
\begin{aligned}
&\mathbf{E}_x \left[e^{-\int_0^t \left(\alpha(1-\alpha)\gamma\tilde{r}T^{-1}\tilde{r}-\alpha \mathrm{Tr}(\gamma I)\right)\,ds} e^{\theta(G(x(t))-G(x))} \right] \\
&= e^{t\gamma \mathrm{Tr}(\theta T+\alpha I)} \mathbf{E}_x \left[e^{-\int_0^t \tilde{r}\left(\alpha(1-\alpha)\gamma T^{-1}-\gamma\theta(1-2\alpha)\right)\tilde{r}\,ds} \times \right. \\
&\qquad\qquad\qquad\qquad \left. \times e^{\int_0^t \theta\sqrt{2\gamma T}\tilde{r}\,d\omega} \right] . \qquad (27)
\end{aligned}
$$

Using the Hölder's inequality we find that the expectation on the r.h.s of Eq. (27) can be estimated by

$$
\begin{aligned}
&\mathbf{E}_x \left[e^{-q\int_0^t \tilde{r}\left(\alpha(1-\alpha)\gamma T^{-1}-\gamma\theta(1-2\alpha)\right)\tilde{r}\,ds} e^{\frac{qp\theta^2}{2}\int_0^t (\sqrt{2\gamma T}\tilde{r})^2\,ds} \right]^{1/q} \\
&\quad \times \mathbf{E}_x \left[e^{-\frac{p^2\theta^2}{2}\int_0^t (\sqrt{2\gamma T}\tilde{r})^2\,ds} e^{p\int_0^t \theta(2\gamma T)^{1/2}\tilde{r}\,d\omega)} \right]^{1/p} \\
&= \mathbf{E}_x \left[e^{-q\gamma\int_0^t \tilde{r}\left(\alpha(1-\alpha)T^{-1}-\theta(1-2\alpha)+p\theta^2 T\right)\tilde{r}\,ds} \right]^{1/q} . \qquad (28)
\end{aligned}
$$

where we have used that the second factor is the expectation of a martingale with expectation 1.

If θ and α satisfy the condition (23), then, by choosing p sufficiently close to 1, the quadratic form in the right side of Eq. (28) is negative definite. Using Theorem 2.12 as in Theorem 3.11 of [26] we obtain

$$
\begin{aligned}
&\sup_{x\in U^C} \mathbf{E}_x \left[e^{-\int_0^t \left(\alpha(1-\alpha)\tilde{r}T^{-1}\tilde{r}-\alpha \mathrm{Tr}(\gamma I)\right)\,ds} e^{\theta(G(x(t))-G(x))} \right] \\
&\leq e^{\gamma \mathrm{Tr}(\theta T+\alpha I)} e^{-CE^{2/k_2}\gamma \mathrm{Tr}(\alpha(1-\alpha)T^{-1}-(1-2\alpha)\theta+p\theta^2 T)} \\
&\leq c_1 e^{-c_2 E^{2/k_2}} .
\end{aligned}
$$

and this concludes the proof of Theorem 2.14. ■

As in Theorem 2.1 we obtain

Theorem 2.15 *If α and θ satisfy the condition Eq.(23), then $e^{t\overline{L}_\alpha}$ extends to a strongly continuous quasi-bounded semigroup on $\mathcal{H}_{p,\theta}$ for $1 \leq p < \infty$ and on $\mathcal{H}^0_{\infty,\theta}$. Moreover $e^{t\overline{L}_\alpha}$ is compact on $\mathcal{H}_{p,\theta}$, $1 < p \leq \infty$ and on $\mathcal{H}^0_{\infty,\theta}$.*

Proof: The proof is a repetition of the proof of Theorem 2.1 and is left to the reader. ■

As a consequence of Theorem 2.15 and of the theory of semigroup of positive operators [11] we obtain

Theorem 2.16 *If*

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

then

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

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

Proof: By Theorem 2.15, $e^{t\overline{L}_\alpha}$ generates a strongly continuous semigroup on $\mathcal{H}^0_{\infty,\theta}$ if

$$-\alpha < \theta T_i < 1-\alpha \, . \tag{29}$$

If $\alpha \leq 0$, this implies that $|\alpha| < \theta T_{\min} < \theta T_{\max} < 1+|\alpha|$ and so the set of θ we can choose is non-empty provided

$$\alpha > -\frac{T_{\min}}{T_{\max}-T_{\min}} \, .$$

If $0 < \alpha < 1$, we can always find θ such that (29) is satisfied. Finally if $\alpha > 1$ then (29) implies that that

$$\alpha < 1 + \frac{T_{\min}}{T_{\max}-T_{\min}} \, .$$

By the definition of R_i, Eq. (10), $e^{-\alpha R_i} \in \mathcal{H}^0_{\infty,\theta}$ since $-\alpha+\theta T_i < 0$. Using now Lemma 2.7, we see that $\Gamma_x^i(t,\alpha)$ exists and is given by

$$\Gamma_x^i(t,\alpha) \; = \; e^{t(L-\alpha\sigma)} 1(x) \; = \; e^{\alpha R_i} e^{t\overline{L}_\alpha} e^{-\alpha R_i}(x) \, .$$

From Theorem 2.11 the semigroup $e^{t\overline{L}_\alpha}$ is an *irreducible* semigroup of *compact* operators on the Banach space $\mathcal{H}^0_{\infty,\theta}$. From the cyclicity properties of the spectrum of irreducible operators and from the compactness it follows (see [11], Chapter C-III) that there is exactly one eigenvalue $e^{-te(\alpha)}$ with maximal modulus and this eigenvalue is real and simple. The corresponding eigenfunction f_α is strictly positive and we denote as P_α the one-dimensional projection on the eigenspace spanned by f_α. In particular if $g \geq 0$, then $P_\alpha g(x) > 0$.

From compactness it follows that the complementary projection $(1-P_\alpha)$ satisfies the bound

$$\left| e^{t\overline{L}_\alpha}(1-P_\alpha) f(x) \right| \; \leq \; C e^{-td(\alpha)} \|f\|_{\infty,\theta} e^{\theta G(x)} \, . \tag{30}$$

for some constants $C > 0$ and $d(\alpha) > e(\alpha)$ and for all $t > 0$.

From Lemma 2.7 and Eq. (30) we obtain, for all $x \in X$, that

$$\begin{aligned}
&\lim_{t\to\infty} -\frac{1}{t}\log \Gamma_x^i(t,\alpha) \\
&= \lim_{t\to\infty} -\frac{1}{t}\log e^{t(L-\alpha\sigma_i)}1(x) \;=\; \lim_{t\to\infty} -\frac{1}{t}\log e^{\alpha R_i} e^{t\overline{L}_\alpha} e^{-\alpha R_i}(x) \qquad (31)\\
&= \lim_{t\to\infty}\left(-\frac{1}{t}\alpha R_i(x)\right) + e(\alpha) \\
&\quad + \lim_{t\to\infty} -\frac{1}{t}\log\left(P_\alpha e^{-\alpha R_i}(x) + e^{te(\alpha)}e^{t\overline{L}_\alpha}(1-P_\alpha)e^{-\alpha R_i}(x)\right) \\
&= e(\alpha)\,.
\end{aligned}$$

This concludes the proof of Theorem 2.16. ■

Using now the identity (14) we can prove the symmetry of $e(\alpha)$. Theorem 1.1 is then an immediate consequence of the following result.

Theorem 2.17 *If*

$$\alpha \in \left(-\frac{T_{\min}}{T_{\max}-T_{\min}}\,,\,1+\frac{T_{\min}}{T_{\max}-T_{\min}}\right)\,, \qquad (32)$$

then

$$e(\alpha) = e(1-\alpha)\,.$$

Proof: If α is in the interval (32) and $-\alpha < \theta T_i < 1-\alpha$ then $e^{t\overline{L}_\alpha}$ is a strongly continuous compact semigroup on $\mathcal{H}^0_{\infty,\theta}$. By Lemma 2.7

$$e^{t(L-\alpha\sigma_i)} \;=\; e^{\alpha R_i}e^{t\overline{L}_\alpha}e^{-\alpha R_i}$$

is also a strongly continuous compact semigroup on the Banach space $\mathcal{H}^0_{\infty,\theta,\alpha} = \{f\,;\,|f|e^{-\theta G+\alpha R_i} \in C_0(x)\}$ with the norm $\|f\|_{\infty,\theta,\alpha} = \sup|f|e^{\theta G+\alpha R_i}$.

The dual semigroup $(e^{t(L-\alpha\sigma_i)})^*$ is a compact semigroup on the Banach space (of measures) $(\mathcal{H}^0_{\infty,\theta,\alpha})^*$. By Theorem 2.11 $(e^{t(L-\alpha\sigma_i)})^*$ maps $(\mathcal{H}^0_{\infty,\theta,\alpha})^*$ into measures with smooth densities and on densities $(e^{t(L-\alpha\sigma_i)})^*$ acts as

$$(e^{t(L-\alpha\sigma_i)})^*(\rho(x)dx) \;=\; (e^{t(L^T-\alpha\sigma_i)}\rho(x))dx\,.$$

By Lemma 2.5 we have

$$e^{-R_i}e^{t(L-(1-\alpha)\sigma_i)}1(x) \;=\; Je^{t(L^T-\alpha\sigma_i)}Je^{-R}(x)\,. \qquad (33)$$

Since $-\alpha < \theta T_i < 1-\alpha$, e^{-R_i} is a density of a measure in $(\mathcal{H}^0_{\infty,\theta,\alpha})^*$. Since $(e^{t(L-\alpha\sigma_i)})^*$ is compact and irreducible with spectral radius $e(\alpha)$ we obtain using

Eq. (33)

$$\begin{aligned} e(\alpha) &= \lim_{t\to\infty} -\frac{1}{t}\log \|J(e^{t(L^T-\alpha\sigma_i)}Je^{-R_i})dx\| \\ &= \lim_{t\to\infty} -\frac{1}{t}\log\left(\sup_{f\leq e^{\theta G+\alpha R_i}}\int fe^{-R_i}e^{t(L-(1-\alpha)\sigma_i)}1\,dx\right), \\ &= e(1-\alpha)\,. \end{aligned}$$

In the last equality we have used Theorem 2.16 and the fact that fe^{-R_i} is a finite measure. This concludes the proof of Theorem 2.17. ∎

We finally obtain the Gallavotti-Cohen fluctuation theorem

Theorem 2.18 *There is a neighborhood O of the interval $[-\langle\sigma\rangle_\nu\,,\langle\sigma\rangle_\nu]$ such that for $A\subset O$ the fluctuations of σ_i in A satisfy the large deviation principle with a large deviation functional $I(w)$ obeying*

$$I(w)-I(-w) \;=\; -w\,,$$

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

Proof: First we note that $e(\alpha)$ is a real analytic function since it is identified with an eigenvalue of a compact operator. A simple computation gives that

$$\left.\frac{d}{d\alpha}e(\alpha)\right|_{\alpha=0} \;=\; \langle\sigma\rangle_\nu\,.$$

The function $e(\alpha)$ is analytic and convex. By the result of [7] it is not identically zero, and so the symmetry the symmetry $e(\alpha)=e(1-\alpha)$ implies that the set of the values of $\frac{d}{d\alpha}e(\alpha)$ is a neighborhood of $[-\langle\sigma\rangle_\nu\,,\langle\sigma\rangle_\nu]$.

The large deviation principle is a direct application of the Gärtner-Ellis theorem, [4], Theorem 2.3.6. The large deviation functional is given by the Legendre transform of $e(\alpha)$ and so we have

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

∎

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