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Non-equilibrium Thermodynamics of Piecewise Deterministic Markov Processes

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Abstract We consider a class of stochastic dynamical systems, called piecewise deterministic Markov processes, with states $(x, \sigma) \in \Omega \times \Gamma$, Ω being a region in $\mathbb{R}^d$ or the d-dimensional torus, Γ being a finite set. The continuous variable x follows a piecewise deterministic dynamics, the discrete variable σ evolves by a stochastic jump dynamics and the two resulting evolutions are fully-coupled. We study stationarity, reversibility and time-reversal symmetries of the process. Increasing the frequency of the σ-jumps, the system behaves asymptotically as deterministic and we investigate the structure of its fluctuations (i.e. deviations from the asymptotic behavior), recovering in a non Markovian frame results obtained by Bertini et al. (Phys. Rev. Lett. 87(4):040601, 2001; J. Stat. Phys. 107(3–4):635–675, 2002; J. Stat. Mech. P07014, 2007; Preprint available online at http://www.arxiv.org/abs/0807.4457, 2008), in the context of Markovian stochastic interacting particle systems. Finally, we discuss a Gallavotti–Cohen-type symmetry relation with involution map different from time-reversal.

Keywords Piecewise deterministic Markov processes · Large deviations · Stationary states · Non-equilibrium processes

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1 Introduction

Piecewise deterministic Markov processes (PDMPs) are stochastic dynamical systems whose state is described by a pair (x, σ), where x is a continuous variable and σ is a discrete variable. We take $x \in \Omega$ and $\sigma \in \Gamma$, Ω being a region in $\mathbb{R}^d$ or the d-dimensional torus, Γ being a finite set. Motivated by applications to biochemical processes [13], we call x and σ the mechanical and the chemical variable (or state) of the system, respectively. The chemical state σ evolves by a random jump dynamics, while in the time intervals in which the chemical state is kept constant and equal to some σ, the mechanical state x evolves according to the deterministic σ-dependent ODE $\dot{x}(t) = F_\sigma(x(t))$. Since the probability rates of chemical jumps can depend on x, the mechanical state x and the chemical one σ are dynamically fully-coupled. In our analysis, we restrict to time-homogeneous PDMPs, i.e. both the vector fields $F_\sigma(x)$ and the probability rate $\lambda r(\sigma, \sigma'|x)$ for a chemical jump from σ to σ' at the x-mechanical state are time-independent. Above, λ is a positive parameter we will play with in order to analyze some special regime. The above models can be used to describe the overdamped motion of a particle in a viscous fluid under alternating force fields, as well as some biochemical processes like molecular motors and gene regulation (see [13]; for a detailed discussion of molecular motors see [15, 20, 22, 23]).

PDMPs are broadly used in applied sciences and engineering, and are a typical example of what is called a *stochastic hydrid system* in control theory [8]. A mathematical analysis of PDMPs has been started by Davis in [9] and the interested reader can find a detailed mathematical treatment in [10]. Our interest here is mainly theoretical and inspired by the physics of out-of-equilibrium systems. In particular, our investigation concerns the steady state, the time-reversed process, the deviations of the system from its typical behavior at large λ, a special fluctuation–dissipation relation and a Gallavotti–Cohen-type symmetry relation. We discuss our results in more detail.

In general, under mixing assumptions, the steady state (stationary probability measure) is unique and has density $\rho_\lambda(x, \sigma)$ on $\Omega \times \Gamma$ which solves a system of differential equations with zero-flux boundary conditions. We give exact solutions in dimension one, while for any dimension we isolate a class of exactly solvable models for which ρ_λ has the special form

$$\rho_\lambda(x, \sigma) = c(\lambda) e^{-\lambda S(x)} \rho(x, \sigma), \tag{1.1}$$

where $c(\lambda)$ is a normalization factor depending only on λ. Given the stationary measure ρ_λ, we consider the time-reversed (adjoint) version of the PDMP and we show that it is again a PDMP, with inverted vector fields and transition rates λr^+ which depend on the direct rates r and on the stationary measure ρ_λ. In particular, our PDMPs typically describe out-of-equilibrium systems, since reversibility appears only in the trivial case of vanishing force fields. For exactly solvable models as in (1.1) we show that $r^+(\cdot, \cdot|x)$ does not depend on λ and that special symmetry relations hold.

In order to study the deviations of the system from its typical behavior, we introduce a scaling procedure forcing the system to behave deterministically in the asymptotic limit. Simply, we take the limit $\lambda \uparrow \infty$. As result, the timescale of chemical jumps becomes infinitesimal w.r.t. the timescale of the mechanical evolution and the dynamics is a combination of slow and fast motions. As one would expect, an *averaging principle* holds: the slow motion is well approximated by averaging the effect of the fast motion, considering the fast (chemical) variable as locally equilibrated. In order to be more precise, let us assume that for any $x \in \Omega$ the continuous-time Markov chain on Γ with jump rates $r(\cdot, \cdot|x)$ (x being interpreted as frozen variable) is irreducible and therefore has a unique invariant probability measure $\mu(\cdot|x)$ on Γ. Then the above high frequency limit implies that, whenever the

mechanical state of the PDMP is x, the chemical state is given by σ with probability well approximated by $\mu(\sigma|x)$, while with probability tending to 1 the mechanical evolution $x(t)$ is well approximated by the deterministic path $x_*(t)$ solving the Cauchy system

$$\begin{cases} \dot{x}_*(t) = \bar{F}(x_*(t)), \\ x_*(0) = x_0, \end{cases} \tag{1.2}$$

x_0 being the initial mechanical state and $\bar{F}$ being the averaged vector field

$$\bar{F}(x) = \sum_{\sigma \in \Gamma} \mu(\sigma|x) F_\sigma(x).$$

The above averaging principle corresponds to a law of large numbers for the mechanical evolution and, introducing suitable spaces and topologies, it can be extended to the joint evolution $(x(t), \sigma(t))$ (see Sect. 3.4). A rigorous derivation of the averaging principle as well as the large deviations (LD) principle for PDMPs can be found in the companion paper [12].

Considering the chemical variable as hidden and taking the limit $\lambda \uparrow \infty$, we analyze the structure of fluctuations of the mechanical variable, i.e. deviations from its asymptotic deterministic behavior (1.2), following ideas and results of [1, 2, 4, 5] for stochastic interacting particle systems. A key identity observed in [2] is the Fluctuation–Dissipation (FD) relation

$$\mathcal{L}(x, \dot{x}) = \nabla V(x) \cdot \dot{x} + \mathcal{L}^+(x, -\dot{x}), \tag{1.3}$$

where V denotes the static LD functional of the steady state (in exactly solvable models as in (1.1), $V = S$), while $\mathcal{L}$ and $\mathcal{L}^+$ are such that the LD functionals for the mechanical dynamics of the PDMP and its time-reversed version are obtained by integrating along the mechanical trajectories $x(t)$ the functions $\mathcal{L}(x, \dot{x})$ and $\mathcal{L}^+(x, \dot{x})$, respectively. As observed in [1, 2, 4, 5] and recalled in Sect. 10, whenever the FD relation is satisfied, several physical properties concerning the relaxation of the system hold. In [2] the authors derive the above FD relation from the definition of the time-reversed process and from the Markov property of the processes under considerations (the direct one and the time-reversed one). In our case, the mechanical evolution $x(t)$ is typically non Markovian, hence the validity of the FD relation has to be investigated. When the dependence on the parameter λ of the transition rates λr^+ is linear or almost linear, as in the case of 1D system or in the case of exactly solvable model with stationary measure (1.1), we can apply again our LD principle for λ-rescaled PDMPs. Then, we show the validity of the FD relation for the entire class of solvable PDMPs whose stationary measures satisfies (1.1) as well for PDMPs with two chemical states on the one dimensional torus for which the stationary measure is not of the form (1.1).

We briefly discuss a Gallavotti–Cohen-type symmetry relation for PDMPs. The natural symmetry for this class of processes is different from time-reversal and the corresponding action functional has a direct physical interpretation. We obtain in this way examples answering a question raised at the end of Sect. 2.2 in [18]. See also [17] and [19] for other examples and for more details and references on the Gallavotti–Cohen symmetry in the framework of stochastic dynamics.

The paper is organized as follows. In Sect. 2 we give a detailed description of the model and comment our basic assumptions. In Sect. 3 we collect and comment all the results of the paper. Proofs and details are contained in the subsequent sections.

We conclude with a remark. Being stochastic dynamical systems, PDMPs can have very different behaviors and show special features. When possible we have tried to keep our analysis at a general level, thus requiring some mathematical abstraction. On the other hand, special dynamical mechanisms have been discussed directly by means of examples. Moreover, even in very simple examples standard stochastic tools used in the paper as the Markov generator can become very delicate and subtle. The interested reader can find some insights in Appendix and can refer to [10] for a general theory.

2 The Model

We consider stochastic models with state space $\Omega \times \Gamma$, where Γ is a finite set and Ω is either a domain (i.e. open and connected subset) of $\mathbb{R}^d$ with regular boundary $\partial\Omega$, or the closure of a domain of $\mathbb{R}^d$ with regular boundary, or the d-dimensional torus $\mathbb{R}^d/\mathbb{Z}^d$. A generic element of the state space is denoted by (x, σ). Inspired by power-stroke models of molecular motors, we call the variables $x \in \Omega$ and $\sigma \in \Gamma$ the *mechanical state* and the *chemical state* of the system, respectively. Their joint stochastic evolution can be described as follows. The mechanical state x evolves continuously, while the chemical state σ jumps at random times. When the chemical state is σ, the mechanical state evolves according to the ordinary differential equation

$$\dot{x}(t) = F_\sigma(x(t)), \tag{2.1}$$

where, for any $\sigma \in \Gamma$, $F_\sigma(x) \in \mathbb{R}^d$ is a vector field. If Ω is the d-dimensional torus, in the above equation x is thought of as element of a box in $\mathbb{R}^d$ with periodic boundary conditions. We assume that the vector fields F_σ have continuous extension to the closure $\overline{\Omega}$ and satisfy the Lipschitz condition

$$|F_\sigma(x) - F_\sigma(y)| \le K_\sigma |x - y|, \quad \forall x, y \in \Omega, \tag{2.2}$$

for appropriate constants K_σ. Moreover, we assume that the mechanical evolution remains confined inside the region Ω. This assumption together with (2.2) implies existence and uniqueness of the mechanical trajectory.

The chemical state σ performs a jump stochastic dynamics with rates depending on the mechanical state. More precisely, the jump rates are continuous functions $r(\sigma, \sigma'|x) : \Gamma \times \Gamma \times \Omega \to [0, \infty)$. Without loss of generality we assume that

$$r(\sigma, \sigma|x) = 0, \quad \forall (x, \sigma) \in \Omega \times \Gamma.$$

Moreover, we set

$$\gamma(\sigma|x) = \sum_{\sigma' \in \Gamma} r(\sigma, \sigma'|x). \tag{2.3}$$

Given the initial state $(x_0, \sigma_0) \in \Omega \times \Gamma$, we consider the random variable τ_1 with distribution

$$\mathbb{P}(\tau_1 > t) = \begin{cases} e^{-\lambda \int_0^t \gamma(\sigma_0|x_0(s))ds}, & t \ge 0, \\ 1, & t < 0. \end{cases}$$

In the above formula λ is a positive parameter and $x_0(s)$ is the solution of the Cauchy problem

$$\begin{cases} \dot{x}(t) = F_{\sigma_0}(x(t)), \\ x(0) = x_0. \end{cases} \tag{2.4}$$

The evolution of the system (mechanical state and chemical state) in the time interval $[0, \tau_1)$ is given by $(x_0(s), \sigma_0)$. The chemical state $\sigma(\tau_1)$ is then chosen in Γ according to the distribution

$$\mathbb{P}(\sigma(\tau_1) = \sigma) = \frac{r(\sigma_0, \sigma|x(\tau_1))}{\gamma(\sigma_0|x(\tau_1))}.$$

In general, we denote by τ_k the random time of the k-th chemical jump and by $(x_k(s), \sigma(\tau_k))$ the state of the system at time $s \in [\tau_k, \tau_{k+1})$. We have that $x_k(s)$ solves (2.4) for the vector field $F_{\sigma(\tau_k)}$ with initial condition $x_k(\tau_k) := x_{k-1}(\tau_k)$ and that τ_{k+1} is a random variable with distribution

$$\mathbb{P}(\tau_{k+1} > t) = \begin{cases} e^{-\lambda \int_{\tau_k}^t \gamma(\sigma(\tau_k)|x_k(s))ds}, & t \geq \tau_k, \\ 1, & t < \tau_k. \end{cases} \tag{2.5}$$

The chemical state $\sigma(\tau_{k+1})$ is then chosen in Γ according to the distribution

$$\mathbb{P}(\sigma(\tau_{k+1}) = \sigma) = \frac{r(\sigma(\tau_k), \sigma|x(\tau_{k+1}))}{\gamma(\sigma(\tau_k)|x(\tau_{k+1}))}.$$

In order to have a well-defined dynamics for all positive times we require that a.s. the family of jump times τ_k has no accumulation point. This is always true if $\lim_{k\uparrow\infty} \tau_k = +\infty$ a.s.

The natural path space of the process $(x(\cdot), \sigma(\cdot))$ is given by the cartesian product

$$C([0, T], \Omega) \times D([0, T], \Gamma). \tag{2.6}$$

The first component is the space of continuous functions from $[0, T]$ to Ω, while the second component is the Skorokhod space of functions from $[0, T]$ to Γ, which are right continuous and have left limits. We note that, due to relation (2.1), the mechanical trajectory $\{x(t)\}_{t\in[0,T]}$ is a piecewise differentiable function and it holds

$$\dot{x}(s) = F_{\sigma(s)}(x(s)), \tag{2.7}$$

for any $s \in [0, T]$ where $\{\sigma(t)\}_{t\in[0,T]}$ is continuous.

Given a point $(x, \sigma) \in \Omega \times \Gamma$, we denote by $\mathbb{P}^\lambda_{x,\sigma}$ and $\mathbb{E}^\lambda_{x,\sigma}$ the law of the process $(x(\cdot), \sigma(\cdot))$ starting in (x, σ) and the associated expectation, respectively. When the initial condition is a probability measure ν on $\Omega \times \Gamma$ we use the symbols $\mathbb{P}^\lambda_\nu$ and $\mathbb{E}^\lambda_\nu$ respectively.

The above stochastic process $(x(\cdot), \sigma(\cdot))$ is called *Piecewise Deterministic Markov Process* (PDMP) [9, 10]. In control theory, it is a typical example of *stochastic hybrid system* [8]. Although the evolution of the mechanical state as well the evolution of the chemical state are not Markovian, as proven in [9, 10] the joint evolution $(x(\cdot), \sigma(\cdot))$ is a strong Markov process, whose Markov generator is formally

$$Lf(x, \sigma) = F_\sigma(x) \cdot \nabla f(x, \sigma) + \lambda \sum_{\sigma' \in \Gamma} r(\sigma, \sigma'|x) \big(f(x, \sigma') - f(x, \sigma)\big) \tag{2.8}$$

where $f : \Omega \times \Gamma \to \mathbb{R}$. For any fixed $x \in \Omega$, we call the x-dependent Markov generator $L_c[x]$ on Γ given by

$$L_c[x]f(\sigma) = \sum_{\sigma' \in \Gamma} r(\sigma, \sigma'|x)\big(f(\sigma') - f(\sigma)\big) \tag{2.9}$$

as *chemical part* of the generator L. Hence, we can write

$$Lf(x, \sigma) = F_\sigma(x) \cdot \nabla f(x, \sigma) + \lambda L_c[x]f(x, \sigma).$$

Note that $L_c[x]$ is the Markov generator of a continuous-time Markov chain on Γ where jumps from σ to σ' take place with probability rate $r(\sigma, \sigma'|x)$. We will assume that for any fixed $x \in \Omega$, this Markov chain is irreducible and consequently has a unique stationary measure $\mu(\cdot|x)$, that we call *quasistationary measure*. In the particular case of two chemical states, e.g. $\Gamma = \{0, 1\}$, this condition reduces to the positivity of the rates $r(0, 1|x)$ and $r(1, 0|x)$. In this case, the quasistationary measure is also reversible w.r.t. the Markov chain on Γ with generator $L_c[x]$ and is given by

$$\mu(0|x) = \frac{r(1, 0|x)}{r(0, 1|x) + r(1, 0|x)}, \qquad \mu(1|x) = \frac{r(0, 1|x)}{r(0, 1|x) + r(1, 0|x)}. \tag{2.10}$$

2.1 Absence of Accumulation Points in $\{\tau_k\}_k$

As already stated, in order to have a well-defined dynamics for all positive times we require that a.s. the family of random jump times τ_k has no accumulation point. This fact is implied for example by the condition

$$\sup_{\{x \in \Omega\}} \max_{\{\sigma \in \Gamma\}} \gamma(\sigma|x) < \infty. \tag{2.11}$$

Indeed, calling C the l.h.s. of (2.11), due to (2.5) we get that $\mathbb{P}(\tau_{k+1} - \tau_k > t) \geq e^{-C\lambda t}$. This allows to build a coupling between the family of random jump times τ_k and a Poisson point process (PPP) on $(0, \infty)$ with density $C\lambda$ such that all jump times τ_k belong to the PPP. Since a.s. the PPP has no accumulation point, the same property holds for the family of jump times τ_k and this proves our claim.

One can even weaken condition (2.11). Due to the irreducibility assumption for $L_c[x]$, the absence of accumulation points for the family of jump times τ_k is implied by the condition

$$\sup_{\{x \in \Omega\}} \min_{\{\sigma \in \Gamma\}} \gamma(\sigma|x) < +\infty \tag{2.12}$$

and some other additional assumptions. Without trying to give some general criterion, in order to explain the mechanism we have in mind we discuss in Appendix A an example where (2.12) is valid and (2.11) is violated, while the family of jump times τ_k has no accumulation point.

We will mainly be interested in models such that a.s. the family of random jumps times τ_k is infinite. A sufficient condition to obtain this behavior is given by

$$\inf_{\{x \in \Omega\}} \min_{\{\sigma \in \Gamma\}} \gamma(\sigma|x) > 0. \tag{2.13}$$

In fact, with arguments similar to the ones after (2.11), it can be shown that the family of jump times dominates a PPP. We discuss in Appendix B an example of a PDMP that violates (2.13) and has a.s. a finite number of chemical jumps.

2.2 Confinement in Ω

As already stated, we assume that the mechanical trajectory $x(t)$ remains confined inside Ω. If Ω is the d-dimensional torus, this assumption is trivially satisfied. Let us consider the case $\Omega \subset \mathbb{R}^d$. Then, it is necessary that there is zero flux through the boundary. A sufficient condition is given by

$$F_\sigma(x) \cdot n(x) \leq 0, \quad \forall \sigma \in \Gamma,\ x \in \partial\Omega, \tag{2.14}$$

where $\cdot$ denotes the Euclidean scalar product in $\mathbb{R}^d$, while $n(x)$ denotes the outward normal to $\partial\Omega$. If Ω includes its boundary $\partial\Omega$, the above condition is enough to have confinement, otherwise one can require in addition to (2.14) that

$$F_\sigma(x) = 0 \quad \forall x \in \partial\Omega \quad \text{s.t.} \quad F_\sigma(x) \cdot n(x) = 0. \tag{2.15}$$

This condition excludes the presence of orbits tangent to the boundary at some point.

Another condition assuring the confinement of $x(t)$ is the following. We take $\Omega \subset \mathbb{R}^d$ open for simplicity. For any $\sigma \in \Gamma$ and $x_0 \in \partial\Omega$, consider the trajectory $x(t)$ starting in x_0 with reversed vector field $-F_\sigma(x)$, namely $\dot{x}(t) = -F_\sigma(x(t))$. If this trajectory is well defined in some time interval $[0, t_0)$ such that $x(t) \in \Omega$ for all $t \in (0, t_0)$, then one can require that

$$\int_0^{t_0} \gamma(\sigma|x(s))ds = +\infty. \tag{2.16}$$

We claim that the mechanical evolution is kept bounded inside Ω by a stochastic mechanism. In fact, condition (2.16) guarantees that if the mechanical trajectory is pointing towards x_0, with probability one there is a jump to a new chemical state before reaching x_0. Now again, if the mechanical trajectory associated to the new chemical state is pointing towards a point $x_1 \in \partial\Omega$, with probability one there is a jump to a new chemical state before reaching x_1. In order to reach the boundary $\partial\Omega$ in a finite time, the system should perform infinite chemical jumps in that time interval, which is not possible due to our assumptions. In the examples discussed below, the above two criteria for the mechanical confinement inside open Ω's are often dual: if the system is confined due to (2.14) and (2.15), the time-reversed system will be confined due to (2.16).

2.3 Markov Generator

As discussed in [10], if the jump rates $r(\sigma, \sigma'|x)$ are not uniformly bounded, it is a difficult task to characterize exactly the domain $\mathcal{D}(L)$ of the generator L. Moreover, $\mathcal{D}(L)$ could not contain very regular functions. Let us stress this last point by means of a simple example discussed in detail in Appendix A. We take $\Omega = (0, 1)$, $\Gamma = \{0, 1\}$, $F_0(x) = -1$, $F_1(x) = 1$, $r(0, 1|x) = 1/x$, $r(1, 0|x) = 1/(1 - x)$. The associated PDMP satisfies all our assumptions. Indeed, $L_c[x]$ has a unique invariant measure, the number of jumps in a finite interval is finite a.s. due to (2.12) (see Appendix A), while the mechanical confinement in Ω is implied by (2.16). As discussed in Appendix A, the very regular function $f(x, \sigma) = \sigma$ does not belong to the domain $\mathcal{D}(L)$.

We will see that the time-inversion of a mechanically confined PDMP is a PDMP with unbounded jump rates, hence this case cannot be considered as exceptional in our analysis. On the other hand, all the above technical problems concerning the Markov generator can be avoided by working with a weaker notion of generator, the *extended generator*, introduced by Davis. We refer the interested reader to [9, 10], while for the sake of

simplicity we will often keep the discussions involving the Markov generators at a formal level.

3 Main Results

In this section we present and comment our main results. We collect them into several *Propositions*, some of which are real mathematical propositions with a rigorous proof, while others are facts derived by arguments outlined in a more physical style, which anyway can be made rigorous. The results concerning large deviations and fluctuation theory are stated with a sloppy notation, avoiding some mathematical technicalities. Again, with additional work one can fill the gaps. Finally, in order to shorten formulas from now on we write $\{x(t), \sigma(t)\}_{t\in[0,T]}$ for the trajectory of the PDMP in the time interval $[0, T]$, omitting the brackets in $(x(t), \sigma(t))$.

3.1 Stationarity

Our results concerning stationarity are derived by standard methods in the theory of stochastic processes. The details are discussed in Sect. 5.

A probability measure (distribution) ρ_λ on $\Omega \times \Gamma$ is called *invariant*, or *stationary*, if for any time $t \geq 0$ the pair $(x(t), \sigma(t))$ is distributed according to ρ_λ when the process has initial distribution ρ_λ. In this case, the process can be univocally defined for all times $t \in \mathbb{R}$ requiring that its law does not change under time-shifts.

Existence and uniqueness of the stationary distribution of a PDMP can be non trivial and the analysis can be very model-dependent. If Ω is bounded one can deduce the existence of a stationary distribution as follows. Fixed any initial distribution ν, we write ν_s for the law of $(x(s), \sigma(s))$ under $\mathbb{P}^\lambda_\nu$. By compactness arguments (cf. [6]), the family of Cesaro averages $\tilde{\nu}_t := t^{-1}\int_0^t \nu_s ds$ admits a subsequence $\tilde{\nu}_{t_n}$, with $t_n \uparrow \infty$, converging to some probability measure ν_* on $\bar{\Omega} \times \Gamma$. If Ω is closed or if Ω is open and $\nu_*(\partial\Omega) = 0$, then by standard arguments one can show that ν_* is a stationary probability measure for the PDMP. The fact that $\nu_*(\partial\Omega) = 0$ for $\Omega \subset \mathbb{R}^d$ can be verified for example if, when approaching the boundary, the system typically jumps to a chemical state σ with a vector field F_σ of order one pointing inside Ω. We will come back to this mechanism in Appendix A. Other existence criteria are given in [10].

The following differential characterization of ρ_λ holds:

Proposition 3.1 *Suppose that $\rho_\lambda = \sum_\sigma \rho_\lambda(x, \sigma)dx\delta_\sigma$ is an invariant distribution for the PDMP such that $\rho_\lambda(\cdot, \sigma) \in C^1(\Omega)$ for all $\sigma \in \Gamma$. Then*

$$\lambda \sum_{\sigma'\in\Gamma} \big(\rho_\lambda(x, \sigma')r(\sigma', \sigma|x) - \rho_\lambda(x, \sigma)r(\sigma, \sigma'|x)\big) = \nabla \cdot \big(\rho_\lambda(x, \sigma)F_\sigma(x)\big) \tag{3.1}$$

for all $(x, \sigma) \in \Omega^\circ \times \Gamma$, Ω° being the interior part of Ω. Moreover, if Ω is an open subset of $\mathbb{R}^d$ and $\sup_{\sigma,\sigma',x} r(\sigma, \sigma'|x) < \infty$, then

$$\big(\rho_\lambda(x, \sigma)F_\sigma(x) \cdot n(x)\big)\big|_{x\in\partial\Omega} = 0, \quad \forall \sigma \in \Gamma. \tag{3.2}$$

If Ω is the closure of a domain in $\mathbb{R}^d$ the boundary condition can differ from (3.2), depending on the dynamics of the PDMP at the boundary.

3.2 Reversibility

The results of this subsection are direct consequence of the general theory of Markov processes but reveal some interesting and hidden symmetries of PDMPs. The proofs are discussed in Sect. 6.

If the PDMP is stationary we can define its time-reversed version. To this aim, we introduce the *time-reversal operator* $\mathcal{T}$ on $C(\mathbb{R},\Omega)\times D(\mathbb{R},\Gamma)$ setting

$$\mathcal{T}\big[\{x(t),\sigma(t)\}_{t\in\mathbb{R}}\big]:=\{x(-t),\sigma(-t)\}_{t\in\mathbb{R}}. \tag{3.3}$$

Above we understand that the path we take in the r.h.s. of (3.3) is the unique path in $C(\mathbb{R},\Omega)\times D(\mathbb{R},\Gamma)$ given by $(x(-t),\sigma(-t))$ at all continuity points t. If $\mathbb{P}^{\lambda}_{\rho_\lambda}$ is the law of the original process, then $\mathbb{P}^{\lambda,+}_{\rho_\lambda}:=\mathbb{P}^{\lambda}_{\rho_\lambda}\circ\mathcal{T}^{-1}$ is the law of the *time-reversed* (*adjoint*) process. If the two laws coincide, one says that the process with law $\mathbb{P}^{\lambda}_{\rho_\lambda}$ is *reversible* and that ρ_λ is a reversible measure for the process.

Proposition 3.2 *If the process $\mathbb{P}^{\lambda}_{\rho_\lambda}$ is stationary, then $\mathbb{P}^{\lambda,+}_{\rho_\lambda}$ is the law of the PDMP with state space $\Omega\times\Gamma$, initial distribution ρ_λ, force fields*

$$F^{+}_{\sigma}(x):=-F_\sigma(x) \tag{3.4}$$

and jump rates $\lambda r^{+}(\sigma,\sigma'|x)$ where

$$r^{+}(\sigma,\sigma'|x):=r(\sigma',\sigma|x)\frac{\rho_\lambda(x,\sigma')}{\rho_\lambda(x,\sigma)}. \tag{3.5}$$

Since by the above proposition $\mathbb{P}^{\lambda,+}_{\rho_\lambda}$ is a PDMP, by considering the transition probability kernels of $\mathbb{P}^{\lambda,+}_{\rho_\lambda}$ one can easily define the adjoint process with arbitrary initial distribution ν. We will denote $\mathbb{P}^{\lambda,+}_{\nu}$ its law on $C(\mathbb{R}_+,\Omega)\times D(\mathbb{R}_+,\Gamma)$.

We point out that for the definition (3.5) of the reversed rates one has to assume some spatial irreducibility of the system implying the positivity of $\rho_\lambda(x,\sigma)$. Moreover, due to the above result, the generator of the adjoint process can be written as

$$L^{+}f(x,\sigma)=-F_\sigma(x)\cdot\nabla f(x,\sigma)+\lambda\sum_{\sigma'\in\Gamma}r(\sigma',\sigma|x)\frac{\rho_\lambda(x,\sigma')}{\rho_\lambda(x,\sigma)}\big(f(x,\sigma')-f(x,\sigma)\big). \tag{3.6}$$

We can write (3.6) as

$$L^{+}f(x,\sigma)=-F_\sigma(x)\cdot\nabla f(x,\sigma)+\lambda L^{+}_{c}[x]f(x,\sigma). \tag{3.7}$$

We stress that $L^{+}_{c}[x]$ denotes the chemical part of the adjoint generator L^{+}. In general, this is different from the operator $L_c[x]^{+}$, defined as the adjoint in $L^2(\mu(\cdot|x))$ of the chemical part $L_c[x]$ of the generator L:

$$L^{+}_{c}[x]\neq L_c[x]^{+}. \tag{3.8}$$

Note that in general the reversed rates can be λ-dependent, thus implying that the chemical part $L^{+}_{c}[x]$ of the adjoint generator can also be λ-dependent. Due to the irreducibility of $L_c[x]$ and identity (3.5), $L^{+}_{c}[x]$ is irreducible for all $x\in\Omega$. We call $\mu^{+}(\cdot|x)$ the quasistationary measure associated to $L^{+}_{c}[x]$ and we remark that it can be λ dependent. The following result holds:

Proposition 3.3 *If for any fixed $x \in \Omega$ the chemical part $L_c[x]$ of the direct generator L is reversible with respect to the quasistationary measure $\mu(\cdot|x)$, then also the chemical part of the adjoint process $L_c^+[x]$ is reversible with respect to its quasistationary measure $\mu^+(\cdot|x)$ for any $x \in \Omega$ and moreover it holds*

$$\mu^+(\sigma|x) = \frac{\rho_\lambda^2(x,\sigma)}{\mu(\sigma|x)Z_\lambda(x)}, \tag{3.9}$$

where $Z_\lambda(x)$ is the normalization constant.

Finally, a comment about reversibility: due to our results, the direct PDMP can be reversible only if all the vector fields F_σ are identically zero. In this case the mechanical state remains constant and the model reduces to the continuous time Markov chain $\sigma(\cdot)$.

3.3 Exactly Solvable Models

In this subsection we present our first main result concerning a class of models whose invariant distribution can be explicitely computed by a method outiled below. All proofs are postponed to Sect. 8, while examples and applications are discussed in Sect. 9.

In Sect. 7 we discuss some 1D models (Ω interval or 1D torus) with two chemical states, for which it is possible to compute explicitly the invariant distribution. In the general case this can be a very difficult task, but our exact solutions of the 1D models suggest to look for invariant distributions of the form

$$\rho_\lambda(x,\sigma) = c(\lambda)e^{-\lambda S(x)}\rho(x,\sigma), \tag{3.10}$$

where $c(\lambda)$ is a normalization factor depending only on λ, $S(x)$ is a function depending only on x and $\rho(x,\sigma)$ is a measure density on $\Omega \times \Gamma$ non depending on λ.

If the PDMP has invariant distribution of the form (3.10), then due to Proposition 3.2 the rates r^+ of the adjoint process do not depend on λ:

$$r^+(\sigma,\sigma'|x) = r(\sigma',\sigma|x)\frac{\rho(x,\sigma')}{\rho(x,\sigma)}. \tag{3.11}$$

In particular, the chemical part $L_c^+[x]$ of the adjoint generator L^+ as well as its quasistationary measure $\mu^+(\cdot|x)$ do not depend on λ. Moreover, if $L_c[x]$ is reversible with respect to the quasistationary measure $\mu(\cdot|x)$, then (3.9) becomes

$$\mu^+(\sigma|x) = \frac{\rho^2(x,\sigma)}{\mu(\sigma|x)Z(x)}. \tag{3.12}$$

Let us now analyze when (3.10) can be a solution of the stationary equations (3.1):

Proposition 3.4 *The function (3.10) solves (3.1) for any $\lambda > 0$ if and only if for any $\sigma \in \Gamma$ it holds*

$$\begin{cases} \nabla \cdot (\rho(x,\sigma)F_\sigma(x)) = 0, \\ \sum_{\sigma' \in \Gamma}(\rho(x,\sigma)r(\sigma,\sigma'|x) - \rho(x,\sigma')r(\sigma',\sigma|x)) = \nabla S(x) \cdot (\rho(x,\sigma)F_\sigma(x)). \end{cases} \tag{3.13}$$

The first equation in (3.13), one for any fixed $\sigma \in \Gamma$, can be written as

$$\nabla\varphi(x,\sigma)\cdot F_\sigma(x) = -\nabla\cdot F_\sigma(x), \tag{3.14}$$

where we set $\varphi(x,\sigma) = \log\rho(x,\sigma)$ (here and below we suppose that $\rho(x,\sigma) > 0$ for all $(x,\sigma) \in \Omega\times\Gamma$ due to some mixing property of the system). Under the same assumption, the second equation, one for any fixed $\sigma \in \Gamma$, can be written in the equivalent form

$$\gamma(\sigma|x) - \gamma^+(\sigma|x) = \nabla S(x)\cdot F_\sigma(x). \tag{3.15}$$

Equation (3.14) is a non-homogeneous transport equation along the orbits of the vector fields F_σ. The important fact is that, as σ varies, these equations are uncoupled, hence one can easily integrate them, as discussed in Sect. 8.2, and determine $\rho(x,\sigma)$ up to arbitrary initial data.

Once determined $\rho(x,\sigma)$, we need to find a function S satisfying the second group of equations in (3.13). To this aim let us set

$$D(x,\sigma) := \sum_{\sigma'\in\Gamma}\big(\rho(x,\sigma)r(\sigma,\sigma'|x) - \rho(x,\sigma')r(\sigma',\sigma|x)\big). \tag{3.16}$$

Proposition 3.5 *Assume that there exists $\Gamma(x) \subseteq \Gamma$ with the property that the vectors $\{\rho(x,\sigma)F_\sigma(x)\}_{\sigma\in\Gamma(x)}$, are linearly independent and satisfy*

$$\mathrm{Span}\{\rho(x,\sigma)F_\sigma(x)\}_{\sigma\in\Gamma(x)} = \mathrm{Span}\{\rho(x,\sigma)F_\sigma(x)\}_{\sigma\in\Gamma} = \mathbb{R}^d, \tag{3.17}$$

where span denotes the spanned vector space. For any $\sigma^* \notin \Gamma(x)$ denote by $c_\sigma(\sigma^*,x)$ the unique real numbers such that

$$\rho(x,\sigma^*)F_{\sigma^*}(x) = \sum_{\sigma\in\Gamma(x)} c_\sigma(\sigma^*,x)\rho(x,\sigma)F_\sigma(x). \tag{3.18}$$

Moreover, let $\{A_{i,\sigma}(x)\}_{i\in\{1,\dots,d\}}^{\sigma\in\Gamma(x)}$ be the $d\times d$ matrix such that $A_{i,\sigma}(x) = \rho(x,\sigma)F_\sigma(x)\cdot e_i$, where $(e_i, 1\le i\le d)$ denotes the canonical basis of $\mathbb{R}^d$.

Then there exists a function $S:\Omega\to\mathbb{R}$ solving the second group of equations in (3.13) if and only if

$$D(x,\sigma^*) = \sum_{\sigma\in\Gamma(x)} c_\sigma(\sigma^*,x)D(x,\sigma) \quad \forall\sigma^*\notin\Gamma(x) \tag{3.19}$$

and the differential form ω on Ω defined as

$$\omega = \sum_{i=1}^d\Big(\sum_{\sigma\in\Gamma(x)} A^{-1}_{\sigma,i}(x)D(x,\sigma)\Big)dx_i \tag{3.20}$$

is exact. In this case it holds

$$S(x) = \int_{\gamma_{x^*,x}}\omega + S(x^*), \tag{3.21}$$

where x^* is an arbitrary point in Ω and $\gamma_{x^*,x}$ is an arbitrary path in Ω from x^* to x, while $S(x^*)$ can be arbitrarely chosen.

We recall that, when the domain Ω is simply connected, exactness of ω is equivalent to say that

$$\partial_{x_i}\Big(\sum_{\sigma\in\Gamma(x)} A^{-1}_{\sigma,j}(x)D(x,\sigma)\Big) = \partial_{x_j}\Big(\sum_{\sigma\in\Gamma(x)} A^{-1}_{\sigma,i}(x)D(x,\sigma)\Big), \quad \forall i\neq j. \tag{3.22}$$

Above we have outlined a method to construct solutions of (3.1) having the special form (3.10). To ensure that these solutions coincide with the invariant distributions of the PDMP, one has to impose the boundary conditions (3.2) if Ω is a bounded domain in $\mathbb{R}^d$, or periodic boundary conditions in x if Ω is the d-dimensional torus. This has to be done, when possible, using the arbitrariness in the initial data in the above construction. Several examples will be discussed in Sect. 9.

We end with some remarks. The assumption (3.17) together with independence implies that $d = |\Gamma(x)|$. Moreover, since $\rho(x,\sigma) > 0$, (3.17) is equivalent to the condition

$$\mathrm{Span}\{F_\sigma(x)\}_{\sigma\in\Gamma(x)} = \mathrm{Span}\{F_\sigma(x)\}_{\sigma\in\Gamma} = \mathbb{R}^d. \tag{3.23}$$

Since by definition (3.16) the sum $\sum_{\sigma\in\Gamma} D(x,\sigma)$ must be zero and since by (3.13) it holds $D(x,\sigma) = \nabla S(x)\cdot(\rho(x,\sigma)F_\sigma(x))$, it must be

$$\nabla S(x)\cdot\Big(\sum_{\sigma\in\Gamma}\rho(x,\sigma)F_\sigma(x)\Big) = 0. \tag{3.24}$$

In particular, the orbits of the vector field $\sum_{\sigma\in\Gamma}\rho(x,\sigma)F_\sigma(x)$ must lie inside the level curves of S.

3.4 Averaging and Large Deviation Principles in the High Frequency Limit

We concentrate now on the asymptotic behavior of our PDMPs and their time-reversed versions as the parameter λ diverges to infinity. By this limit, the frequency of chemical jumps diverges and the timescale of chemical jumps becomes infinitesimal w.r.t. the relaxation time of the mechanical state. In this subsection we recall some of our results rigorously proved in [12], concerning the high frequency regime. This results will be the starting point for the fluctuation theory presented in the next subsections.

Let us first fix some notation. Writing $\Gamma = \{\sigma_1,\dots,\sigma_{|\Gamma|}\}$, we associate to a chemical trajectory $\{\sigma(t)\}_{t\in[0,T]} \in D([0,T],\Gamma)$ the following time-dependent d-dimensional vector

$$\big\{\sigma(t)\big\}_{t\in[0,T]} \to \big\{\chi(t)\big\}_{t\in[0,T]} = \big\{\big(\chi_{\sigma_1}(t),\dots,\chi_{\sigma_{|\Gamma|}}(t)\big)\big\}_{t\in[0,T]},$$

where

$$\chi_\sigma(t) = \begin{cases} 1, & \text{if } \sigma(t) = \sigma,\\ 0, & \text{if } \sigma(t)\neq\sigma.\end{cases}$$

We denote by $\mathcal{M}([0,T])$ the space of nonnegative finite measures on the interval $[0,T]$, endowed with the weak convergence topology. Then we isolate the subspace $\mathcal{M}_0([0,T]) \subset \mathcal{M}([0,T])$ given by the measures that are absolutely continuous w.r.t. the Lebesgue measure. We can interpret $\{\chi(t)\}_{t\in[0,T]}$ as an element of the cartesian product $\mathcal{M}_0([0,T])^\Gamma$ by identifying $\chi_\sigma(t)$ with the measure $\chi_\sigma(t)dt$. If our PDMP starts in the state (x_0,σ_0),

we can think its evolution $\{x(t), \chi(t)\}_{t\in[0,T]}$ as an element of the following subset $\mathcal{Y}_{x_0}$ of $C([0,T],\Omega)\times\mathcal{M}_0([0,T])^\Gamma$:

$$\mathcal{Y}_{x_0}=\Big\{\{x(t),\chi(t)\}_{t\in[0,T]}\in C([0,T],\Omega)\times\mathcal{M}_0([0,T])^\Gamma:\\ \sum_{\sigma\in\Gamma}\chi_\sigma(t)=1 \text{ a.e., } x(t)=x_0+\int_0^t\sum_{\sigma\in\Gamma}\chi_\sigma(s)F_\sigma(x(s))ds\Big\}. \tag{3.25}$$

In the above formula and hereafter we identify measures in $\mathcal{M}_0([0,T])$ with their corresponding densities. It can be proved (cf. [12]) that $\mathcal{Y}_{x_0}$ is a compact subspace of $C[0,T]\times\mathcal{M}[0,T]^\Gamma$, with the topology defined from the metric

$$d\left(\{x(t),\chi(t)\}_{t\in[0,T]},\{\bar{x}(t),\bar{\chi}(t)\}_{t\in[0,T]}\right)\\ =\sup_{t\in[0,T]}|x(t)-\bar{x}(t)|+\sum_{\sigma\in\Gamma}\sup_{0\le t\le T}\left|\int_0^t\left[\chi_\sigma(s)-\bar{\chi}_\sigma(s)\right]ds\right|. \tag{3.26}$$

The following averaging and dynamic large deviations principles hold:

Proposition 3.6 [12]

(i) *Given $(x,\sigma)\in\Omega\times\Gamma$, define the mean vector field $\bar{F}(x)$ as*

$$\bar{F}(x)=\sum_{\sigma\in\Gamma}\mu(\sigma|x)F_\sigma(x). \tag{3.27}$$

Given the initial state (x_0,σ_0) of the PDMP, call $\{x^*(t),\chi^*(t)\}_{t\in[0,T]}$ the unique element of $\mathcal{Y}_{x_0}$ such that

$$\begin{cases}\dot{x}^*(t)=\bar{F}(x^*(t)),\\ x^*(0)=x_0,\\ \chi^*_\sigma(t)=\mu(\sigma|x^*(t)).\end{cases} \tag{3.28}$$

Then,

$$\lim_{\lambda\to\infty}\mathbb{P}^\lambda_{x_0,\sigma_0}\Big[\{x(t),\chi(t)\}_{t\in[0,T]}\in\mathcal{Y}_{x_0}:\\ d\left(\{x(t),\chi(t)\}_{t\in[0,T]},\{x^*(t),\chi^*(t)\}_{t\in[0,T]}\right)>\delta\Big]=0,\quad\forall\delta>0, \tag{3.29}$$

where the law $\mathbb{P}^\lambda_{x_0,\sigma_0}$ of the PDMP starting at (x_0,σ_0) and having parameter λ is thought of as a probability distribution on $\mathcal{Y}_{x_0}$.

(ii) *Set $W:=\{(\sigma,\sigma')\in\Gamma\times\Gamma:\sigma\neq\sigma'\}$ and, for any $(x,\chi)\in\Omega\times[0,1]^\Gamma$ define*

$$j(x,\chi):=\sup_{z\in(0,\infty)^\Gamma}\sum_{(\sigma,\sigma')\in W}\chi_\sigma r(\sigma,\sigma'|x)\left[1-\frac{z_{\sigma'}}{z_\sigma}\right]. \tag{3.30}$$

Then, for any fixed path $\{\hat{x}(t),\hat{\chi}(t)\}\in\mathcal{Y}_{x_0}$, it holds

$$\mathbb{P}^\lambda_{x_0,\sigma_0}\Big[\{x(t),\chi(t)\}_{t\in[0,T]}\in\mathcal{Y}_{x_0}:\{x(t),\chi(t)\}_{t\in[0,T]}\approx\{\hat{x}(t),\hat{\chi}(t)\}_{t\in[0,T]}\Big]$$

$$\sim e^{-\lambda J_{[0,T]}(\{\hat{x}(t),\hat{\chi}(t)\}_{t\in[0,T]})}, \tag{3.31}$$

where the rate functional $J_{[0,T]} : \mathcal{Y}_{x_0} \to [0,\infty)$ *is given by*

$$J_{[0,T]}\big(\{x(t),\chi(t)\}_{t\in[0,T]}\big) := \int_0^T j\big(x(t),\chi(t)\big)dt. \tag{3.32}$$

In the above formula (3.31) the symbol $\approx$ means closeness in the metric of $\mathcal{Y}_{x_0}$ while the symbol $\sim$ means asymptotic logarithmic equivalence in the limit of diverging λ. A more precise statement can be found in [12].

If, given $x \in \Omega$, the chemical part $L_c[x]$ of the generator is reversible w.r.t. the quasi-stationary measure $\mu(\cdot|x)$, then one can solve the variational problem (3.30) (see [12] for details) getting

$$j(x,\chi) = \sum_\sigma \gamma(\sigma|x)\chi_\sigma - \sum_{(\sigma,\sigma')\in W} \sqrt{\frac{\mu(\sigma|x)}{\mu(\sigma'|x)}}\, r(\sigma,\sigma'|x)\sqrt{\chi_\sigma}\sqrt{\chi_{\sigma'}}. \tag{3.33}$$

In particular if $\Gamma = \{0,1\}$ one gets

$$j(x,\chi) = \Big(\sqrt{\chi_0 r(0,1|x)} - \sqrt{\chi_1 r(1,0|x)}\Big)^2. \tag{3.34}$$

3.5 LDP for the Mechanical State

It is natural to analyze the statistical behavior of the mechanical variables alone, since often the chemical variables remain hidden to direct observations. The following result can be easily obtained from the LD Principle in Proposition 3.6 by means of the contraction principle [11] and we omit the proof:

Proposition 3.7 *Given an element* $\{\hat{x}(t)\}_{t\in[0,T]} \in C([0,T],\Omega)$, *for each initial state* (x_0,σ_0) *it holds*

$$\mathbb{P}^\lambda_{x_0,\sigma_0}\left(\{x(t)\}_{t\in[0,T]} : \{x(t)\}_{t\in[0,T]} \approx \{\hat{x}(t)\}_{t\in[0,T]}\right) \sim e^{-\lambda J^m_{[0,T]}(\{\hat{x}(t)\}_{t\in[0,T]})}, \tag{3.35}$$

where the rate functional $J^m_{[0,T]} : C([0,T],\Omega) \to [0,\infty]$ *is defined as*

$$J^m_{[0,T]}\big(\{x(t)\}_{t\in[0,T]}\big) := \inf_{\{\{\chi(t)\}_{t\in[0,T]} : \{x(t),\chi(t)\}_{t\in[0,T]}\in\mathcal{Y}_{x_0}\}} J_{[0,T]}\left(\{x(t),\chi(t)\}_{t\in[0,T]}\right). \tag{3.36}$$

In particular,

$$J^m_{[0,T]}\left(\{x(t)\}_{t\in[0,T]}\right) = \begin{cases} \int_0^T j_m(x(t),\dot{x}(t))dt, & \text{if } x(\cdot)\in\mathcal{Y}^m_{x_0}, \\ +\infty, & \text{otherwise}, \end{cases} \tag{3.37}$$

where

$$\mathcal{Y}^m_{x_0} := \Big\{\{x(t)\}_{t\in[0,T]} : \exists\{\chi(t)\}_{t\in[0,T]} \text{ s.t. } \{x(t),\chi(t)\}_{t\in[0,T]}\in\mathcal{Y}_{x_0}\Big\},$$

and the density $j_m(x,\dot{x})$ *is given by*

$$j_m(x,\dot{x}) = \inf_{\{\chi:\ \dot{x}=\sum_\sigma \chi_\sigma F_\sigma(x)\}} j(x,\chi). \tag{3.38}$$

In the above formula, χ *varies among vectors in* $[0,1]^\Gamma$ *such that* $\sum_\sigma \chi_\sigma = 1$.

In general an explicit computation of j_m depends on the specific model we are dealing with. In formula (3.38) we are minimizing over all possible convex decompositions of the vector $\dot{x}$ with respect to the collection of vectors $\{F_\sigma(x)\}_{\sigma\in\Gamma}$. A special case is when for any $x \in \Omega$ the collection of vectors $\{F_\sigma(x)\}_{\sigma\in\Gamma}$ are the vertices of a simplex, i.e. the vectors $\{F_{\sigma_j} - F_{\sigma_1} : 2 \le j \le |\Gamma|\}$ are independent (writing $\Gamma = \{\sigma_j : 1 \le j \le |\Gamma|\}$). In this case if the vector $\dot{x}$ belong to $\mathcal{C}(\{F_\sigma(x)\}_{\sigma\in\Gamma})$, where the symbol $\mathcal{C}(\cdot)$ denotes the *convex hull*, then there exists a unique probability measure on Γ, $\chi^F(\dot{x})$, such that $\dot{x} = \sum_\sigma \chi^F_\sigma(\dot{x})F_\sigma(x)$. The $\chi^F(\dot{x})$ are called the *barycentric coordinates* of $\dot{x}$ with respect to the collection of vectors $\{F_\sigma(x)\}_{\sigma\in\Gamma}$. The upper index F indicates the dependence on the vector fields, the dependence on x is understood. When $\dot{x} \notin \mathcal{C}(\{F_\sigma(x)\}_{\sigma\in\Gamma})$ then the infimum in (3.38) is over an empty set and we obtain

$$j_m(x,\dot{x}) = \begin{cases} j(x,\chi^F(\dot{x})), & \text{if } \dot{x} \in \mathcal{C}\left(\{F_\sigma(x)\}_{\sigma\in\Gamma}\right), \\ +\infty, & \text{otherwise.} \end{cases} \tag{3.39}$$

We will compute the rate density $j_m(x,\dot{x})$ in specific examples.

3.6 LDP for the Time-Reversed Process

In this subsection we compute large deviation rate functionals for the time-reversed version of the PDMPs in the class of exactly solvable models introduced in Sect. 3.3. This computation follows from the results mentioned in Sect. 3.4, since for our exactly solvable models the chemical part of the adjoint generator is λ-independent. In this investigation, a key role is played by the symmetries pointed out in Sect. 3.3

Since the adjoint (time-reversed) process of our PDMP is again a PDMP with reversed vector fields, the space on which it is natural to study the adjoint process and its limiting behavior is $\mathcal{Y}^+_{x_0}$ having the same definition of $\mathcal{Y}_{x_0}$ (cf. (3.25)) but with F_σ replaced by $-F_\sigma$. For models having invariant measure of the form (3.10), the rates r^+ of the adjoint process do not depend on λ so that a LDP for the adjoint process can be obtained using again the results of [12]:

Proposition 3.8 *Consider a PDMP having an invariant measure of the form* (3.10)*. Then we have*

$$\begin{aligned} &\mathbb{P}^{\lambda,+}_{x_0,\sigma_0}\left(\left\{x(t),\chi(t)\right\}_{t\in[0,T]} \in \mathcal{Y}^+_{x_0} : \left\{x(t),\chi(t)\right\}_{t\in[0,T]} \approx \left\{\hat{x}(t),\hat{\chi}(t)\right\}_{t\in[0,T]}\right) \\ &\quad \sim e^{-\lambda J^+_{[0,T]}(\{\hat{x}(t),\hat{\chi}(t)\}_{t\in[0,T]})}, \end{aligned} \tag{3.40}$$

where

$$\begin{aligned} J^+_{[0,T]}\left(\left\{x(t),\chi(t)\right\}_{t\in[0,T]}\right) &:= \int_0^T j^+\left(x(t),\chi(t)\right)dt, \\ j^+(x,\chi) &:= \sup_{z\in(0,\infty)^\Gamma} \sum_{(\sigma,\sigma')\in W} \chi_\sigma r^+(\sigma,\sigma'|x)\left[1 - \frac{z_{\sigma'}}{z_\sigma}\right]. \end{aligned} \tag{3.41}$$

In the above formula $\mathbb{P}^{\lambda,+}_{x_0,\sigma_0}$ is the probability measure on $\mathcal{Y}^+_{x_0}$ induced by the adjoint process with parameter λ and initial condition (x_0,σ_0).

Let us assume now, as done for (3.33), that for all $x \in \Omega$ the chemical part $L_c[x]$ of the direct generator is reversible w.r.t. the quasistationary measure $\mu(\cdot|x)$. Then we know that the same property holds for the adjoint process with $\mu(\cdot|x)$ replaced by $\mu^+(\cdot|x)$. In this case, similarly to (3.33) and using relations (3.11) and (3.12), we obtain

$$j^+(x,\chi) = \sum_\sigma \gamma^+(\sigma|x)\chi_\sigma - \sum_{(\sigma,\sigma')\in W} \sqrt{\frac{\mu(\sigma|x)}{\mu(\sigma'|x)}} r(\sigma,\sigma'|x)\sqrt{\chi_\sigma}\sqrt{\chi_{\sigma'}}. \tag{3.42}$$

As the reader can check, the proof of the LDP in [12] remains valid for PDMPs with λ-dependent rates $r(\sigma,\sigma',\lambda|x)$ obtained as perturbation of λ-independent rates, i.e. $r(\sigma,\sigma',\lambda|x) = r(\sigma,\sigma'|x)(1+o(1))$. Hence, the above result (3.40) can be extended to more general processes with invariant measures not of the form (3.10). We will discuss an example in Sect. 11.2.

Similarly to Proposition 3.7 one can consider the LD rate functional $J^{m,+}_{[0,T]} : C([0,T],\Omega) \to [0,\infty]$ for the evolution of the mechanical state in the adjoint process.

Proposition 3.9 *Consider a PDMP having an invariant distribution of the form (3.10). Given an element $\{\hat{x}(t)\}_{t\in[0,T]} \in C([0,T],\Omega)$, for each initial state (x_0,σ_0) it holds*

$$\mathbb{P}^{\lambda,+}_{x_0,\sigma_0}\left(\{x(t)\}_{t\in[0,T]} : \{x(t)\}_{t\in[0,T]} \approx \{\hat{x}(t)\}_{t\in[0,T]}\right) \sim e^{-\lambda J^{m,+}_{[0,T]}(\{\hat{x}(t)\}_{t\in[0,T]})}, \tag{3.43}$$

where the rate functional $J^{m,+}_{[0,T]} : C([0,T],\Omega) \to [0,\infty]$ is defined as

$$J^{m,+}_{[0,T]}\big(\{x(t)\}_{t\in[0,T]}\big) = \inf_{\{\{\chi(t)\}_{t\in[0,T]} : \{x(t),\chi(t)\}_{t\in[0,T]}\in\mathcal{Y}^+_{x_0}\}} J^+_{[0,T]}(\{x(t),\chi(t)\}_{t\in[0,T]}). \tag{3.44}$$

In particular,

$$J^{m,+}_{[0,T]}\left(\{x(t)\}_{t\in[0,T]}\right) = \begin{cases} \int_0^T j^+_m(x(t),\dot{x}(t))dt, & \text{if } x(\cdot)\in\mathcal{Y}^{m,+}_{x_0}, \\ +\infty, & \text{otherwise}, \end{cases} \tag{3.45}$$

where

$$\mathcal{Y}^{m,+}_{x_0} := \left\{\{x(t)\}_{t\in[0,T]} : \exists\{\chi(t)\}_{t\in[0,T]} \text{ s.t. } \{x(t),\chi(t)\}_{t\in[0,T]}\in\mathcal{Y}^+_{x_0}\right\}$$

and the density $j^+_m(x,\dot{x})$ is given by

$$j^+_m(x,\dot{x}) = \inf_{\{\chi:\ \dot{x}=-\sum_\sigma \chi_\sigma F_\sigma(x)\}} j^+(x,\chi). \tag{3.46}$$

In the above formula, χ varies among vectors in $[0,1]^\Gamma$ such that $\sum_\sigma \chi_\sigma = 1$.

If the collection of vectors $\{F_\sigma(x)\}_{\sigma\in\Gamma}$ are the vertices of a simplex for any $x\in\Omega$, then this holds also for the vectors $\{-F_\sigma(x)\}_{\sigma\in\Gamma}$ and consequently we have

$$j^+_m(x,\dot{x}) = \begin{cases} j(x,\chi^{-F}(\dot{x})), & \text{if } \dot{x}\in\mathcal{C}\left(\{-F_\sigma(x)\}_{\sigma\in\Gamma}\right), \\ +\infty, & \text{otherwise.} \end{cases} \tag{3.47}$$

Trivially, $\mathcal{C}(\{-F_\sigma(x)\}_{\sigma\in\Gamma}) = -\mathcal{C}(\{F_\sigma(x)\}_{\sigma\in\Gamma})$ and $\chi^{-F}(\dot{x}) = \chi^F(-\dot{x})$.

3.7 Fluctuation Theory

In this subsection we present our second main result concerning the fluctuations of the mechanical state of our PDMPs, following ideas and results developed in [1, 2, 4, 5] for interacting particle systems and inspired by the Freidlin and Wentzell theory for diffusion processes [14]. As we will show, PDMPs are a natural source of examples where the macroscopic fluctuation theory applies. A key identity in this theory is given by the Fluctuation–Dissipation (FD) relation (1.3). In [2] this relation is a direct consequence of the Markov property, while the mechanical evolution of our PDMPs is not Markov. Hence, the FD relation cannot be taken for granted in our case. On the other hand, as stressed in Sect. 4, its validity automatically implies several interesting consequences without any request of Markovianity.

Proofs and details are given in Sects. 4 and 10. In particular, in Sect. 4 we review the main ideas of the *macroscopic fluctuation theory* of Bertini et al. in the framework of stochastic processes having continuous trajectories in Ω. In Sects. 10.1 and 10.2 we prove respectively Propositions 3.10 and 3.11. In Sect. 10.3 we propose a conjecture concerning the FD relation. Finally, in Sect. 10.4 we discuss as example the FD relation in the case of 1D PDMPs with two chemical states. Other results related to fluctuations in 1D PDMP are presented in the next subsection.

Since $\{x(t)\}_{t\geq 0}$ is not Markov, there is not a natural notion of invariant distribution. This has to be replaced by the projection $\hat{\rho}_\lambda$ on the x component of the invariant distribution of the PDMP:

$$\hat{\rho}_\lambda(x) := \sum_\sigma \rho_\lambda(x,\sigma). \tag{3.48}$$

The following static LDP holds:

Proposition 3.10 *Consider a PDMP having an invariant measure of the form* (3.10). *Then for any fixed* $x_* \in \Omega$ *it holds*

$$\hat{\rho}_\lambda\big(x \in \Omega : x \approx x_*\big) \sim e^{-\lambda V(x_*)}, \tag{3.49}$$

where the rate functional V *is given by*

$$V(x) = S(x) - \inf_{y\in\Omega} S(y). \tag{3.50}$$

The above proposition states that, up to an additive constant, the function S coincides with the rate functional V. As the reader can easily check, this fact together with the following main result implies the FD relation (1.3) with Lagrangians given by j_m and j_m^+:

Proposition 3.11 *Consider a PDMP having an invariant measure of the form* (3.10). *Then for any* $x \in \Omega$ *and* $\dot{x} \in \mathbb{R}^d$, *the following symmetry relation holds*

$$j_m(x,\dot{x}) = \nabla S(x)\cdot\dot{x} + j_m^+(x,-\dot{x}). \tag{3.51}$$

3.8 One Dimensional Models

We present the third group of our main results concerning exactly computations for 1D PDMPs with two chemical states. The proofs of Proposition 3.12 and of the first two points of Proposition 3.13 are given in Sect. 7, while the third point of Proposition 3.13 is proved in Sect. 11.2.

We first consider the case $\Omega = (a, b)$ and $\Gamma = \{0, 1\}$. For simplicity we restrict to non vanishing vector fields (the general case leads to a much richer discussion, cf. [21]). Trivially, if the vector fields have the same sign, then a mechanical drift is present and no stationarity can exist. The case of opposing vector fields and Ω-confinement due to (2.14) is treated in the next proposition:

Proposition 3.12 *Take $\Omega = (a, b) \subset \mathbb{R}$ and $\Gamma = \{0, 1\}$. Consider vector fields F_0, F_1 such that* (i) *$F_0(x) < 0$ and $F_1(x) > 0$ for all $x \in (a, b)$*, (ii) *$F_0(a) = F_1(b) = 0$, and assume that the jump rates $r(0, 1|x)$, $r(1, 0|x)$ are positive and bounded from above. Then the PDMP has a unique stationary distribution and this has density*

$$\rho_\lambda(x, i) = \frac{e^{-\lambda \int_{x_*}^{x} (\frac{r(0,1|z)}{F_0(z)} + \frac{r(1,0|z)}{F_1(z)}) dz}}{Z|F_i(x)|}, \quad i = 0, 1, \tag{3.52}$$

where x_* is a generic element of (a, b), when the normalization constant Z exists.

If the jump rates vary in the interval (c_1, c_2) with $c_1, c_2 > 0$, while $F_1(x)$ and $F_0(x)$ are of order one near a and b respectively, then Z is well defined.

Note that for the 1D example in Appendix B the normalization of (3.52) is not possible and the invariant probability measures are not absolutely continuous.

We point out the above stationary distribution has the form (3.10). Moreover, due to (3.5) the λ-independent jump rates of the time-reversed process are

$$\begin{cases} r^+(0, 1|x) = r(1, 0|x) \frac{|F_0(x)|}{|F_1(x)|}, \\ r^+(1, 0|x) = r(0, 1|x) \frac{|F_1(x)|}{|F_0(x)|}. \end{cases}$$

Due to the above formula, if $F_0(b) < 0$ and $F_1(a) > 0$, then the Ω-confinement of the time-reversed process is related to (2.16), while in the direct process the Ω-confinement is related by (2.14).

We consider now the toroidal case $\Omega = \mathbb{R}/\mathbb{Z}$. In the formulas below we will think of the jump rates and of the vector fields also as periodic functions on $\mathbb{R}$, with period 1.

Proposition 3.13 *Let Ω be the 1D torus $\mathbb{R}/\mathbb{Z}$ and let $\Gamma = \{0, 1\}$. Consider non vanishing vector fields F_0, F_1 on Ω and assume that $r(0, 1|x), r(1, 0|x) > 0$ for all $x \in \Omega$. Define $S : \mathbb{R} \to \mathbb{R}$ as*

$$S(x) := \int_0^x \left(\frac{r(0, 1|z)}{F_0(z)} + \frac{r(1, 0|z)}{F_1(z)} \right) dz, \quad x \in \mathbb{R}. \tag{3.53}$$

Then the following holds:

(i) *The PDMP has a unique invariant distribution, and this has density*

$$\begin{cases} \rho_\lambda(x, 0) := \frac{k}{F_0(x)} \int_x^{x+1} [\frac{r(1,0|y)}{F_1(y)} e^{\lambda(S(y)-S(x))}] dy, \\ \rho_\lambda(x, 1) := \frac{k}{F_1(x)} \int_x^{x+1} [\frac{r(0,1|y)}{F_0(y)} e^{\lambda(S(y)-S(x))}] dy, \end{cases} \tag{3.54}$$

where k is the normalizing constant, always well defined.

(ii) *if the function S is periodic with period 1, or equivalently if the equilibrium condition*

$$\int_0^1 \left(\frac{r(0, 1|z)}{F_0(z)} + \frac{r(1, 0|z)}{F_1(z)} \right) dz = 0 \tag{3.55}$$

is satisfied, then setting $C(\lambda) = \int_0^1 \frac{r(1,0|y)}{F_1(y)} e^{\lambda S(y)} dy$ (3.54) *read*

$$\begin{cases} \rho_\lambda(x,0) = \frac{kC(\lambda)}{F_0(x)} e^{-\lambda S(x)}, \\ \rho_\lambda(x,1) = \frac{-kC(\lambda)}{F_1(x)} e^{-\lambda S(x)}, \end{cases} \tag{3.56}$$

and in particular the invariant distribution is of the form (3.10).

(iii) *For any fixed* $x_* \in \Omega$ *it holds*

$$\hat{\rho}_\lambda\big(x \in \Omega : x \approx x_*\big) \sim e^{-\lambda W(x_*)}, \tag{3.57}$$

where the rate functional W *is given by*

$$W(x) = \inf_{y \in [x, x+1]} \big(S(x) - S(y)\big) - \inf_{x \in [0,1]} \inf_{y \in [x, x+1]} \big(S(x) - S(y)\big). \tag{3.58}$$

Moreover for any point $x \in \Omega$ *where* W *is differentiable it holds the FD relation*

$$j_m(x, \dot{x}) = \nabla W(x) \cdot \dot{x} + j_m^+(x, -\dot{x}). \tag{3.59}$$

We point out that condition (3.55) can hold only if the vector fields F_0 and F_1 have opposite sign. We will show that, independently from the periodicity of S, the function W is always periodic in such a way that it can be interpreted as a function on the torus Ω. When S is periodic then $W = S$ up to an additive constant. Finally we remark that in general W has flat parts. In fact it is possible to show that the geometric construction by which W is obtained coincides with the Freidlin and Wentzell construction for a one dimensional diffusion on the one dimensional torus. This is discussed at pp. 191–192 in [14]. Formula (3.58) gives a compact and simple representation for this construction.

3.9 A Gallavotti–Cohen-Type Symmetry

In this subsection we exhibit in the framework of PDMPs a Gallavotti–Cohen (G-C) symmetry with involution different from time reversal. Other examples of this type have been discussed for example in [17] and [19]. Details are postponed to Sect. 12.

Let us briefly recall a result of [18]. Consider an involution $\mathcal{R}$ on the path space of a stochastic process, i.e. a map from the path space into itself such that $\mathcal{R}^2 = \mathbb{1}$. Assume also that the measure $\mathbb{P}_{st} \circ \mathcal{R}^{-1}$ is absolutely continuous w.r.t. $\mathbb{P}_{st}$, where $\mathbb{P}_{st}$ denotes the stationary law of the process. Then the random variable

$$W_T := -\frac{1}{2T} \log \frac{d(\mathbb{P}_{st} \circ \mathcal{R}^{-1})}{d\mathbb{P}_{st}}\bigg|_{t \in [-T,T]} \tag{3.60}$$

satisfies the G-C-type symmetry

$$\mathbb{E}_{st}\big(e^{-sW_T}\big) = \mathbb{E}_{st}\big(e^{-(1-s)W_T}\big), \tag{3.61}$$

where $\mathbb{E}_{st}$ denotes the expectation w.r.t. $\mathbb{P}_{st}$ and s is a real parameter.

Differently from the examples discussed in [18], for PDMPs it is natural to consider involutions $\mathcal{R}$ different from time reversal. Indeed, given a trajectory $\{x(t), \sigma(t)\}_{t \in [-T,T]}$ of the PDMP, solving in particular $\dot{x}(t) = F_{\sigma(t)}(x(t))$, then the time reversed trajectory is typically not a trajectory of the PDMP if the vector fields F_σ are not identically zero. In the case of PDMPs one needs to find an involution $\mathcal{R}$ on the path space preserving the relation $\dot{x}(t) = F_{\sigma(t)}(x(t))$. This is easily done for a suitable class of models:

Lemma 3.14 *Consider a PDMP such that for any $\sigma \in \Gamma$ and any $x \in \Omega$ there exists a unique $\sigma' \in \Gamma$ such that $F_{\sigma'}(x) = -F_\sigma(x)$. Call R_x the involution on Γ that associates to every σ the corresponding σ' characterized as above. Then the map $\mathcal{R}$ defined as*

$$\mathcal{R}\big[\{x(t), \sigma(t)\}_{t\in[-T,T]}\big] := \{x(-t), R_{x(-t)}\sigma(-t)\}_{t\in[-T,T]} \tag{3.62}$$

is an involution on the path space preserving the relation $\dot{x}(t) = F_{\sigma(t)}(x(t))$.

The proof of the above lemma is omitted since very simple. An example of such a PDMP is given by $\Omega = \mathbb{R}^2/\mathbb{Z}^2$, $\Gamma = \{1, 2, 3, 4\}$ and vector fields $F_i = e_i$, where e_1 and e_2 constitute the canonical basis of $\mathbb{R}^2$ and $e_3 = -e_1$, $e_4 = -e_2$. Then $\mathcal{R}_x 1 = 3$, $\mathcal{R}_x 2 = 4$, $\mathcal{R}_x 3 = 1$ and $\mathcal{R}_x 4 = 2$.

If we consider models satisfying additional assumptions we obtain an explicit form of the functional (3.60) having a direct physical interpretation:

Proposition 3.15 *In the same setting of Lemma 3.14, assume that the jump rates satisfy the generalized detailed balance condition*

$$r(\sigma, \sigma'|x) = \exp\{H(\sigma, x) - H(\sigma', x)\} r(R_x\sigma', R_x\sigma|x), \tag{3.63}$$

for a suitable bounded energy function $H : \Gamma \times \Omega \to \mathbb{R}$, and that the function $\gamma(\cdot|\cdot)$ satisfies

$$\gamma(\sigma|x) = \gamma(R_x\sigma|x), \quad \forall (x, \sigma) \in \Omega \times \Gamma. \tag{3.64}$$

Then, as $T \to \infty$,

$$\begin{aligned} W_T &= \frac{1}{2T}\int_{-T}^{T} \nabla H(\sigma(s), x(s)) \cdot \dot{x}(s) ds + o(1) \\ &= \frac{1}{2T}\int_{-T}^{T} \nabla H(\sigma(s), x(s)) \cdot F_{\sigma(s)}(x(s)) ds + o(1), \end{aligned} \tag{3.65}$$

which is the averaged mechanical work done on the system by the external force fields ∇H apart negligible errors as $T \uparrow \infty$.

We note that conditions (3.63) and (3.64) are satisfied if the rates are defined as

$$r(\sigma, \sigma'|x) := \exp\big\{[H(\sigma, x) - H(\sigma', x)]/2\big\}, \tag{3.66}$$

for an energy function H satisfying the symmetry condition

$$H(\sigma, x) = H(R_x\sigma, x), \quad \forall (x, \sigma) \in \Omega \times \Gamma. \tag{3.67}$$

4 Fluctuation Theory for Stochastic Processes on Ω

We reformulate the results of [1, 2, 4, 5] in the simpler context of processes with trajectories in $C([0, T], \Omega)$ and discuss consequences of the FD relation (1.3).

We consider a λ-parameterized family of Markov stochastic processes with trajectories in $C([0, T], \Omega)$, satisfying a sample path LD principle as the parameter λ diverges to $+\infty$. This means that, fixed $\{\hat{x}(t)\}_{t\in[0,T]} \in C([0, T], \Omega)$, it holds

$$\mathbb{P}^{\lambda}_{x_0}\Big(\{x(t)\}_{t\in[0,T]} : \{x(t)\}_{t\in[0,T]} \approx \big\{\hat{x}(t)\big\}_{t\in[0,T]}\Big) \sim e^{-\lambda I^{x_0}_{[0,T]}(\{\hat{x}(t)\}_{t\in[0,T]})}, \tag{4.1}$$

where $\mathbb{P}^{\lambda}_{x_0}$ denotes the law on $C([0,T],\Omega)$ induced by the λ-parameterized process with initial configuration $x_0 \in \Omega$. As a prototype one can take diffusions on $\Omega = \mathbb{R}^d$ with noise of order $\sqrt{1/\lambda}$ as in the Freidlin and Wentzell theory [14].

We further assume that for any fixed λ the λ-parameterized process admits a unique invariant distribution ρ_λ. Then the adjoint process can be defined and has ρ_λ as unique invariant distribution. We assume that also the λ-parameterized family of adjoint processes satisfies a LD principle as λ diverges, i.e. (4.1) remains valid with $\mathbb{P}^{\lambda}_{x_0}$ and $I^{x_0}_{[0,T]}$ replaced by $\mathbb{P}^{\lambda,+}_{x_0}$ and $I^{x_0,+}_{[0,T]}$, respectively. In addition, we assume that there exist densities $\mathcal{L}(x,\dot{x}), \mathcal{L}^+(x,\dot{x}) : \Omega \times \mathbb{R}^d \to [0,\infty)$ such that for any initial configuration x_0 the rate functionals $I^{x_0}_{[0,T]}$ and $I^{x_0,+}_{[0,T]}$ admit an integral representation of the form

$$I^{x_0}_{[0,T]}\left(\{x(t)\}_{t\in[0,T]}\right) = \begin{cases} \int_0^T \mathcal{L}(x(t),\dot{x}(t))dt, & \text{if } x(\cdot) \in \mathcal{X}_{x_0}, \\ +\infty, & \text{otherwise}, \end{cases} \tag{4.2}$$

$$I^{x_0,+}_{[0,T]}\left(\{x(t)\}_{t\in[0,T]}\right) = \begin{cases} \int_0^T \mathcal{L}^+(x(t),\dot{x}(t))dt, & \text{if } x(\cdot) = \mathcal{X}^+_{x_0}, \\ +\infty, & \text{otherwise}, \end{cases} \tag{4.3}$$

for suitable subspaces $\mathcal{X}_{x_0}, \mathcal{X}^+_{x_0} \subset C([0,T],\Omega)$. This assumption implies in particular that all paths in $\mathcal{X}_{x_0}$ and $\mathcal{X}^+_{x_0}$ starts in x_0.

The functions $\mathcal{L}$ and $\mathcal{L}^+$ are called Lagrangians. Typically, $\mathcal{L}(x,\dot{x}) = 0$ if and only if $\dot{x} = \bar{F}(x)$ for a suitable vector field $\bar{F}(x)$ that identifies the law of large numbers of the model in the limit of diverging λ. In fact, in this case we derive from (4.1) that

$$\lim_{\lambda\to+\infty} \mathbb{P}^{\lambda}_{x_0}\Big(\sup_{t\in[0,T]} |x(t) - \bar{x}(t)| > \delta\Big) = 0, \quad \forall \delta > 0, \tag{4.4}$$

where $\{\bar{x}(t)\}_{t\in[0,T]} \in C([0,T],\Omega)$ solves the Cauchy problem

$$\begin{cases} \dot{\bar{x}}(t) = \bar{F}(\bar{x}(t)), \\ \bar{x}(0) = x_0. \end{cases} \tag{4.5}$$

Similarly we require that $\mathcal{L}^+$ vanishes along a path $\{x(t)\}_{t\in[0,T]}$ if and only if $\dot{x}(t) = \bar{F}^+(x(t))$, where the vector field $\bar{F}^+$ identifies the law of large numbers of the adjoint process in the limit of diverging λ.

Finally we assume that the family of invariant distributions ρ_λ satisfy a LD principle on Ω as λ diverges, with rate function $V(x)$. This means that for any fixed t and for any fixed $x \in \Omega$ it holds

$$\mathbb{P}^{\lambda}_{\rho_\lambda}\left(x(t) \approx x\right) \sim e^{-\lambda V(x)}, \tag{4.6}$$

where $\mathbb{P}^{\lambda}_{\rho_\lambda}$ denotes the law of the stationary process with parameter λ and initial distribution ρ_λ. Below we will denote by $\mathbb{P}^{\lambda,+}_{\rho_\lambda}$ the law of its adjoint process.

Let us now derive some consequences from our assumptions. By definition we have for any fixed path $\hat{x}(\cdot) \in C([-T,T],\Omega)$ that

$$\mathbb{P}^{\lambda}_{\rho_\lambda}\left(\{x(t)\}_{t\in[-T,T]} \approx \left\{\hat{x}(t)\right\}_{t\in[-T,T]}\right) = \mathbb{P}^{\lambda,+}_{\rho_\lambda}\left(\{x(t)\}_{t\in[-T,T]} \approx \left\{\hat{x}(-t)\right\}_{t\in[-T,T]}\right). \tag{4.7}$$

Due to the fact that the processes are Markov and that the path $\{x(t-T)\}_{t\in[0,2T]}$ belongs to the path space $\mathcal{X}_{x(-T)}$ (referred to the time interval $[0,2T]$), while the path $\{x(T-t)\}_{t\in[0,2T]}$

belongs to the path space $\mathcal{X}_{x(T)}$ (referred to the time interval $[0, 2T]$), (4.7) implies the following relation concerning the LD rate functionals:

$$V(\hat{x}(-T)) + \int_{-T}^{T} \mathcal{L}(\hat{x}(t), \dot{\hat{x}}(t))dt = V(\hat{x}(T)) + \int_{-T}^{T} \mathcal{L}^+(\hat{x}(-t), -\dot{\hat{x}}(-t))dt. \tag{4.8}$$

Dividing both sides of (4.8) by $2T$ and taking the limit $T \downarrow 0$ we obtain FD relation

$$\mathcal{L}(x, \dot{x}) = \nabla V(x) \cdot \dot{x} + \mathcal{L}^+(x, -\dot{x}), \tag{4.9}$$

valid for any $x, \dot{x}$ corresponding to the values $\hat{x}(0), \dot{\hat{x}}(0)$ for some path $\hat{x}(\cdot)$ as above.

From now on we suppose that the FD relation (4.9) holds, without assuming that the processes under consideration are Markov. Following [2] we derive some consequences of (4.9).

A point $x_* \in \Omega$ is called *equilibrium point* for the λ-parameterized family of processes if $\bar{F}(x_*) = 0$. Then, by the LLN (4.4), the trajectory $\bar{x}(t) \equiv x_*$ is the limiting path for the process starting in x_*, thus implying that $I^{x_*}_{[0,T]}(\bar{x}(\cdot)) = 0$, i.e. $\mathcal{L}(x_*, 0) = 0$. By means of the FD relation we obtain that $\mathcal{L}^+(x_*, 0) = 0$ and consequently x_* is an equilibrium point also for the family of adjoint processes, i.e. we have $\bar{F}^+(x_*) = 0$. We restrict now to the case that the vector field $\bar{F}$ has a unique equilibrium point x_*, which is a global attractor. This means that

$$\lim_{t \to +\infty} x(t) = x_*$$

for any $t\{x(t)\}_{t \in [0,+\infty)}$ solving $\dot{x} = \bar{F}(x)$. Note that, due to the previous argument, x_* is also the unique equilibrium point of the vector field $\bar{F}^+$. We assume that it is also a global attractor for $\bar{F}^+$. As simple example satisfying all the above assumptions, consider the family of reversible diffusions on $\Omega = \mathbb{R}^d$ descried by the SDE

$$\dot{x} = -\nabla U(x) + \lambda^{-\frac{1}{2}} \dot{w},$$

where U is a single well potential and w is a standard Brownian motion. In this case

$$\mathcal{L}(x, \dot{x}) = \mathcal{L}^+(x, \dot{x}) = \frac{1}{2} |\dot{x} + \nabla U(x)|^2,$$

and $V(x) = 2U(x)$.

Let us introduce the *quasi-potential* $Q(x)$ as function on Ω defined by

$$Q(x) = \inf_{\mathcal{A}_x} \int_{-\infty}^{0} \mathcal{L}(x(t), \dot{x}(t))dt, \tag{4.10}$$

where

$$\mathcal{A}_x = \Big\{ \{x(t)\}_{t \in (-\infty, 0]} \,:\, x(0) = x,\ \lim_{t \to -\infty} x(t) = x_* \Big\}.$$

In the case of multiple equilibrium points and different basins of attraction the definition has to be suitably modified. We will not consider this situation here, referring to [14] the interested reader.

Remark 1 We point out that the rigorous definition of quasi-potential is slightly different from (4.10). Indeed, since the dynamic LD principles with rate functionals (4.2), (4.3) hold for finite time intervals, one has to define the quasi-potential as

$$Q(x) = \inf_{T\geq 0} \inf_{\mathcal{A}_x^T} \int_{-T}^{0} \mathcal{L}(x(t), \dot{x}(t))dt, \tag{4.11}$$

where

$$\mathcal{A}_x^T = \left\{ \{x(t)\}_{t\in[-T,0]} \,:\, x(0) = x \,,\; x(-T) = x_* \right\}.$$

We use definition (4.10) to simplify our discussion, while the interested reader can adapt our arguments in order to obtain rigorous proofs (see for example [3]).

We now derive an *H-Theorem* for the quasi-potential. More precisely, we show that the quasi-potential is a decreasing Lyapunov functional for both the vector field $\bar{F}$ and for the vector field $\bar{F}^+$. This means that $t \to Q(x(t))$ is a decreasing function if $\dot{x}(t) = \bar{F}(x(t))$ or if $\dot{x}(t) = \bar{F}^+(x(t))$, respectively. In order to justify our claim, we take a path $\{x(t)\}_{t\geq 0}$ such that $\dot{x}(t) = \bar{F}(x(t))$. Let $x = x(0)$ and $x' = x(t')$, with $t' > 0$. Given $\varepsilon > 0$ we fix an element $\{\tilde{x}(t)\}_{t\in[-\infty,0]} \in \mathcal{A}_x$ such that $Q(x)$ differs from $I_{(-\infty,0]}(\tilde{x}(\cdot))$ at most ε. Then we construct the following element of $\mathcal{A}_{x'}$

$$\bar{x}(t) = \begin{cases} \tilde{x}(t+t'), & \text{if } \; t \leq -t', \\ x(t+t'), & \text{if } t \in (-t', 0]. \end{cases}$$

Since $\mathcal{L}(x(t), \dot{x}(t)) = 0$ for all $t \geq 0$, we have

$$\begin{aligned} Q(x') &\leq \int_{-\infty}^{0} \mathcal{L}(\bar{x}(t), \dot{\bar{x}}(t))dt \\ &= \int_{-\infty}^{-t'} \mathcal{L}(\tilde{x}(t+t'), \dot{\tilde{x}}(t+t'))dt + \int_{-t'}^{0} \mathcal{L}(x(t+t'), \dot{x}(t+t'))dt \\ &= \int_{-\infty}^{0} \mathcal{L}(\tilde{x}(t), \dot{\tilde{x}}(t))dt \leq Q(x) + \varepsilon. \end{aligned}$$

By the arbitrariness of ε, we deduce that $Q(x') \leq Q(x)$. Therefore, it must be $\nabla Q(x) \cdot \bar{F}(x) \leq 0$ for all $x \in \Omega$. The same kind of argument can be used for the vector fields $\bar{F}^+$, thus implying that $\nabla Q(x) \cdot \bar{F}^+(x) \leq 0$.

Let us now show that the quasi-potential $Q(x)$ coincides with the LD rate functional $V(x)$ of the invariant measures ρ_λ:

$$Q(x) = V(x) \quad \forall x \in \Omega.$$

Since $\mathcal{L}^+$ is nonnegative, using the FD relation we get for any $\{x(t)\}_{t\in[-\infty,0]} \in \mathcal{A}_x$ that

$$\int_{-\infty}^{0} \mathcal{L}(x(t), \dot{x}(t))dt \geq \int_{-\infty}^{0} \nabla V(x(t)) \cdot \dot{x}(t)dt = V(x) - V(x_*) = V(x). \tag{4.12}$$

The last equality follows from the fact that the rate functional V is zero on the unique equilibrium point x_*. Indeed, the function V is nonnegative due to the fact that it is a rate

functional, moreover it must be zero only at x_* in agreement with the law of large numbers. Due to the definition of the quasi-potential Q, the above bound (4.12) implies that $Q(x) \geq V(x)$. In order to prove the reversed inequality, let $\{x^+(t)\}_{t\in[0,\infty)}$ be the solution of the Chauchy problem

$$\begin{cases} \dot{x}^+(t) = \bar{F}^+(x^+(t)), \\ x^+(0) = x. \end{cases} \tag{4.13}$$

Due to the global attractiveness of x_* we have

$$\lim_{t\to+\infty} x^+(t) = x_*,$$

so that $\mathcal{T}[\{x^+(t)\}_{t\in[0,\infty)}] = \{x^+(-t)\}_{t\in(-\infty,0]} \in \mathcal{A}_x$ and, by definition of $Q(x)$ and due to the FD relation (4.9),

$$Q(x) \leq \int_{-\infty}^{0} \mathcal{L}(x^+(-t), -\dot{x}^+(-t))dt = V(x),$$

thus concluding the proof that $Q(x) = V(x)$. Coming back to the above expression, we then conclude that the path $\{x^+(-t)\}_{t\in(-\infty,0]}$ is the minimizer in (4.10). Hence, we arrive at the following key observation. Starting from equilibrium at time zero, for λ and T large, if the system at time T is in state x then with high probability its evolution for times $t \in [0, T]$ is well approximated by the path $x^+(T - \cdot)$, where $x^+(\cdot)$ solves (4.13). More precisely:

$$\begin{aligned} &\lim_{T\uparrow\infty} \lim_{\lambda\uparrow\infty} \mathbb{P}^{\lambda}_{\rho_\lambda}\big(\{x(t)\}_{t\in[0,T]} \approx \{x^+(T-t)\}_{t\in[0,T]} \big| x(T) = x\big) \\ &\quad = \lim_{T\uparrow\infty} \lim_{\lambda\uparrow\infty} \mathbb{P}^{\lambda}_{\rho_\lambda}\big(\{x(t)\}_{t\in[-T,0]} \approx \{x^+(-t)\}_{t\in[-T,0]} \big| x(0) = x\big) = 1. \end{aligned} \tag{4.14}$$

We call $\{x^+(-t)\}_{t\in(-\infty,0]}$ the *exit trajectory*, while we call the path $\{\bar{x}(t)\}_{t\in[0,\infty)}$ solving (4.5) the *relax trajectory* (motivated by the LLN). When the vector fields $\bar{F}$ and $\bar{F}^+$ coincide, i.e.

$$\bar{F}(x) = \bar{F}^+(x), \quad \forall x \in \Omega, \tag{4.15}$$

then the exit/relax trajectories are related by time reversal and using the terminology of [1, 2] we say that an *Onsager-Machlup symmetry* holds. When condition (4.15) does not hold, the exit/relax trajectories are not necessarily related by time reversal and according to [1, 2] we say that a *generalized Onsager-Machlup symmetry* holds.

We conclude this subsection justifying the name "Lagrangian" given to $\mathcal{L}(x, \dot{x})$. From classical arguments in variational analysis it follows that the quasi-potential $Q(x)$ as defined in (4.10) solves the Hamilton–Jacobi equation

$$\mathcal{H}(x, \nabla Q(x)) = 0, \tag{4.16}$$

where the Hamiltonian $\mathcal{H}$ is obtained as Legendre transform of $\mathcal{L}$ as

$$\mathcal{H}(x, p) = \sup_{y\in\mathbb{R}^d} (p \cdot y - \mathcal{L}(x, y)). \tag{4.17}$$

It can be shown (see [2] for details) that Q is the maximal solution of (4.16). The l.h.s. of (4.16) must be zero for the following reason. Due to (4.17) it must be $\mathcal{H}(x_*, 0) = 0$, while due to the fact that $Q(x) \geq Q(x_*)$ it must be $\nabla Q(x_*) = 0$. Hence, $\mathcal{H}(x_*, \nabla Q(x_*)) = 0$.

Clearly the above arguments hold also for the family of adjoint processes. In particular, the quasi-potential Q solves also Hamilton–Jacobi equation

$$\mathcal{H}^+(x, \nabla Q(x)) = 0, \tag{4.18}$$

where the Hamiltonian $\mathcal{H}^+$ is obtained as Legendre transform of $\mathcal{L}^+$ as

$$\mathcal{H}^+(x, p) = \sup_{y\in\mathbb{R}^d} \big(p \cdot y - \mathcal{L}^+(x, y)\big). \tag{4.19}$$

Note that due to the validity of the FD relation (4.9) we have

$$\begin{aligned}\mathcal{H}(x, p) &= \sup_{y\in\mathbb{R}^d} (p \cdot y - \mathcal{L}(x, y)) \\ &= \sup_{y\in\mathbb{R}^d} \big(p \cdot y - \nabla V(x) \cdot y - \mathcal{L}^+(x, -y)\big) \\ &= \sup_{y\in\mathbb{R}^d} \big((\nabla V(x) - p) \cdot y - \mathcal{L}^+(x, y)\big) = \mathcal{H}^+(x, \nabla V(x) - p).\end{aligned}$$

Finally we point out that for PDMPs the vector fields $\bar{F}$ and $\bar{F}^+$ mentioned above become

$$\begin{cases} \bar{F}(x) = \sum_\sigma \mu(\sigma|x) F_\sigma(x), \\ \bar{F}^+(x) = -\sum_\sigma \mu^+(\sigma|x) F_\sigma(x), \end{cases}$$

where $\mu(\cdot|x)$ and $\mu^+(\cdot|x)$ are the unique invariant measures of $L_c[x]$ and $L_c^+[x]$, respectively.

5 Stationarity: Proof of Proposition 3.1

We give here the proof of Proposition 3.1. Let us fist suppose that Ω is an open subset of $\mathbb{R}^d$ such that $\sup_{\sigma,\sigma',x} r(\sigma, \sigma'|x) < \infty$, or that Ω is a d-dimensional torus. Due to the stationary of ρ_λ it must be

$$\rho_\lambda(Lf) = 0 \tag{5.1}$$

for all functions f in the domain of the Markov generator. Let us denote here by $\mathbb{F}$ the family of functions f which are C^1 in x, have continuous extension to $\partial\Omega$ and satisfy for some σ the property: $f(x, \sigma') = 0$ if $\sigma' \neq \sigma$. Then, (5.1) for $f \in \mathbb{F}$ reads

$$\begin{aligned}&\int_\Omega dx \rho_\lambda(x, \sigma) F_\sigma(x) \cdot \nabla f(x, \sigma) \\ &\quad + \lambda \sum_{\sigma'\in\Gamma} \int_\Omega dx f(x, \sigma)\big(\rho_\lambda(x, \sigma') r(\sigma', \sigma) - \rho_\lambda(x, \sigma) r(\sigma, \sigma')\big) = 0.\end{aligned} \tag{5.2}$$

By the Gauss–Green formula, the first integral in the l.h.s. equals

$$\int_{\partial\Omega} dS(x) f(x, \sigma) \rho_\lambda(x, \sigma) F_\sigma(x) \cdot n(x) - \int_\Omega dx f(x, \sigma) \nabla \cdot \big(\rho_\lambda(x, \sigma) F_\sigma(x)\big), \tag{5.3}$$

where dS denotes the $(d-1)$-dimensional surface measure on $\partial\Omega$ and $n(x)$ denotes the outward normal to $\partial\Omega$ in x. Since (5.2) must hold in particular for all functions $f \in \mathbb{F}$ with x-support given by a compact subset of Ω, we conclude that (3.1) must be satisfied. Then, due to (5.2), (5.3) and (3.1), the boundary integral in (5.3) must be zero for all functions $f \in \mathbb{F}$. This forces ρ_λ to have zero flux across the boundary $\partial\Omega$, thus leading to (3.2). Note that if Ω is the closure of a domain in $\mathbb{R}^d$, the system of identities (3.1) must still be valid for $(x,\sigma) \in \Omega^\circ \times \Gamma$, Ω° being the interior part of Ω, since it follows from (5.1) by taking arbitrary functions f which are bounded, C^1 in x and with x-support strictly included in Ω°.

6 Reversibility: Proof of Propositions 3.2 and 3.3

Let us first prove Proposition 3.2. Being aware of the subtle difficulties concerning the domain of definition of the generator, we keep this analysis at a very heuristic level. The generator L^+ of the time-reversed process must be the adjoint in $L^2(\rho_\lambda)$ of the generator L of the direct process, namely

$$\mathbb{E}_{\rho_\lambda}(gLf) = \mathbb{E}_{\rho_\lambda}\left(fL^+g\right) \tag{6.1}$$

for all f, g good enough. Let us take f, g with compact support included in the interior part Ω° of Ω. Then the l.h.s. of (6.1) can be written as

$$\sum_{\sigma\in\Gamma}\int_\Omega dx\rho_\lambda(x,\sigma)g(x,\sigma)\Big[F_\sigma(x)\cdot\nabla f(x,\sigma)+\lambda\sum_{\sigma'\in\Gamma}r(\sigma,\sigma'|x)\big(f(x,\sigma')-f(x,\sigma)\big)\Big].$$

By a change of variable in the discrete sum and an integration by parts in the mechanical variable, we obtain

$$\sum_{\sigma\in\Gamma}\int_\Omega dx f(x,\sigma)\Big\{-\nabla\cdot\big(\rho_\lambda(x,\sigma)g(x,\sigma)F_\sigma(x)\big)$$
$$+\lambda\sum_{\sigma'\in\Gamma}\big(r(\sigma',\sigma|x)\rho_\lambda(x,\sigma')g(x,\sigma')-r(\sigma,\sigma'|x)\rho_\lambda(x,\sigma)g(x,\sigma)\big)\Big\}.$$

Using now (3.1) we get

$$\sum_{\sigma\in\Gamma}\int_\Omega dx f(x,\sigma)\Big\{-\nabla\cdot\big(\rho_\lambda(x,\sigma)g(x,\sigma)F_\sigma(x)\big)+g(x,\sigma)\nabla\cdot\big(\rho_\lambda(x,\sigma)F_\sigma(x)\big)$$
$$+\rho_\lambda(x,\sigma)\lambda\sum_{\sigma'\in\Gamma}\Big(r(\sigma',\sigma|x)\frac{\rho_\lambda(x,\sigma')}{\rho_\lambda(x,\sigma)}g(x,\sigma')-r(\sigma',\sigma|x)\frac{\rho_\lambda(x,\sigma')}{\rho_\lambda(x,\sigma)}g(x,\sigma)\Big)\Big\},$$

that finally becomes

$$\sum_{\sigma\in\Gamma}\int_\Omega dx\rho_\lambda(x,\sigma)f(x,\sigma)\Big[-F_\sigma(x)\cdot\nabla g(x,\sigma)+\lambda\sum_{\sigma'\in\Gamma}r(\sigma',\sigma|x)\frac{\rho_\lambda(x,\sigma')}{\rho_\lambda(x,\sigma)}$$
$$\times\big(g(x,\sigma')-g(x,\sigma)\big)\Big].$$

This ends the proof of (3.6) and therefore of Proposition 3.2.

Let us face now with Proposition 3.3. In order to justify (3.9), one can argue as follows. The reversibility of $L_c[x]$ is equivalent to the detailed balance condition

$$\mu(\sigma|x)r(\sigma,\sigma'|x) = \mu(\sigma'|x)r(\sigma',\sigma|x), \quad \forall\sigma,\sigma',\ \forall x \in \Omega. \tag{6.2}$$

Due to (3.5), this relation is equivalent to

$$\mu(\sigma|x)r^+(\sigma',\sigma|x)\frac{\rho_\lambda(x,\sigma')}{\rho_\lambda(x,\sigma)} = \mu(\sigma'|x)r^+(\sigma,\sigma'|x)\frac{\rho_\lambda(x,\sigma)}{\rho_\lambda(x,\sigma')},$$

that can be written as

$$\frac{\rho_\lambda^2(x,\sigma')}{\mu(\sigma'|x)}r^+(\sigma',\sigma|x) = \frac{\rho_\lambda^2(x,\sigma)}{\mu(\sigma|x)}r^+(\sigma,\sigma'|x).$$

This equation states that the rates r^+ at x satisfy the detailed balance condition with respect to a measure on Γ proportional to $\frac{\rho_\lambda^2(x,\sigma)}{\mu(\sigma|x)}$. The proportionality factor can depend on x and on λ. This is exactly the content of (3.9).

7 Invariant Distributions of 1D Models with Two Chemical States

In this section we prove Proposition 3.12 and the first two points of Proposition 3.13.

Let us first consider Proposition 3.12. The stationarity equations (3.1) are given by

$$\begin{cases} \lambda(\rho_\lambda(x,1)r(1,0|x) - \rho_\lambda(x,0)r(0,1|x)) = \partial_x(\rho_\lambda(x,0)F_0(x)), \\ \lambda(\rho_\lambda(x,0)r(0,1|x) - \rho_\lambda(x,1)r(1,0|x)) = \partial_x(\rho_\lambda(x,1)F_1(x)), \end{cases} \tag{7.1}$$

from which we obtain

$$\partial_x\big(\rho_\lambda(x,0)F_0(x) + \rho_\lambda(x,1)F_1(x)\big) = 0,$$

and consequently

$$\rho_\lambda(x,0)F_0(x) + \rho_\lambda(x,1)F_1(x) = c. \tag{7.2}$$

Due to the boundary condition (3.2), we know that c must be zero. Then relation (7.2) allows to solve (7.1) by separation of variables, leading to (3.52), which is meaningful as soon as the normalizing constant Z exists. Note that solution (3.52) automatically satisfies the boundary condition (3.2), since by construction the constant c in (7.2) is zero and by assumption $F_0(a) = F_1(b) = 0$. As the reader can check, (3.52) is the only solution of (3.1) compatible with the boundary condition (3.2). The last statement in Proposition 3.12 can be easily verified by the interested reader.

We now prove the first two points in Proposition 3.13. The equations for the stationary distribution are still (7.1) to which we have to add the periodic boundary conditions

$$\rho_\lambda(0,i) = \rho_\lambda(1,i), \quad i = 0,1. \tag{7.3}$$

It is easy to check that, for any constant k, the expressions in (3.54) are solutions of (7.1) satisfying the boundary conditions (7.3), since for any $x, y \in \mathbb{R}$ it holds

$$S(y) - S(x) = S(y+1) - S(x+1). \tag{7.4}$$

Moreover, there exists a unique value of k such that the expressions in the r.h.s. of (3.54) are positive functions, satisfying the normalization condition $\sum_{\sigma=0,1}\int_0^1 \rho_\lambda(x,\sigma)dx = 1$. On the other hand, it is simple to check that the above solution is the only one satisfying (3.1) and the periodic boundary conditions. This concludes the proof of point (i).

Let us now prove point (ii). Trivially, the equilibrium condition is equivalent to the fact that S is periodic with period 1. From this periodicity we obtain that

$$\int_x^{x+1}\left[\left(\frac{r(1,0|y)}{F_1(y)}+\frac{r(0,1|y)}{F_0(y)}\right)e^{\lambda S(y)}\right]dy=\frac{1}{\lambda}\left(e^{\lambda S(x+1)}-e^{\lambda S(x)}\right)=0. \tag{7.5}$$

The above identity together with (3.54) implies (3.56).

8 Exactly Solvable Models: Some Proofs

8.1 Proof of Proposition 3.4

Inserting (3.10) in (3.1), we obtain that for any $\sigma\in\Gamma$ it must hold

$$\begin{aligned}&\lambda c(\lambda)e^{-\lambda S(x)}\sum_{\sigma'\in\Gamma}\big(\rho(x,\sigma')r(\sigma',\sigma|x)-\rho(x,\sigma)r(\sigma,\sigma'|x)\big)\\&\quad=-\lambda c(\lambda)e^{-\lambda S(x)}\nabla S(x)\cdot\big(\rho(x,\sigma)F_\sigma(x)\big)+c(\lambda)e^{-\lambda S(x)}\nabla\cdot\big(\rho(x,\sigma)F_\sigma(x)\big).\end{aligned} \tag{8.1}$$

Dividing by nonzero terms we get

$$\begin{aligned}&\lambda\Big[\sum_{\sigma'\in\Gamma}\big(\rho(x,\sigma')r(\sigma',\sigma|x)-\rho(x,\sigma)r(\sigma,\sigma'|x)\big)+\nabla S(x)\cdot\big(\rho(x,\sigma)F_\sigma(x)\big)\Big]\\&\quad+\nabla\cdot\big(\rho(x,\sigma)F_\sigma(x)\big)=0.\end{aligned} \tag{8.2}$$

In the above formula we have a first order polynomial in λ and we have equality to zero for any value of λ if and only if the coefficients of the zero and first order terms are equal to zero separately. This observation leads to (3.13).

8.2 Integration of (3.14) Along Orbits of F_σ

We distinguish between closed and open orbits.

Closed Orbits Let $\gamma\subseteq\Omega$ be a closed orbit of the vector field F_σ, let x_0 be any element of γ and let $x_\gamma(t)$ be the parametrization of γ such that $x_\gamma(0)=x_0$ and $\dot{x}_\gamma(t)=F_\sigma(x_\gamma(t))$ for all $t\in[0,T]$, where T is the period of the orbit (note that $x_\gamma(0)=x_\gamma(T)=x_0$). Given $x'\in\gamma$, let t' be the only time in $[0,T]$ such that $x'=x_\gamma(t')$. Then (3.14) implies that

$$\begin{aligned}\varphi(x',\sigma)-\varphi(x_0,\sigma)&=\int_0^{t'}\nabla\varphi(x_\gamma(s),\sigma)\cdot\dot{x}_\gamma(s)ds\\&=\int_0^{t'}\nabla\varphi(x_\gamma(s),\sigma)\cdot F_\sigma(x_\gamma(s))ds\end{aligned}$$

$$= -\int_0^{t'} \nabla \cdot F_\sigma(x_\gamma(s))ds. \tag{8.3}$$

This implies that a function φ satisfying (3.14) can be constructed along γ if and only if the univalued condition

$$\int_0^T \nabla \cdot F_\sigma(x_\gamma(s))ds = 0 \tag{8.4}$$

is satisfied. Moreover the values of φ on γ are uniquely determined from (8.3) once the initial condition $\varphi(x_0, \sigma)$ has been arbitrarily fixed.

Open Orbits Let $\gamma \subseteq \Omega$ be an open orbit of the vector field F_σ and consider $x_0 \in \gamma$. Let $x_\gamma(t)$ be a parametrization of γ such that $\dot{x}_\gamma(t) = F_\sigma(x_\gamma(t))$ and $x(0) = x_0$. Given $x' \in \gamma$, let t' be the unique time such that $x_\gamma(t') = x'$. Then (8.3) continues to hold and we can determine the value of $\varphi(x', \sigma)$ for any $x' \in \gamma$ starting from the arbitrary initial condition $\varphi(x_0, \sigma)$.

8.3 Proof of Proposition 3.5

Let us first assume that S solves the second group of equations in (3.13). Due to definition (3.16), this group of equations reads

$$D(x, \sigma) = \nabla S(x) \cdot \big(\rho(x, \sigma) F_\sigma(x)\big), \quad \forall (x, \sigma) \in \Omega \times \Gamma. \tag{8.5}$$

This means that, for any $\sigma \in \Gamma$, $D(x, \sigma)$ is the directional derivative of S at x along the vector $\rho(x, \sigma) F_\sigma(x)$. We recall that, given vectors $v, v_1, \ldots, v_k$ such that $v = \sum_i c_i v_i$, it holds

$$\lim_{t\to 0} \frac{S(x + tv) - S(x)}{t} = \sum_i c_i \nabla S(x) \cdot v_i = \sum_i c_i \lim_{t\to 0} \frac{S(x + tv_i) - S(x)}{t}. \tag{8.6}$$

From (3.18) and (8.6) we get that (3.19) is a necessary condition for the existence of the function S solving (3.13).

The definition of the matrix $\{A_{i,\sigma}(x)\}_{i\in\{1,\ldots,d\}}^{\sigma\in\Gamma(x)}$ implies that

$$\rho(x, \sigma) F_\sigma(x) = \sum_{i=1}^{d} A_{i,\sigma}(x) e_i, \quad \forall \sigma \in \Gamma(x), \tag{8.7}$$

as well as

$$e_i = \sum_{\sigma\in\Gamma(x)} A^{-1}_{\sigma,i}(x) \rho(x, \sigma) F_\sigma(x), \quad \forall i : 1 \le i \le d. \tag{8.8}$$

Since $\{D(x, \sigma)\}_{\sigma\in\Gamma(x)}$ must correspond to directional derivatives of a function S on Ω, due to (8.6) and (8.8) it must be

$$\partial_{x_i} S(x) = \sum_{\sigma\in\Gamma(x)} A^{-1}_{\sigma,i}(x) D(x, \sigma). \tag{8.9}$$

Consider a closed curve $\gamma \subseteq \Omega$ with parametrization $\{x_\gamma(t)\}_{t\in[0,T]}$. Since γ is closed, it must be $0 = \int_0^T \nabla S(x_\gamma(s)) \cdot \dot{x}_\gamma(s) ds$. Using (8.9) the above identity becomes

$$0 = \int_0^T \sum_{i=1}^d \Big(\sum_{\sigma\in\Gamma(x_\gamma(s))} A^{-1}_{\sigma,i}(x_\gamma(s)) D(x_\gamma(s),\sigma) \Big) \dot{x}_{\gamma,i}(s) ds = \oint_\gamma \omega, \tag{8.10}$$

where ω is the differential form defined in (3.20). The validity of condition (8.10) for any closed curve γ is equivalent to require that the ω is exact. Since (8.9) means that $dS = \omega$, this implies (3.21) and concludes the proof in the case that S is a solution of the second group of equations in (3.13).

Vice versa, let us prove that all the conditions appearing in Proposition 3.5 imply that any function S satisfying (3.21) is a solution of (3.13). Since ω is exact, (3.21) is equivalent to the identity $dS = \omega$, which is equivalent of (8.9). Since by (8.7)

$$\nabla S(x) \cdot \big(\rho(x,\sigma) F_\sigma(x)\big) = \sum_{i=1}^d A_{i,\sigma}(x) \partial_{x_i} S(x),$$

from (8.9) we derive (8.5) for all (x,σ) such that $\sigma \in \Gamma(x)$. Due to (3.18), (3.19) and additivity, identity (8.5) extends to all $\sigma \in \Gamma$.

9 Examples of Application of Proposition 3.5

We now exhibit solutions of (3.1) in specific examples by means of the construction outlined in Proposition 3.5. The reader can easily check that our solutions satisfy the appropriate boundary conditions so that they correspond to the invariant measure of the PDMPs under consideration.

9.1 Interval

We apply Proposition 3.5 in order to check Proposition 3.12, of which we keep the assumptions. We fix an arbitrary point $x_* \in (a,b)$. Given $x(t)$ the solution of $\dot{x} = F_1(x)$ with $x(0) = x_*$, due to (3.14) for any $x \in (a,b)$ the function $\varphi(x,1) = \log \rho(x,1)$ satisfies

$$\varphi(x,1) = \phi(x_*) - \int_0^t \nabla \cdot F_1(x(s)) ds \tag{9.1}$$

where the time t is such that $x(t) = x$ and $\phi(x_*)$ is an arbitrary constant. Since by differentiation it must be $\ddot{x}(s)/\dot{x}(s) = \nabla \cdot F_1(x(s))$, inserting this identity in (9.1) gives

$$\varphi(x,1) = \phi(x_*) - \int_0^t \frac{d}{ds} (\log \dot{x}(s))\, ds = \phi(x_*) + \log \frac{F_1(x_*)}{F_1(x)}.$$

The above identity and similar arguments applied to the vector field F_0 imply that

$$\begin{cases} \rho(x,1) = e^{\phi(x_*)} \frac{F_1(x_*)}{F_1(x)}, \\ \rho(x,0) = e^{\psi(x_*)} \frac{F_0(x_*)}{F_0(x)}, \end{cases} \tag{9.2}$$

where also $\psi(x_*)$ is an arbitrary constant. It remains now to determine the function S and afterwards to fix the arbitrary constants. Taking $\Gamma(x) = \{1\}$ for any $x \in \Omega$, condition (3.23) is satisfied. Due to (9.2), we can express the constant $c_1(0, x)$ in (3.18) as

$$c_1(0, x) = \frac{\rho(x, 0)F_0(x)}{\rho(x, 1)F_1(x)} = \frac{e^{\psi(x_*)}F_0(x_*)}{e^{\phi(x_*)}F_1(x_*)}. \tag{9.3}$$

Since in addition $D(x, 0) = -D(x, 1)$, condition (3.19) is satisfied if and only if $c_1(0, x) \equiv -1$. To this aim we take $e^{\psi(x_*)} = -1/F_0(x_*)$ and $e^{\phi(x_*)} = 1/F_1(x_*)$. By this choice, the differential form (3.20) is given by

$$\omega = \frac{D(x, 1)}{\rho(x, 1)F_1(x)}dx = \left(\frac{r(0, 1|x)}{F_0(x)} + \frac{r(1, 0|x)}{F_1(x)}\right)dx. \tag{9.4}$$

The form ω is trivially exact, being a 1D form on a simply connected domain. Then, by formula (3.21) and the previous computations, we get (3.52) as a special case of (3.10).

9.2 1D Torus

Let us keep the same assumptions as in Proposition 3.13. Then both F_0 and F_1 have a closed orbit that coincide with Ω. In both cases the univalued condition (8.4) is satisfied due to the fact that on the periodic orbit $x(t)$ solution of $\dot{x} = F_i(x)$ with period T we have

$$\int_0^T \nabla \cdot F_i(x(s))ds = \int_0^T \frac{d}{ds}(\log \dot{x}(s))\, ds = 0.$$

We can repeat all the arguments and computations of the case $\Omega = (a, b)$. The only exception is that now the form ω given by (9.4) is not automatically exact, since Ω is not simply connected. The requirement that $\oint_\Omega \omega = 0$ is exactly the equilibrium condition (3.55). The final result coincides with (3.56).

9.3 Triangular Domain

Let us now discuss a simple but non trivial example in dimension $d = 2$ of a PDMP with an invariant measure of the form (3.10). Let $\Omega \subseteq \mathbb{R}^2$ be the open triangle with vertices $(0, 0)$, $(1, 0)$, $(0, 1)$ and let (x, y) denote a generic element of Ω. The set of chemical states is $\Gamma = \{1, 2, 3\}$. The vector fields associated to the chemical states are obtained from the gradients of quadratic potentials centered at the vertices of the triangle. More precisely

$$\begin{cases} F_1(x, y) = -\frac{1}{2}\nabla(x^2 + y^2) = (-x, -y), \\ F_2(x, y) = -\frac{1}{2}\nabla((x-1)^2 + y^2) = (1-x, -y), \\ F_3(x, y) = -\frac{1}{2}\nabla(x^2 + (y-1)^2) = (-x, 1-y). \end{cases}$$

All the orbits of the above vector fields are open and condition (2.14) is satisfied. Moreover the orbits of the vector fields F_i exit from $\partial\Omega_i^+ \subset \partial\Omega$, where $\partial\Omega_1^+$ is the segment with extrema $(0, 1)$ and $(1, 0)$; $\partial\Omega_2^+$ is the segment with extrema $(0, 0)$ and $(0, 1)$; $\partial\Omega_3^+$ is the segment with extrema $(0, 0)$ and $(1, 0)$. Let us determine the function $\varphi(x, y, 1) = \log \rho(x, y, 1)$ by means of the discussion following (3.14). To this aim, we observe that given $(x, y) \in \Omega$

the path $(x(t), y(t)) := (e^{-t}, e^{-t}y/x)$ satisfies

$$\begin{cases} (\dot{x}(t), \dot{y}(t)) = F_1(x(t), y(t)), \quad \forall t \geq t_0, \\ (x(t_0), y(t_0)) = (x/(x+y), y/(x+y)) \in \partial\Omega_1^+, \\ (x(t_1), y(t_1)) = (x, y), \end{cases}$$

where $t_0 := \log\big((x+y)/x\big)$ and $t_1 := \log(1/x)$. In particular, the above path parameterized by $t \geq t_0$ is an orbit of F_1 exiting from $\partial\Omega_1^+$ and passing through the point (x, y). Fixed an arbitrary function $\phi_1 : (0, 1) \to \mathbb{R}$ we obtain using (8.3)

$$\varphi(x, y, 1) - \phi_1\left(\frac{x}{x+y}\right) = 2\int_{\log\frac{x+y}{x}}^{\log\frac{1}{x}} dt = -2\log(x+y),$$

so that $\rho(x, y, 1) = \frac{e^{\phi_1(\frac{x}{x+y})}}{(x+y)^2}$. Note that this can be rewritten as $\rho(x, y, 1) = a_1(x/(x+y))/x^2$ for a suitable function $a_1 : (0, 1) \to \mathbb{R}$. In conclusion, by similar arguments, we get that

$$\begin{cases} \rho(x, y, 1) = a_1(\frac{x}{x+y})\frac{1}{x^2}, \\ \rho(x, y, 2) = a_2(\frac{y}{1-x})\frac{1}{y^2}, \\ \rho(x, y, 3) = a_3(\frac{x}{1-y})\frac{1}{x^2}, \end{cases} \tag{9.5}$$

for positive functions a_1, a_2, a_3, which can be chosen arbitrarily. Note that the point $(0, y/(1-x))$ is the exit point in $\partial\Omega_2^+$ of the F_2-orbit passing through the point $(x, y) \in \Omega$, while $(x/(1-y), 0)$ is the exit point in $\partial\Omega_3^+$ of the F_3-orbit passing through the point $(x, y) \in \Omega$.

In order to determine the function S of (3.10), for any $(x, y) \in \Omega$ we take $\Gamma(x, y) = \{2, 3\}$. Trivially condition (3.23) is satisfied. Moreover, we can compute $c_2(1, x, y)$ and $c_3(1, x, y)$ of (3.18):

$$\begin{cases} c_2(1, x, y) = \frac{x}{x+y-1}\frac{\rho(x,y,1)}{\rho(x,y,2)}, \\ c_3(1, x, y) = \frac{y}{x+y-1}\frac{\rho(x,y,1)}{\rho(x,y,3)}. \end{cases} \tag{9.6}$$

At this point, the check of condition (3.19) depends strongly from the form of the rates $r(\cdot, \cdot|x, y)$. Indeed, omitting the dependence from the point (x, y) (for the sake of simplicity) condition (3.19) becomes

$$\begin{aligned} &r(1,2) + r(1,3) - \frac{\rho(2)}{\rho(1)}r(2,1) - \frac{\rho(3)}{\rho(1)}r(3,1) \\ &\quad = \frac{x}{x+y-1}\left[r(2,1) + r(2,3) - \frac{\rho(1)}{\rho(2)}r(1,2) - \frac{\rho(3)}{\rho(2)}r(3,2)\right] \\ &\qquad + \frac{y}{x+y-1}\left[r(3,1) + r(3,2) - \frac{\rho(1)}{\rho(3)}r(1,3) - \frac{\rho(2)}{\rho(3)}r(2,3)\right]. \end{aligned} \tag{9.7}$$

As the reader can easily check, the above identity is automatically satisfied for all kind of jump rates if

$$\frac{\rho(1)}{\rho(3)} = \frac{1-x-y}{y}, \qquad \frac{\rho(2)}{\rho(3)} = \frac{x}{y}, \qquad \frac{\rho(1)}{\rho(2)} = \frac{1-x-y}{x}. \tag{9.8}$$

In order to satisfy the above identities it is enough to take a_1, a_2, a_3 in (9.5) as $a_i(u) = \frac{u}{1-u}$. By this choice, (9.5) reads

$$\begin{cases} \rho(x, y, 1) = 1/(xy), \\ \rho(x, y, 2) = 1/[y(1-x-y)], \\ \rho(x, y, 3) = 1/[x(1-x-y)]. \end{cases} \tag{9.9}$$

It remains now to compute the form ω given by (3.20), check when it is exact and afterwards check the boundary condition (3.2). First we observe that

$$A(x, y) = \frac{1}{1-x-y} \begin{pmatrix} \frac{1-x}{y} & -1 \\ -1 & \frac{1-y}{x} \end{pmatrix}, \qquad A^{-1}(x, y) = \begin{pmatrix} y(1-y) & xy \\ xy & x(1-x) \end{pmatrix}.$$

Therefore

$$\omega = \big[y(1-y)D(x, y, 2) + xyD(x, y, 3)\big]dx + \big[xyD(x, y, 2) + x(1-x)D(x, y, 3)\big]dy.$$

We have

$$\omega = B(x, y)dx + C(x, y)dy$$

where (omitting the dependence on (x, y) for simplicity)

$$\begin{aligned} B(x, y) &= \frac{1-y}{1-x-y} r(2, 1) - \frac{1-y}{x} r(1, 2) \\ &\quad + \frac{y}{1-x-y} r(3, 1) - r(1, 3) + r(2, 3) - \frac{y}{x} r(3, 2), \\ C(x, y) &= \frac{1-x}{1-x-y} r(3, 1) - \frac{1-x}{y} r(1, 3) \\ &\quad + \frac{x}{1-x-y} r(2, 1) - r(1, 2) + r(3, 2) - \frac{x}{y} r(2, 3). \end{aligned}$$

Note that $C(x, y)$ can be obtained from $B(x, y)$ by exchanging x with y and 2 with 3.

If, motivated by the geometric symmetries of Ω, we assume that

$$r(1, 2|x, y) = r(1, 3|y, x), \qquad r(2, 1|x, y) = r(3, 1|y, x), \qquad r(2, 3|x, y) = r(3, 2|y, x)$$

then

$$\omega = B(x, y)dx + B(y, x)dy.$$

In this case, since Ω is simply connected, ω is exact if and only if $\partial_y B(a, b) = \partial_y B(b, a)$ (cf. (3.22)), i.e. the function $\partial_y B$ is symmetric.

Let us discuss an example, where the above condition is satisfied. We take $r(\sigma, \sigma'|x, y) = 1$ for all $\sigma \neq \sigma'$. Then one easily compute the above $B(x, y)$ and $C(x, y)$, getting

$$\omega = \frac{2x + y - 1}{x(1-x-y)} dx + \frac{2y + x - 1}{y(1-x-y)} dy, \tag{9.10}$$

which is exact since the domain Ω is simply connected and condition (3.22) is satisfied. Integrating the form ω as in (3.21), we obtain up to an arbitrary constant

$$S(x, y) = \int_\gamma \omega = -\log x - \log y - \log(1-x-y). \tag{9.11}$$

By collecting our results (9.9) and (9.11), we obtain that the invariant measure is of the form (3.10) and that

$$\begin{aligned}\rho_\lambda &= \big(\rho_\lambda(x,y,1), \rho_\lambda(x,y,2), \rho_\lambda(x,y,3)\big)\\ &= c(\lambda)\left(x^{\lambda-1}y^{\lambda-1}(1-x-y)^{\lambda}, x^{\lambda}y^{\lambda-1}(1-x-y)^{\lambda-1}, x^{\lambda-1}y^{\lambda}(1-x-y)^{\lambda-1}\right).\end{aligned}$$

Above, $c(\lambda)$ is the normalization constant, which is well-defined as the reader can easily check. Finally, we observe that the above invariant measure satisfies the boundary condition (3.2).

Note that, due to (9.5), (3.2) can be satisfied only if S diverges to $-\infty$ when approaching the boundary of the triangle Ω. This is a strong restriction. For example, if we tale $r(3,2|x,y) = r(2,3|x,y) = 0$, $r(2,1|x,y) = r(3,1|x,y) = 1-x-y$, $r(1,2|x,y) = r(1,3|y,x) = x$, we obtain that $\omega = dS$ where S is a constant function, thus leading to a solution of the stationary equations (3.1), but not satisfying the boundary condition (3.2).

9.4 2D Torus

We take $\Omega = \mathbb{R}^2/\mathbb{Z}^2$ and $\Gamma = \{0,1\}$. We call (x,y) a generic element of Ω and choose vector fields

$$\begin{cases} F_0(x,y) = (f(x,y),0),\\ F_1(x,y) = (0,g(x,y)),\end{cases}$$

where f and g are regular functions which never vanish on Ω. The chemical part of the generator is determined by the transition rates $r(i,i-1|x,y)$ $i=0,1$. The first group of equations in (3.13) can be easily solved:

$$\begin{cases} \rho(x,y,0) = \frac{\phi(y)}{f(x,y)},\\ \rho(x,y,1) = \frac{\tilde\phi(x)}{g(x,y)};\end{cases}$$

where ϕ and $\tilde\phi$ are arbitrary functions. Moreover we have that

$$A^{-1}(x,y) = \begin{pmatrix} \frac{1}{\phi(y)} & 0\\ 0 & \frac{1}{\tilde\phi(x)}\end{pmatrix},$$

hence ω can be written as

$$\omega = \left(\frac{r(0,1|x,y)}{f(x,y)} - \frac{\tilde\phi(x) r(1,0|x,y)}{\phi(y) g(x,y)}\right)dx + \left(\frac{r(1,0|x,y)}{g(x,y)} - \frac{\phi(y) r(0,1|x,y)}{\tilde\phi(x) f(x,y)}\right)dy. \quad (9.12)$$

Fix arbitrary points $x^*, y^* \in [0,1]$ and consider the associated fundamental cycles on Ω

$$\begin{cases} \gamma^1(t) = (t, y^*), & t\in[0,1],\\ \gamma^2(t) = (x^*, t), & t\in[0,1].\end{cases}$$

The exactness of (9.12) is equivalent to imposing conditions (3.22) with the additional conditions

$$\oint_{\gamma^1}\omega = \oint_{\gamma^2}\omega = 0. \quad (9.13)$$

If we call $H(x,y)=\phi(y)r(0,1|x,y)/f(x,y)$ and $G(x,y)=\tilde{\phi}(x)r(1,0|x,y)/g(x,y)$, then we can write ω as

$$\omega=\frac{H(x,y)-G(x,y)}{\phi(y)}dx+\frac{G(x,y)-H(x,y)}{\tilde{\phi}(x)}dy,$$

hence the above exactness conditions become

$$\begin{cases}\int_0^1 H(x^*,y)dy=\int_0^1 G(x^*,y)dy,\\ \int_0^1 H(x,y^*)dx=\int_0^1 G(x,y^*)dx,\\ \partial_x(\frac{G(x,y)-H(x,y)}{\tilde{\phi}(x)})=\partial_y(\frac{H(x,y)-G(x,y)}{\phi(y)}).\end{cases}$$

Examples of rates $r(i,i-1|x,y)$ satisfying these conditions can be easily constructed.

9.5 Square Domain

We consider the open square $\Omega\subseteq\mathbb{R}^2$ with vertices $(0,0)$, $(0,1)$, $(1,0)$ and $(1,1)$. The chemical states are $\Gamma=\{0,1,2,3\}$ with associated vector fields

$$F_0(x,y)=(-x,-y),\qquad F_1(x,y)=(1-x,-y),$$
$$F_2(x,y)=(-x,1-y),\qquad F_3(x,y)=\alpha(1-x,1-y),$$

where α is a positive parameter and (x,y) is a generic element of Ω. We choose the jump rates as

$$r(0,1|x,y)=r(0,2|y,x)=q(x,y),\qquad r(1,0|x,y)=r(2,0|y,x)=r(x,y),$$
$$r(1,3|x,y)=r(2,3|y,x)=Q(x,y),\qquad r(3,1|x,y)=r(3,2|y,x)=R(x,y),$$

where q, r, Q and R are arbitrary positive functions and moreover $r(1,2|x,y)=r(2,1|x,y)=0$.

Proceeding as in the previous examples we obtain a solution of the form (3.10) if we require that the rates satisfy the following relations: there exists a function $G(x,y)$ such that

$$\begin{cases}q(x,y)-Q(x,y)=G(x,y)x,\\ r(x,y)-\frac{R(x,y)}{\alpha}=G(x,y)(1-x)\end{cases}$$

and there exists a symmetric function $s(x,y)$ and a function ϕ such that

$$xR(x,y)-\alpha(1-x)Q(x,y)=\alpha x(1-x)\left(\int_z^y dus(x,u)+\phi(x)\right),$$

where $z\in(0,1)$. Under the above conditions we have a solution of the form (3.10) with

$$S(x,y)=\int_z^x dw\int_z^y dus(w,u)+\int_z^x dw\phi(w)+\int_z^y du\phi(u),$$

and

$$\rho(x,y,0)=\frac{1}{xy},\qquad \rho(x,y,1)=\frac{1}{y(1-x)},$$

$$\rho(x,y,2)=\frac{1}{x(1-y)},\qquad \rho(x,y,3)=\frac{1}{\alpha(1-x)(1-y)}.$$

Boundary conditions (3.2) are not necessarily satisfied.

10 Fluctuation Theory: Proof of Propositions 3.10 and 3.11

10.1 Proof of Proposition 3.10

It is easy to compute $\lim_{\lambda\to\infty}\lambda^{-1}\log\hat{\rho}_\lambda(x)$, and derive a LD principle for $\hat{\rho}$. To this aim, first observe that the function S in (3.10) is univocally determined up to an additive constant. From now on, we denote by S the unique function satisfying (3.10) normalized in such a way that $\inf_{x\in\Omega}S(x)=0$. By this choice, it is simple to see that

$$\lim_{\lambda\to\infty}\lambda^{-1}\log\hat{\rho}_\lambda(x)=-S(x).$$

Comparing with (4.6), we deduce that $S(x)=V(x)$, namely the function S coincides with the LD rate functional of the measures $\hat{\rho}_\lambda$.

10.2 Proof of Proposition 3.11

We first establish for the class of models satisfying (3.10), a special symmetry concerning the rate densities j and j^+ defined in (3.30) and (3.41):

Lemma 10.1 *Suppose that the invariant distribution ρ_λ of the PDMP satisfies (3.10). Then, it holds*

$$j(x,\chi)-j^+(x,\chi)=\sum_\sigma\chi_\sigma(\gamma(\sigma|x)-\gamma^+(\sigma|x)). \tag{10.1}$$

Proof If $L_c[x]$ and consequently also $L_c^+[x]$ are reversible w.r.t. the corresponding quasi-stationary measures, then (10.1) follows directly from the explicit expressions (3.33) and (3.42). In the general case, using also (3.5), we can write the variational expressions (3.30) and (3.41) as

$$j(x,\chi)=\sum_\sigma\chi_\sigma\gamma(\sigma|x)-\inf_{z\in(0,+\infty)^\Gamma}\Big(\sum_{(\sigma,\sigma')\in W}\chi_\sigma r(\sigma,\sigma'|x)\frac{z_{\sigma'}}{z_\sigma}\Big), \tag{10.2}$$

$$j^+(x,\chi)=\sum_\sigma\chi_\sigma\gamma^+(\sigma|x)-\inf_{z\in(0,+\infty)^\Gamma}\Big(\sum_{(\sigma,\sigma')\in W}\chi_{\sigma'}r(\sigma,\sigma'|x)\frac{\rho(x,\sigma)z_\sigma}{\rho(x,\sigma')z_{\sigma'}}\Big). \tag{10.3}$$

Let us first assume that $\chi_\sigma>0$ for any $\sigma\in\Gamma$. Setting $\widetilde{z}_\sigma:=\frac{\chi_\sigma}{\rho(x,\sigma)z_\sigma}$, the variational expression in (10.3) can then be written as

$$\inf_{\widetilde{z}\in(0,+\infty)^\Gamma}\Big(\sum_{(\sigma,\sigma')\in W}\chi_\sigma r(\sigma,\sigma'|x)\frac{\widetilde{z}_{\sigma'}}{\widetilde{z}_\sigma}\Big),$$

that coincides with the variational expression in (10.2). Relation (10.1) now follows immediately.

We consider now the case that there exists some $\sigma \in \Gamma$ for which $\chi_\sigma = 0$. For simplicity we assume $\chi_{\sigma_1} = 0$ and $\chi_\sigma > 0$ for any $\sigma \neq \sigma_1$. The general case can be proved in the same way. Let us define $\Gamma^1 := \{\sigma \in \Gamma : \sigma \neq \sigma_1\}$ and $W^1 := \{(\sigma, \sigma') \in W : \sigma \neq \sigma_1, (\sigma' \neq \sigma_1)\}$. We want to show that

$$\inf_{z \in (0,+\infty)^\Gamma} \sum_{(\sigma,\sigma') \in W} \chi_\sigma r(\sigma, \sigma'|x) \frac{z_{\sigma'}}{z_\sigma} = \inf_{z \in (0,+\infty)^{\Gamma^1}} \sum_{(\sigma,\sigma') \in W^1} \chi_\sigma r(\sigma, \sigma'|x) \frac{z_{\sigma'}}{z_\sigma}. \tag{10.4}$$

The r.h.s. of (10.4) is clearly less or equal than the l.h.s. To prove the opposite inequality take $z \in (0, +\infty)^{\Gamma^1}$ and consider $z^\epsilon := (\epsilon, z) \in (0, +\infty)^\Gamma$. We have that

$$\lim_{\epsilon \to 0} \sum_{(\sigma,\sigma') \in W} \chi_\sigma r(\sigma, \sigma'|x) \frac{z^\epsilon_{\sigma'}}{z^\epsilon_\sigma} = \sum_{(\sigma,\sigma') \in W^1} \chi_\sigma r(\sigma, \sigma'|x) \frac{z_{\sigma'}}{z_\sigma},$$

and this implies (10.4). This argument shows that we can write (10.2) and (10.3) as

$$j(x, \chi) = \sum_\sigma \chi_\sigma \gamma(\sigma|x) - \inf_{z \in (0,+\infty)^{\Gamma^1}} \sum_{(\sigma,\sigma') \in W^1} \chi_\sigma r(\sigma, \sigma'|x) \frac{z_{\sigma'}}{z_\sigma}, \tag{10.5}$$

$$j^+(x, \chi) = \sum_\sigma \chi_\sigma \gamma^+(\sigma|x) - \inf_{z \in (0,+\infty)^{\Gamma^1}} \sum_{(\sigma,\sigma') \in W^1} \chi_{\sigma'} r(\sigma, \sigma'|x) \frac{\rho(x, \sigma) z_\sigma}{\rho(x, \sigma') z_{\sigma'}}. \tag{10.6}$$

If we introduce $\widetilde{z}_\sigma := \frac{\chi_\sigma}{\rho(x,\sigma) z_\sigma}$ for any $\sigma \in \Gamma^1$ the variational expression in (10.6) can be written as

$$\inf_{z \in (0,+\infty)^{\Gamma^1}} \sum_{(\sigma,\sigma') \in W^1} \chi_\sigma r(\sigma, \sigma'|x) \frac{\widetilde{z}_{\sigma'}}{\widetilde{z}_\sigma},$$

which coincides with the variational expression in (10.5). Relation (10.1) now follows directly. □

Using (3.15) (valid for each $\sigma \in \Gamma$), which are equivalent to the second group of identities in (3.13), we obtain that (10.1) of the above lemma can be written as

$$j(x, \chi) - j^+(x, \chi) = \nabla S(x) \cdot \left(\sum_\sigma \chi_\sigma F_\sigma \right). \tag{10.7}$$

Observe that in order to compute both $j_m(x, \dot{x})$ and $j^+_m(x, -\dot{x})$ we need to minimize respectively j and j^+ over χ subject to the same constraint $\sum_s \chi_s F_\sigma(x) = \dot{x}$. Recalling (10.7), we get for any fixed x and $\dot{x}$ that

$$\begin{aligned} j_m(x, \dot{x}) &= \inf_{\{\chi : \sum_s \chi_s F_\sigma(x) = \dot{x}\}} j(x, \chi) \\ &= \nabla S(x) \cdot \dot{x} + \inf_{\{\chi : \sum_s \chi_s F_\sigma(x) = \dot{x}\}} j^+(x, \chi) \\ &= \nabla S(x) \cdot \dot{x} + j^+_m(x, -\dot{x}). \end{aligned} \tag{10.8}$$

That corresponds to the FD relation (4.9) since, as already observed, $S(x) = V(x)$. From (10.7) we obtain also that the minimizers χ for the computation of both $j_m(x, \dot{x})$ and $j^+_m(x, -\dot{x})$ coincide. We point out that in the case of computable LD rate functionals as in

(3.39) and (3.47), identity (10.8) follows directly from (3.33), (3.42) and the simple relation $\chi_\sigma^F(\dot{x}) = \chi_\sigma^{-F}(-\dot{x})$.

Remark 2 It is interesting to note that we can obtain a simple explicit expression for the *entropy production*, i.e. the rate of variation of S along the orbits of the vector fields $\bar{F}$ and $\bar{F}^+$. Given $x(t)$ a solution of (4.5), using (3.15) we have

$$\nabla S(x)\cdot\dot{x} = \nabla S(x)\cdot\bar{F}(x) = \sum_\sigma \mu(\sigma|x)\nabla S(x)\cdot F_\sigma(x) = \sum_\sigma \mu(\sigma|\bar{x})(\gamma(\sigma|x) - \gamma^+(\sigma|x)). \tag{10.9}$$

Likewise given x^+ a solution of (4.13) we have

$$\nabla S(x^+)\cdot\dot{x}^+ = \sum_\sigma \mu^+(\sigma|x^+)(\gamma^+(\sigma|x^+) - \gamma(\sigma|x^+)). \tag{10.10}$$

10.3 A Conjecture

As already observed, the validity of the FD relation for PDMPs with invariant measures of the form (3.10) follows from the identity (10.8). This key identity can be rewritten as

$$j_m(x,\dot{x}) = \nabla W\cdot\dot{x} + \mathcal{G}(x,-\dot{x}), \tag{10.11}$$

where $W = S$ and $\mathcal{G}(x,-\dot{x}) = j_m^+(x,-\dot{x})$. In this subsection, we desire to present a conjecture related to (10.11). In general, the computation of the quasi-potential (4.10) for PDMPs not having invariant measure of the form (3.10) is non trivial. We will discuss a specific example of this type in the next subsection. A possible purely variational approach to this problem is as follows. Suppose we can decompose the dynamic LD rate density as in (10.11), where now $\mathcal{G}(x,\dot{x})$ is a nonnegative function, which is zero only when $\dot{x} = G(x)$, with G a vector field having x_* has the unique global attractive equilibrium point. Then from the general arguments in Sect. 4 we have that W coincides in fact with the quasi-potential Q. Inspired by the structure of the rate functionals for PDMPs we can search for $\mathcal{G}$ having a specific form. For simplicity we discuss only the case of computable rates of the form (3.39) when the chemical part of the generator is reversible for any x and consequently j is given by (3.33). In this case given a positive $\psi(\sigma,x)$ we can search for a $\mathcal{G}$ of the form

$$\mathcal{G}(x,\dot{x}) = \sum_\sigma \widetilde{\gamma}(\sigma|x)\chi_\sigma^{-F}(\dot{x}) - \sum_{(\sigma,\sigma')\in W}\sqrt{\frac{\mu(\sigma|x)}{\mu(\sigma'|x)}}r(\sigma,\sigma'|x)\sqrt{\chi_\sigma^{-F}(\dot{x})}\sqrt{\chi_{\sigma'}^{-F}(\dot{x})},$$

where

$$\widetilde{\gamma}(\sigma|x) := \sum_{\sigma'} r(\sigma',\sigma|x)\frac{\psi(\sigma',x)}{\psi(\sigma,x)}.$$

To verify (10.11) we need to find a function W such that for any x, $\dot{x}$ it holds

$$\sum_\sigma (\gamma(\sigma|x) - \widetilde{\gamma}(\sigma|x))\,\chi_\sigma^F(\dot{x}) = \nabla W\cdot\dot{x} = \sum_\sigma (\nabla W\cdot F_\sigma(x))\,\chi_\sigma^F(\dot{x}). \tag{10.12}$$

To derive the above condition we used $\chi_\sigma^F(\dot{x}) = \chi_\sigma^{-F}(-\dot{x})$. Condition (10.12) is verified if and only if for any $\sigma\in\Gamma$ and for any $x\in\Omega$ we have that $\gamma(\sigma|x) - \widetilde{\gamma}(\sigma|x)$ is the directional

derivative of W at x along the direction $F_\sigma(x)$. In this case the vector field G is given by

$$G(x) = -\frac{1}{Z(x)} \sum_\sigma \frac{\psi^2(\sigma, x)}{\mu(\sigma|x)} F_\sigma(x),$$

where $Z(x) := \sum_\sigma \frac{\psi^2(\sigma,x)}{\mu(\sigma|x)}$. If we can find the positive functions ψ in such a way that the above requirements are satisfied then the function W obtained in (10.12), appropriately normalized, coincides with the quasi-potential. In this case we obtain also that $\bar{F}^+$ in fact coincides with G. We do not discuss this issue here.

10.4 An Example

We now illustrate with an example the validity of the general results discussed in Sect. 10.2 and their consequences. We consider the 1D models of Sect. 3.8. The explicit formulas that we obtain will be useful in the discussion of the fluctuation theory for 1D PDMPs on the torus.

In this case the quasistationary measures for the direct and adjoint chemical generators can be easily computed and we have

$$\begin{cases} \bar{F}(x) = \frac{r(1,0|x)}{r(1,0|x)+r(0,1|x)} F_0(x) + \frac{r(0,1|x)}{r(1,0|x)+r(0,1|x)} F_1(x), \\ \bar{F}^+(x) = -\left(\frac{r(1,0|x)F_0^2(x)}{r(1,0|x)F_0^2(x)+r(0,1|x)F_1^2(x)} F_1(x) + \frac{r(0,1|x)F_1^2(x)}{r(1,0|x)F_0^2(x)+r(0,1|x)F_1^2(x)} F_0(x)\right). \end{cases} \tag{10.13}$$

Note that $x \in \Omega$ is an equilibrium point for $\bar{F}$ if and only if $r(1,0|x)F_0(x) + r(0,1|x)F_1(x) = 0$. The same equation characterizes the equilibrium points of $\bar{F}^+$, thus implying that $\bar{F}$ and $\bar{F}^+$ have the same equilibrium points in Ω. Moreover we have that both relations $\bar{F}(x) > 0$ and $\bar{F}^+(x) > 0$ holds if and only if $r(1,0|x)F_0(x) + r(0,1|x)F_1(x) > 0$, so that also the stability of the equilibrium points for both vector fields is the same. We point out that, since $F_0(a) = F_1(b) = 0$, the adjoint vector field $\bar{F}^+$ has two additional equilibrium points at the boundary $\partial\Omega = \{a, b\}$, which are necessary unstable.

Note that there are models such that the vector field $\bar{F}$ has many stable equilibrium points. In this case the definition of the quasi-potential $Q(x)$ in (4.10) has to be modified considering separately the different basin of attraction. We do not discuss this possibility.

For a vector $\dot{x} \in \mathcal{C}\{F_0(x), F_1(x)\}$ we have that

$$\chi_0^F(\dot{x}) = \frac{F_1(x) - \dot{x}}{F_1(x) - F_0(x)}, \qquad \chi_1^F(\dot{x}) = \frac{\dot{x} - F_0(x)}{F_1(x) - F_0(x)}.$$

Using the results of Sect. 3.4 (see (3.34) and (3.39)), we get

$$j_m(x, \dot{x}) = \left(\sqrt{\frac{r(0,1|x)(F_1(x) - \dot{x})}{F_1(x) - F_0(x)}} - \sqrt{\frac{r(1,0|x)(\dot{x} - F_0(x))}{F_1(x) - F_0(x)}} \right)^2 \tag{10.14}$$

for all $x \in \Omega$ and $\dot{x} \in \mathcal{C}(F_0(x), F_1(x))$. Since similarly to (3.34) + (3.39) it holds

$$j_m^+(x, \dot{x}) = \left(\sqrt{\chi_0^{-F}(\dot{x}) r^+(0,1|x)} - \sqrt{\chi_1^{-F}(\dot{x}) r^+(1,0|x)} \right)^2, \tag{10.15}$$

observing that $\chi^{-F}(\dot{x}) = \chi^{F}(-\dot{x})$ for all $\dot{x} \in \mathcal{C}(-F_0(x), -F_1(x))$ we conclude that

$$j_m^+(x,\dot{x}) = \left(\sqrt{\frac{r(1,0|x)|F_0(x)|(F_1(x)+\dot{x})}{F_1(x)(F_1(x)-F_0(x))}} - \sqrt{\frac{r(0,1|x)F_1(x)(-\dot{x}-F_0(x))}{|F_0(x)|(F_1(x)-F_0(x))}} \right)^2 \tag{10.16}$$

for all $x \in \Omega$ and $\dot{x} \in \mathcal{C}(-F_0(x), -F_1(x))$. The validity of the FD relation (4.9) can now be checked directly recalling that in this case

$$\nabla S(x) = \frac{r(0,1|x)}{F_0(x)} + \frac{r(1,0|x)}{F_1(x)}. \tag{10.17}$$

Also the validity of the H-Theorem can be checked directly, we have in fact

$$\nabla S(x) \cdot \bar{F}(x) = -\frac{(r(1,0|x)\sqrt{\frac{|F_0(x)|}{F_1(x)}} + r(0,1|x)\sqrt{\frac{F_1(x)}{|F_0(x)|}})^2}{r(0,1|x)+r(1,0|x)},$$

and

$$\nabla S(x) \cdot \bar{F}^+(x) = -\frac{(r(0,1|x)F_1(x) + r(1,0|x)F_0(x))^2}{r(0,1|x)F_1^2(x) + r(1,0|x)F_0^2(x)},$$

whose non-positivity is immediate. Finally we can also explicitly compute the Hamiltonian

$$\mathcal{H}(x,p) = \sup_{y \in \mathcal{C}\{F_0(x), F_1(x)\}} \big[py - j_m(x,y)\big],$$

and check that (10.17) is its maximal solution. The solution to this variational problem is given by

$$\mathcal{H}(x,p) = p\dot{x}(x,p) - j_m(x,\dot{x}(x,p)),$$

where

$$\dot{x}(x,p) = \frac{1}{2}(F_1(x)+F_0(x)) + \frac{1}{2}(F_1(x)-F_0(x))\frac{\varepsilon(x,p)}{\sqrt{\varepsilon(x,p)^2+4}}$$

and

$$\epsilon(x,p) = \left((F_1(x)-F_0(x))\frac{p}{\sqrt{r(0,1|x)r(1,0)|x)}} + \frac{r(0,1|x)-r(1,0|x)}{\sqrt{r(1,0|x)r(0,1|x)}} \right).$$

It can be checked that the Hamilton–Jacobi equation $\mathcal{H}(x, \nabla S) = 0$ holds. We refer the reader to [21] for these computations and for more details on the one dimensional models on a bounded domain.

11 Fluctuation Theory for the 1D Torus with Two Chemical States

11.1 Time Reversed Process

From the explicit expression (3.54) of the stationary measure ρ_λ, we can compute the jump rates of the time-reversed process:

$$\begin{cases} r^+(0,1|x) = r(1,0|x)\frac{F_0(x)}{F_1(x)}\frac{\int_x^{x+1}[\frac{r(0,1|y)}{F_0(y)}e^{\lambda S(y)}]dy}{\int_x^{x+1}[\frac{r(1,0|y)}{F_1(y)}e^{\lambda S(y)}]dy}, \\ r^+(1,0|x) = r(0,1|x)\frac{F_1(x)}{F_0(x)}\frac{\int_x^{x+1}[\frac{r(1,0|y)}{F_1(y)}e^{\lambda S(y)}]dy}{\int_x^{x+1}[\frac{r(0,1|y)}{F_0(y)}e^{\lambda S(y)}]dy}. \end{cases} \tag{11.1}$$

Note that in general, the above rates are λ-dependent. They are λ-independent when the equilibrium condition (3.55) holds. In this case from (7.5) we conclude that

$$\begin{cases} r^+(0,1|x) = -r(1,0|x)\frac{F_0(x)}{F_1(x)}, \\ r^+(1,0|x) = -r(0,1|x)\frac{F_1(x)}{F_0(x)}. \end{cases} \tag{11.2}$$

Remember that in this case the vector fields have opposite sign so that the above rates are positive.

When condition (3.55) is violated then rates (11.1) can be λ-dependent. In this case we can study the asymptotic behavior of ρ_λ as $\lambda \uparrow \infty$ using some classical results (see for example [7]) that we recall for the reader's convenience. Let f and $\mathcal{S}$ be smooth real functions on the interval $[a,b]$. If $\mathcal{S}(y) < \mathcal{S}(a)$ for any $y \in (a,b]$ and $\mathcal{S}'(a) < 0$, then it holds

$$\lim_{\lambda\to\infty} \frac{\int_a^b f(y)e^{\lambda\mathcal{S}(y)}dy}{e^{\lambda\mathcal{S}(a)}\lambda^{-1}} = -\frac{f(a)}{\mathcal{S}'(a)}. \tag{11.3}$$

If there exists $y^* \in (a,b)$ such that $\mathcal{S}(y) < \mathcal{S}(y^*)$ for any $y \in [a,b]$ different from y^* and moreover $\mathcal{S}''(y^*) < 0$, then it holds

$$\lim_{\lambda\to\infty} \frac{\int_a^b f(y)e^{\lambda\mathcal{S}(y)}dy}{e^{\lambda\mathcal{S}(y^*)}\lambda^{-\frac{1}{2}}} = f(y^*)\sqrt{-\frac{2\pi}{\mathcal{S}''(y^*)}}. \tag{11.4}$$

Let us suppose that the function S defined by (3.53) is regular and that for any $x \geq 0$ the maximum of the function S in the closed interval $[x, x+1]$ is assumed in at most one point of the open interval $(x, x+1)$. This fact is guaranteed if for example $S(z_1) \neq S(z_2)$ for any pair of critical points z_1 and z_2 (i.e. such that $S'(z_1) = S'(z_2) = 0$). If F_0 and F_1 have the same sign, this is always true since the function S is strictly increasing or strictly decreasing. Moreover, note that in general x and $x+1$ cannot be both maximum points of the function S on $[x, x+1]$, since due to (7.4) the identity $S(x) = S(x+1)$ would imply the periodicity of S. In addition to the previous assumptions, we require that $S''(y) < 0$ if the maximum of S on the interval $[x, x+1]$ is reached at the internal point y. We point out that by the methods discussed in [7] more general cases can be considered.

Given $x \geq 0$, we define $y(x) \in [x, x+1]$ as follows. We require that $S(y(x)) = \max_{y\in[x,x+1]} S(y)$. If the maximum point in $[x, x+1]$ is unique, then $y(x)$ is univocally determined from the above condition. The only other possibility is that there is a maximum

point at the boundary and a maximum point in the interior of the interval $[x, x+1]$. In this case, we define $y(x)$ as the unique maximum point inside $(x, x+1)$.

From the results (11.3) and (11.4) it is easy to derive that

$$\begin{cases} r^+(0,1|x) = r(1,0|x)\frac{F_0(x)}{F_1(x)}\frac{r(0,1|y(x))F_1(y(x))}{r(1,0|y(x))F_0(y(x))} + o(1), \\ r^+(1,0|x) = r(0,1|x)\frac{F_1(x)}{F_0(x)}\frac{r(1,0|y(x))F_0(y(x))}{r(0,1|y(x))F_1(y(x))} + o(1), \end{cases} \tag{11.5}$$

where by $o(1)$ we indicate a term which is infinitesimal as λ diverges. Note that the first terms in the r.h.s. of (11.5) are λ-independent.

Note that if $y(x) \in \{x, x+1\}$, by the periodicity of $F_\sigma(x)$ and $r(\sigma, \sigma'|x)$ formula (11.5) reduces to

$$\begin{cases} r^+(0,1|x) = r(0,1|x) + o(1), \\ r^+(1,0|x) = r(1,0|x) + o(1). \end{cases} \tag{11.6}$$

This is always true if the vector fields F_0 and F_1 have the same sign, since in this case the function S is monotone. On the other hand, if $y(x) \in (x, x+1)$, then necessarily it holds

$$\nabla S(y(x)) = \frac{r(0,1|y(x))}{F_0(y(x))} + \frac{r(1,0|y(x))}{F_1(y(x))} = 0, \tag{11.7}$$

and (11.5) reduces to

$$\begin{cases} r^+(0,1|x) = -r(1,0|x)\frac{F_0(x)}{F_1(x)} + o(1), \\ r^+(1,0|x) = -r(0,1|x)\frac{F_1(x)}{F_0(x)} + o(1). \end{cases} \tag{11.8}$$

11.2 Fluctuation Theory

We discuss now the fluctuation theory for our PDMP on the torus, proving between other point (iii) of Proposition 3.13.

If the equilibrium condition (3.55) holds, then we know that the invariant measure has the form (3.10) and therefore the validity of relation (4.9) follows from the general argument of Sect. 10.2. We consider here the general case, without assuming (3.55).

Starting from the exact expression (3.54) of the invariant measure we can derive the LD functional of $\hat{\rho}_\lambda$. We have that

$$\begin{aligned} \lim_{\lambda\to\infty} \lambda^{-1} \log \hat{\rho}_\lambda(x) &= \lim_{\lambda\to\infty} \lambda^{-1} \log\big(\rho_\lambda(x,0) + \rho_\lambda(x,1)\big) \\ &= \sup_{y\in[x,x+1]} \big(S(y) - S(x)\big) + c =: -W(x), \end{aligned} \tag{11.9}$$

where c is an appropriate additive constant related to the normalization factor $k = k(\lambda)$ in (3.54). Formula (11.9) follows from the fact that for arbitrary $a(\lambda)$ and $b(\lambda)$ it holds

$$\lim_{\lambda\to+\infty} \lambda^{-1} \log\big(a(\lambda) + b(\lambda)\big) = \max\Big\{ \lim_{\lambda\to+\infty} \lambda^{-1} \log a(\lambda), \lim_{\lambda\to+\infty} \lambda^{-1} \log b(\lambda) \Big\},$$

and from the Laplace theorem [11]. Note that the function W defined in (11.9), due to the validity of (7.4), satisfy the periodicity condition $W(x) = W(x+1)$ and consequently it can be interpreted as a function on the torus $\Omega = \mathbb{R}/\mathbb{Z}$. The constant c appearing in (11.9)

can be computed observing that, since $\int_\Omega \hat\rho_\lambda(x)dx = 1$, the Laplace theorem implies that $\inf_{x\in[0,1]} W(x) = 0$. Therefore, it must be

$$c = -\sup_{x\in[0,1]} \sup_{y\in[x,x+1]} \big(S(y) - S(x)\big).$$

The above function W is the LD functional for the measure $\hat\rho_\lambda$. If the function S is periodic, then it is simple to check that $W(x) = S(x) - \min_{y\in[0,1]} S(y)$. In the general case, W is a nonnegative function that can be flat on subregions of Ω.

Let us now verify the validity of the FD relation (4.9), with $\mathcal{L}(x,\dot x) = j_m(x,\dot x)$, $\mathcal{L}^+(x,\dot x) = j_m^+(x,\dot x)$ and $V = W$. For simplicity, we assume the same conditions discussed after (11.4). The function $y(x)$ is defined as in the paragraph below (11.4). First we need to compute ∇W. We have that in the points where W is differentiable it holds

$$\nabla W(x) = \nabla S(x) - \nabla S(y(x))\nabla y(x). \tag{11.10}$$

When $y(x) \in (x, x+1)$ we have that (11.10) becomes

$$\nabla W(x) = \nabla S(x), \tag{11.11}$$

due to the fact that $\nabla S(y(x)) = 0$. When $y(x) \in \{x, x+1\}$ then (11.10) becomes

$$\nabla W(x) = 0, \tag{11.12}$$

due to the fact that $\nabla S(x) = \nabla S(x+1)$ and $\nabla y(x) = 1$. Note that this second alternative holds for any x if the vector fields F_0 and F_1 have the same sign so that in this case W is identically zero.

The Lagrangian $j_m(x,\dot x)$ can be computed by means of (3.34) and (3.39), getting that its expression coincides with (10.14). The Lagrangian $j_m^+(x,\dot x)$ can be computed by adapting the arguments in [12]. We get that its expression can be obtained from (10.15) where instead of the λ-dependent rates r^+ we have to use their asymptotic limit value given by (11.5). We obtain for all $x \in \Omega$ and $\dot x \in \mathcal{C}(-F_0(x), -F_1(x))$

$$j_m^+(x,\dot x) = \left(\sqrt{\frac{r(1,0|x)B(x)(F_1(x)+\dot x)}{F_1(x)-F_0(x)}} - \sqrt{\frac{r(0,1|x)(\dot x + F_0(x))}{B(x)(F_0(x)-F_1(x))}}\right)^2, \tag{11.13}$$

where $B(x) := \frac{F_0(x)}{F_1(x)}\frac{r(0,1|y(x))F_1(y(x))}{r(1,0|y(x))F_0(y(x))}$.

We can now compute $j_m(x,\dot x) - j_m^+(x,-\dot x)$ obtaining

$$\dot x \frac{[r(1,0|x)(1+B(x)) - r(0,1|x)(1+B^{-1}(x))]}{F_1(x)-F_0(x)} + \frac{r(0,1|x)(F_1(x)+F_0(x)B^{-1}(x)) - r(1,0|x)(F_0(x)+F_1(x)B(x))}{F_1(x)-F_0(x)}. \tag{11.14}$$

The validity of the FD relation for points x where W is differentiable follows now directly from the fact that if $y(x) \in \{x, x+1\}$ then $B(x) = \frac{r(0,1|x)}{r(1,0|x)}$, while if $y(x) \in (x, x+1)$ then $B(x) = -\frac{F_0(x)}{F_1(x)}$ (recall (11.7)). In particular the second term in (11.14) is identically zero.

Finally we point out that in the general case the quasi-potential cannot be defined directly as in (4.10). Indeed, the hypothesis of existence, uniqueness and global attractiveness of the equilibrium point of $\bar F$ could be violated. We cannot then identify directly W with the quasi-potential.

12 A Gallavotti–Cohen-Type Symmetry: Proof of Proposition 3.15

Assuming (3.63) and (3.64), it is easy to compute (3.60) using standard methods for jump processes (see for example [16]). One gets up to boundary terms

$$W_T = \frac{1}{2T} \sum_i \{H(\sigma(\tau_i^-), x(\tau_i)) - H(\sigma(\tau_i), x(\tau_i))\}. \tag{12.1}$$

The boundary terms are due to the fact that in (3.60) we are considering stationary measures. In the case of compact phase space $\Omega \times \Gamma$ they are negligible in the limit of diverging T. In the above formula (12.1) the sum is over the jump times τ_i of $\{\sigma(t)\}_{t\in[-T,T]}$ and we denote the left limit as $\sigma(t^-) := \lim_{\Delta\downarrow 0} \sigma(t-\Delta)$. Since for any trajectory it holds

$$H(\sigma(T), x(T)) - H(\sigma(-T), x(-T)) = \int_{-T}^{T} \nabla H(\sigma(s), x(s)) \cdot \dot{x}(s) ds + \sum_i \{H(\sigma(\tau_i), x(\tau_i)) - H(\sigma(\tau_i^-), x(\tau_i))\},$$

in the case of bounded energy functions H we can derive from (12.1) the first identity in (3.65). The second identity follows from the relation $\dot{x}(t) = F_\sigma(x(t))$.

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Appendix A: An Example of 1D PDMP with Singular Features

We consider the 1D PDMP such that $\Omega = (0,1)$, $\Gamma = \{0,1\}$, $F_0(x) = -1$, $F_1(x) = 1$, $r(0,1|x) = 1/x$, $r(1,0|x) = 1/(1-x)$. This PDMP satisfies all our assumptions. Indeed, $L_c[x]$ has a unique invariant measure $\mu(\cdot|x)$ given by (2.10), while the mechanical confinement in Ω is implied by (2.16). Moreover, we claim that the number of jumps in a finite interval is finite a.s. due to (2.12) (note that (2.11) is violated). To this aim suppose by contradiction that the family of jump times τ_k is a sequence converging to some $\tau_* < \infty$. Before time τ_* the mechanical state must be eventually in $(0, 3/4]$ or in $[1/4, 1)$ (otherwise it should evolve with arbitrarily large velocity). Let us consider for example the first case. Then, the system must be infinite times in the chemical state $\sigma = 1$ and, once it jumps into $\sigma = 1$, it remains in this chemical state for a random time typically of order one. This is in contradiction with the fact that $\tau_{k+1} - \tau_k$ converges to zero.

Let us now take $\lambda = 1$ and show another special feature of our simple PDMP: the regular function $f(x,\sigma) = \sigma$ does not belong to the domain of the classical (i.e. not extended) Markov generator. To this aim, it is enough to show that starting at $(x_0, 0)$ it holds

$$\limsup_{t\downarrow 0} \sup_{x_0\in(0,1)} t^{-1} \mathbb{P}^1_{x_0,0}(\sigma_t = 1) = \infty. \tag{A.1}$$

To this aim we observe that $\mathbb{P}^1_{x_0,0}(\sigma_t = 1)$ can be bounded from below by the probability that the process makes only one chemical jump in the time interval $[0,t]$ and, as the reader can

compute, this equals

$$x_0^{-1}\int_0^{x_0}\frac{1-x_0+2s-t}{1-x_0+s}ds \geq x_0^{-1}\int_0^{x_0}(1-x_0+2s-t)ds = 1-t$$

for $x_0 < t$. This observation implies (A.1).

Finally, we come back to the observations about the existence of the invariant measure collected in Sect. 3.1. We take (x_0, σ_0) as initial state and write ν_t for the distribution at time t. By compactness arguments, we know that the sequence of probability measures $\tilde{\nu}_t := t^{-1}\int_0^t \nu_s ds$ admits a subsequence weakly converging to a probability measure ν_* on the closure $\bar{\Omega}\times\Gamma$. Let us show that ν_* has support on $\Omega\times\Gamma$, thus implying that ν_* describes a steady state of the PDMP. Consider the interval $I_\varepsilon = (0,\varepsilon)$, $\varepsilon < 1$. When the mechanical state enters in the interval I_ε, the chemical state of the system must be 0. After a time of order $O(\varepsilon)$ the system jumps into the chemical state 1 keeping this value for a time $O(1)$. During this interval $x(t)$ moves on the right with constant velocity, spending at most $O(\varepsilon)$ time inside I_ε. Hence, in a time interval of order $O(1)$ the mechanical state is in I_ε for at most $O(\varepsilon)$ time. This implies that $\tilde{\nu}_t(I_\varepsilon\times\Gamma) \leq c\varepsilon$, for each t. It is simple to conclude that the limiting measure ν_* must give zero weight to $\{0\}\times\Gamma$. The same conclusion holds for the set $\{1\}\times\Gamma$, thus proving that $\nu_*(\{0,1\}\times\Gamma) = 0$.

Appendix B: An Example of 1D PDMP with a Finite Number of Jumps

We take here $\Omega = [0,1]$ and $\Gamma = \{0,1\}$. The vector fields are given by $F_0(x) = -x$ and $F_1(x) = 1-x$ and the jump rates by $r(0,1|x) = x$ and $r(1,0|x) = 1-x$.

Let us consider the process with initial condition given by $(x^*, 0)$, with x^* a generic element of Ω. We can easily compute the probability that there are no chemical jumps

$$\mathbb{P}^{\lambda}_{(x^*,0)}\left(\sigma(t) = 0,\ \forall t\in\mathbb{R}^+\right) = e^{-\lambda x^*\int_0^{+\infty}e^{-t}dt} = e^{-\lambda x^*} \geq e^{-\lambda}. \tag{B.1}$$

A similar estimate can be obtained also if we consider the process starting from the chemical state 1. The above result (B.1) states that every time the process jumps into a new chemical state σ, with positive probability uniformly bounded from below by $e^{-\lambda}$ it will never more change its chemical state and consequently the mechanical variable will definitely evolve according to the ODE $\dot{x} = F_\sigma(x)$. As a consequence it is easy to derive that this PDMP has a.s. a finite number of jumps and that the invariant measures are of the form

$$c\delta(x)\delta_{\sigma,0} + (1-c)\delta(x-1)\delta_{\sigma,1}, \quad c\in[0,1].$$

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