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LJLL

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University Department **Laboratoire Jacques-Louis Lions**

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**Long-time behavior of some Markov
processes, and application to
stochastic algorithms**

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COLOPHON

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Mots clés : probabilités, calcul stochastique, méthodes de couplage, comportement en temps long de processus de markov, inégalité de poincaré, algorithme stochastique, hypocoercivité.

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You can't be what you can't see.

Marian Wright Edelman

LONG-TIME BEHAVIOR OF SOME MARKOV PROCESSES, AND APPLICATION TO STOCHASTIC ALGORITHMS**Abstract**

This thesis is devoted to the study of the long-time behavior of some Markov processes arising in stochastic algorithms. These algorithms are variations of Monte Carlo methods, which constitute a class of techniques for sampling probability measures based on Markov processes. The thesis is structured into three parts, each addressing a different type of algorithm:

1. Chapters 2 and 3 focus on sampling Gibbs measures using two distinct kinetic processes.
2. Chapter 4 explores non-convex and high-dimensional optimization through simulated annealing, while Chapter 5 investigates optimization using a switched process.
3. Chapters 6, 7, and 8 delve into sampling quasi-stationary distributions based on the Fleming-Viot process, a Moran-type particle system.

The motivation for these algorithms, and thus much of the research conducted for this thesis, stems from molecular dynamics and statistics applications. By applying coupling and partial differential equation methods, we aim to establish convergence guarantees for these algorithms.

Keywords: probability theory, stochastic calculus, coupling methods, long time behavior of markov processes, poincaré inequality, stochastic algorithm, hypocoercivity.

Résumé

Cette thèse est consacrée à l'étude du comportement à long terme de certains processus de Markov apparaissant dans les algorithmes stochastiques. Ces algorithmes sont des variations autour des méthodes de Monte Carlo, qui constituent une classe de techniques d'échantillonnage de mesures de probabilité basées sur des processus de Markov. La thèse est structurée en trois parties, chacune traitant d'un type d'algorithme différent :

1. Les chapitres 2 et 3 portent sur l'échantillonnage des mesures de Gibbs à l'aide de deux processus cinétiques différents.
2. Le chapitre 4 traite de l'optimisation non-convexe en grande dimension par recuit simulé, tandis que le chapitre 5 étudie l'optimisation à l'aide d'un processus commuté.
3. Les chapitres 6, 7 et 8 traitent de l'échantillonnage de mesures quasi-stationnaires basé sur le processus de Fleming-Viot, un système de particules de type Moran.

La motivation pour ces algorithmes, et donc pour la plupart des recherches menées dans le cadre de cette thèse, provient de dynamique moléculaire et d'applications en statistiques. En appliquant des méthodes de couplage et d'équations aux dérivées partielles, nous établirons des garanties de convergence pour ces algorithmes.

Mots clés : probabilités, calcul stochastique, méthodes de couplage, comportement en temps long de processus de markov, inégalité de poincaré, algorithme stochastique, hypocoercivité.

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En fait, la réponse, c'est qu'il n'y a plus de pappouths...

Chapter 1

Introduction

Outline of the current chapter

1.1 Markov processes: definitions and basic properties for Monte-Carlo purposes	2
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The topic of this thesis is the application of the study of the long time behavior of Markov processes to the analysis of stochastic algorithms, at the intersection of PDE theory, probability, and applied mathematics. These algorithms are variations of Monte Carlo methods, which constitute a class of techniques for probability measure sampling based on Markov processes. In addition to sampling, stochastic algorithms can also be employed to model physical systems, or in non-convex and high-dimensional optimization problems that cannot be efficiently solved using deterministic algorithms. They offer a compelling compromise between obtaining high-quality results and reducing computation time. The theoretical study of the underlying Markov processes provides essential guarantees of convergence for such algorithms, which are of paramount importance.

The motivation for most of the projects undertaken during the preparation of this thesis stems from molecular dynamics and statistics, yet it can be applied to a broad spectrum of fields, including population dynamics, finance, and biology. Beyond their practical applications, the study of such algorithms gives rise to intriguing theoretical questions in the domain of coupling methods, hypocoercivity, and metastability. Since this thesis focuses on Markov processes in metric spaces (while non-Markovian processes are also of interest for stochastic algorithms, they are not the primary focus of this thesis), which constitute a particular class of stochastic processes, we will first introduce them in Section 1.1. This introduction will then be divided into two parts. Section 1.2 will present two families of methods for the study of the long time behavior of Markov

processes. The final Section 1.3 will introduce some stochastic algorithms, as well as the various contributions of this thesis.

1.1 Markov processes: definitions and basic properties for Monte-Carlo purposes

The goal of Monte Carlo Markov Chains (MCMC) is to sample from a specified probability measure μ using Markov chains or processes. To illustrate how this operates, let's introduce some notations and define Markov processes. For a more in-depth introduction to Markov processes, refer to [58].

Notations: Throughout this introduction, (Ω, \mathcal{F}) will denote a measurable space, and (E, \mathbf{d}) a metric space referred to as the state space. We use \mathcal{B} for the Borel σ -algebra on E . As our focus is on dynamics within a state space, we denote by $\mathcal{C}(\mathbb{R}_+, E)$ (resp. $\mathcal{D}(\mathbb{R}_+, E)$) the set of continuous (resp., right-continuous with left limits at all points, or *cadlag*) functions from \mathbb{R}_+ to E . These two sets are equipped with the product σ -algebra. Let $\mathcal{M}^1(E)$ denotes the set of probability measures on any set E , and if $\mu \in \mathcal{M}^1(E)$ is a measure on E , and $h : E \rightarrow \mathbb{R}$, denote

$$\mu(h) = \int_E h d\mu.$$

Given $d \in \mathbb{N}$, $\mathcal{M}_d(\mathbb{R})$ denote the set of real valued matrix of size $d \times d$.

Definition 1.1.1. We call a continuous (resp. cadlag) Markov process a random variable

$$X : \Omega \rightarrow \mathcal{C}(\mathbb{R}_+, E), \quad \text{resp. } X : \Omega \rightarrow \mathcal{D}(\mathbb{R}_+, E),$$

with a family of probability measures $(\mathbb{P}_x)_{x \in E}$ on (E, \mathcal{B}) such that:

- $\mathbb{P}_x(X_0 = x) = 1$.
- For all $x \in E$, $0 \leq s_1 \leq \dots \leq s_m \leq t \leq t_1 \leq \dots \leq t_n$, $(A_i)_{1 \leq i \leq m} \in \mathcal{B}$, $(B_i)_{1 \leq i \leq n} \in \mathcal{B}$:

$$\begin{aligned} & \mathbb{P}_x(X_{s_1} \in A_1, \dots, X_{s_m} \in A_m, X_{t_1} \in B_1, \dots, X_{t_n} \in B_n | X_t) \\ &= \mathbb{P}_x(X_{s_1} \in A_1, \dots, X_{s_m} \in A_m | X_t) \mathbb{P}_x(X_{t_1} \in B_1, \dots, X_{t_n} \in B_n | X_t). \end{aligned}$$

Informally, a Markov process X is a random function from \mathbb{R}_+ to E , such that, for all $t \geq 0$, knowing X_t , the future is independent of the past. In mathematical terms, it is equivalent to

$$\forall A \in \sigma(X_s, s \geq t), \forall B \in \sigma(X_s, s \leq t), \mathbb{P}(AB | X_t) = \mathbb{P}(A | X_t) \mathbb{P}(B | X_t).$$

The probability \mathbb{P}_x corresponds to the Markov process with initial condition x . Additionally, for any probability measure $\nu \in \mathcal{M}^1(E)$, a process with initial condition ν can be defined by

$$\mathbb{P}_\nu = \int_E \mathbb{P}_x \nu(dx).$$

We denote \mathbb{E}_ν the expectation under \mathbb{P}_ν and simply \mathbb{E}_x when $\nu = \delta_x$. In all of this thesis, a Markov process will be denoted either X or Z . Let's start with a few examples that will arise at some point in this thesis. We will not delve into the construction of such processes or the proof of their Markovian nature, as these may be intricate subjects. Also, note that E is not necessarily complete or separable, as we will see below.

- The simplest Markov processes are jump processes on graphs. Let E be a (finite or countable) set, endowed with the trivial topology, namely $\mathbf{d}(x, y) = \mathbb{1}_{x \neq y}$. For all $x, y \in E$, let $q(x, y) \geq 0$ be a jump rate. A Markov process X on E can be defined as follows: given some initial condition $x \in E$, let J_y be an exponential random variable with parameter $q(x, y)$. Write

$$J^1 = \min_{y \in E} J_y, \quad Y^1 = \arg \min_{y \in E} J_y.$$

Then X jumps from a state x to a state y at rate $q(x, y)$ in the sense that $X_t = x$ for all $t < J^1$ and $X_{J^1} = Y^1$. This defines X until J^1 , and an induction argument then extends X_t for all $t \geq 0$. Such processes will appear exclusively in Chapter 8.

- (Itô-)Diffusion processes on \mathbb{R}^d : this is most important example for this thesis, appearing in Chapters 2,4,6 and 7. They can be defined as the solution to the Itô equation:

$$dZ_t = b(Z_t)dt + \sigma(Z_t)dB_t, \quad (1.1)$$

where B is a Brownian motion, $b : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is the drift, and $\sigma : \mathbb{R}^d \rightarrow \mathcal{M}_d(\mathbb{R})$ is the diffusion coefficient. They are continuous Markov process, see [154]. While they can be defined more generally, this definition is sufficient for our purpose and encompasses the two most crucial examples for this thesis: the overdamped and kinetic Langevin processes (see Section 1.2 and 1.3).

- Switched diffusion process: fix a family of drifts (b_i) and diffusions (σ_i) , $1 \leq i \leq N$, and a Markov chain I on the set $\llbracket 1, N \rrbracket$. Then we say that Z is a switched diffusion if it solves:

$$dZ_t = b_{I_t}(Z_t)dt + \sigma_{I_t}(Z_t)dB_t.$$

Z here is not a Markov process, but (Z, I) is. This represents a less classical class of Markov processes and will be discussed in Chapter 5.

- Piecewise deterministic Markov process (PDMP): fix some flow φ_t on a set E , jump rate $\lambda : E \rightarrow \mathbb{R}_+$, and jump kernel $Q(x) : E \rightarrow \mathcal{M}^1(E)$. Then, X is a PDMP if, by defining the random times T_n by

$$T_{n+1} = \inf \left\{ t \geq T_n, \int_{T_n}^t \lambda(X_s)ds \geq E_n \right\},$$

where $(E_n)_{n \in \mathbb{N}}$ is a family of independent exponential random variable of parameter 1, we have that for all $n \in \mathbb{N}$:

$$X_t = \varphi_{t-T_n}(X_{T_n}), \quad \forall t \in [T_n, T_{n+1}[, \quad X_{T_n} \sim Q(X_{T_n-}).$$

The process X is deterministic between random times, at which it jumps randomly to another location. While such processes were more recently analyzed for sampling purposes and may not directly appear in the thesis, a mixture between PDMP and diffusion processes will be studied in Chapter 3.

For a given Markov process (X_t) , we define its semi-group $(P_t)_{t \geq 0}$ by:

$$P_t f(x) = \mathbb{E}_x(f(X_t)),$$

for any $f : E \rightarrow \mathbb{R}$ bounded and measurable. The process is completely characterized by its semi-group, making it a central object of study. The semi-group also acts on the set of probability

measures $\mathcal{M}^1(E)$ as follows:

$$\int f d(\nu P_t) = \int P_t f d\nu,$$

for any $\nu \in \mathcal{M}^1(E)$. By the definition of the semi-group, νP_t is the law of X_t under \mathbb{P}_ν .

Definition 1.1.2. A measure μ is said to be an invariant (or stationary) measure for the Markov process X if for all $t \geq 0$

$$\mu P_t = \mu.$$

There may exist no, one, or an infinite number of invariant measures. The goal of MCMC is, given a target distribution μ , to design a Markov process X such that μ is its only invariant measure, and X is ergodic, in one of the following senses:

$$\frac{1}{t} \int_0^t \delta_{X_s} ds \xrightarrow[t \rightarrow \infty]{} \mu, \text{ weakly, almost surely,} \quad (1.2)$$

or

$$\mathcal{L}aw(X_t) \xrightarrow[t \rightarrow \infty]{} \mu, \text{ weakly.} \quad (1.3)$$

In these cases, the invariant measure describes the behavior of the process as time goes to infinity. Reciprocally, the simulation of X_t (or of a trajectory $(X_s)_{0 \leq s \leq t}$), for large time $t \geq 0$, yields an approximation of μ . Hence, the analysis of such convergences (under different possible norms) will be the main topic of this thesis.

A powerful tool to study the evolution of the law of a Markov process (and thus its long-time behavior) is its so-called generator (or equivalently the generator of its semi-group).

Definition 1.1.3. Let \mathcal{E} be a Banach space of functions from E to \mathbb{R} , endowed with some norm $\|\cdot\|_{\mathcal{E}}$. The generator of P_t and its domain $(L, \mathcal{D}(L))$ are defined by:

$$f \in \mathcal{D}(L), g = Lf \Leftrightarrow \lim_{t \rightarrow 0} \left\| \frac{P_t f - f}{t} - g \right\|_{\mathcal{E}} = 0.$$

The classical setting is to take \mathcal{E} as the set of bounded functions, endowed with the norm $\|g\|_{\infty} = \sup_E |g|$. In this case, for continuous or *cadlag* process, the generator completely determines the Markov process, and for all $f \in \mathcal{D}(L)$, we have the Kolmogorov equation:

$$\partial_t P_t f = L P_t f = P_t L f.$$

However, in many cases, P_t defines a semi-group in other Banach spaces, see Section 1.2.1. The minimal prerequisite on \mathcal{E} that we need here is that the set of smooth and compactly supported functions is a dense and stable by L subset of \mathcal{E} . The link between the semi-group and the generator (and resolvent) is the subject of the Hille-Yoshida theory, which lies outside the scope of this introduction (see [169]). Let's consider two examples:

- For a diffusion process (1.1) with Lipschitz continuous drift b and diffusion coefficient σ , we have $\mathcal{C}_c^2 \subset \mathcal{D}(L)$, where \mathcal{C}_c^k denotes the k times differentiable functions with compact support, and for $f \in \mathcal{C}^2$:

$$L f = b \cdot \nabla f + \frac{1}{2} \text{tr}(\sigma^t \nabla^2 f \sigma). \quad (1.4)$$

- For a PDMP, we have $\mathcal{C}_c^1 \subset \mathcal{D}(L)$, and for $f \in \mathcal{C}_c^1$:

$$L f(x) = \nabla \varphi(x) \cdot \nabla f(x) + \lambda(x) \int (f(y) - f(x)) Q(x, dy). \quad (1.5)$$

The choice of \mathcal{E} depends on the topology in which the long-term convergence of the semi-group occurs and must be specified. Various topologies, such as weak, Wasserstein, L^2 , H^k , etc., are available, and each require a different method to prove convergence. Depending on the process, understanding which given norm or method is best suited is a critical part of the study.

Now, the remainder of this introduction is divided into two sections: first, Section 1.2 will elaborate on the different methods used to study the convergence of Markov processes towards their invariant probability measure; then, Section 1.3 will introduce the algorithms to which we will apply the previously presented methods, as well as the contributions of this thesis.

1.2 Some methods to study the long-time behavior of Markov processes

Two families of methods are used in this PhD to study the long-time behavior of Markov processes, giving explicit rates in the convergences (1.3). The first family of methods, presented in Section 1.2.1, corresponds to PDE methods, used for the convergence in entropy, and in L^2 or Sobolev spaces. We will then delve into coupling methods in Section 1.2.2.

1.2.1 The PDE methods: Entropy, L^2 , H^k convergence

Link between PDE and Markov process

The first family of methods to study the long-time evolution of the law of a Markov process are based on PDEs, and the use of the generator. As seen previously, the semi-group P of a Markov process which admits a generator L satisfies for $f \in \mathcal{D}(L)$ the Kolmogorov (or Fokker-Planck) equation:

$$\partial_t P_t f = L P_t f = P_t L f. \quad (1.6)$$

Hence, if L is a differential operator, PDE methods can be employed to study the long-time behavior of the semi-group. There is also a dual formulation. Denote by l the Lebesgue measure, g_t the law of the Markov process, and L^* the dual of L in $L^2(l)$. Then, g is a weak solution to the PDE:

$$\partial_t g_t = L^* g_t. \quad (1.7)$$

This provides two points of view for the long-time convergence of a Markov process, depending on the context. For instance, equation (1.6) in Sobolev spaces, as done in Chapters 2 and 3, allows for estimates on $P_t f$, whereas equation (1.7) is better suited for the convergences in entropy (see below), or for the convergence in probability of the process studied in Chapter 4. In the remainder of this section, we will consider for simplicity diffusion processes with an invariant measure μ , but other kinds of processes (such as PDMPs giving rise to integro-differential equations) can be considered. In those cases, we will have $E = \mathbb{R}^d$. We will have a look at two families of diffusions:

Elliptic diffusions: An elliptic diffusion Z is a diffusion in E that solves

$$dZ_t = b(Z_t)dt + \sigma(Z_t)dB_t,$$

where the diffusion matrix satisfies

$$\sigma(x)^T \sigma(x) \geq cI_d,$$

where σ^T denote the adjoint of σ , for some $c > 0$ and all $x \in E$, in the sense that $\sigma^T \sigma - cI_d$ is everywhere positive definite. The generator of these diffusions has a regularizing effect, making

them suitable for PDE methods.

Proposition 1.2.1. *Suppose that $b \in L_{loc}^p$ for some $p > d + 2$, and $\sigma^T \sigma$ and its inverse are bounded. Then the law of Z_t admits a Hölder continuous density g_t with respect to the Lebesgue measure. If, in addition, we suppose b and σ Lipschitz continuous and C^p , then $g_t \in C^p$ and $P_t f \in C^p$.*

Proofs of those statements can be found in [18, 102]. The most important example of an elliptic diffusion in this thesis is given by the so-called overdamped Langevin process

$$dX_t = -\nabla U(X_t)dt + \sqrt{2\beta^{-1}}dB_t, \quad (1.8)$$

where $U : \mathbb{R}^d \rightarrow \mathbb{R}_+$ will usually be taken as a smooth function. This example is crucial as it has an explicit invariant measure given by:

$$\nu_\beta(dx) = Z_\beta^{-1} e^{-\beta U(x)} dx, \quad (1.9)$$

where Z_β is a normalisation constant.

Hypoelliptic diffusions: Since the law of an elliptic diffusion with smooth coefficients at a given time has a smooth density, it is natural to wonder which other kind of generator will generate a smooth density, and hence be adapted to PDE methods. This corresponds to the notion of a parabolic hypoelliptic operator.

Definition 1.2.1. *We say that L is parabolic hypoelliptic or that $\partial_t - L$ is hypoelliptic if for all $u : \mathbb{R}_+ \times \mathbb{R}^d \rightarrow \mathbb{R}$:*

$$\partial_t u - Lu \in C^\infty \implies u \in C^\infty.$$

If L is the generator of the semi-group P and is parabolic hypoelliptic, then Equation (1.6) would yield the smoothness of the semi-group. Let's now give a criterion for parabolic hypoellipticity. Given two vector fields A , and B on \mathbb{R}^d , we denote their Lie bracket as

$$[A, B](x) = DB(x)A(x) - DA(x)B(x),$$

where $(DA)_{i,j} = \partial_j A_i$.

Definition 1.2.2. *For a family of vector fields $(A_i)_{0 \leq i \leq m}$ on \mathbb{R}^d , define*

$$V_0 = \{A_i, i \in \llbracket 1, m \rrbracket\}, V_{k+1} = V_k \cup \{[B, A_i], B \in V_k, i \in \llbracket 0, m \rrbracket\}.$$

We say that $(A_i)_{0 \leq i \leq m}$ satisfies the Hörmander's bracket condition if

$$\text{Span}(\cup_{k=0}^\infty V_k) = \mathbb{R}^d.$$

Proposition 1.2.2 (Hörmander's theorem). *Identify any vector field with the corresponding differential form. Then if $L = A_0 + \sum_{i=1}^m A_i^2$, the $(A_i)_{0 \leq i \leq m}$ are bounded, and satisfy the Hörmander's bracket condition 1.2.2, then L is parabolic hypoelliptic.*

Proof of this theorem and variations can be found in [77, 28]. The most important example of a hypoelliptic process for this thesis is the Langevin one:

$$\begin{cases} dX_t = Y_t dt, \\ dY_t = -\nabla U(X_t)dt - \gamma Y_t dt + \sqrt{2\gamma\beta^{-1}}dB_t. \end{cases} \quad (1.10)$$

Here, $d = 2n$, $X \in \mathbb{R}^n$ and $Y \in \mathbb{R}^n$ are not Markov processes, but (X, Y) is, and the fact that the noise only acts on Y makes this process non-elliptic. Its generator is given by

$$L = y \cdot \nabla_x - \nabla \cdot \nabla_y - \gamma y \cdot \nabla_y + \gamma \beta^{-1} \Delta_y = A_0 + \gamma \beta^{-1} \sum_{i=1}^n \partial_{y_i}^2. \quad (1.11)$$

We have the commutator

$$[\partial_{y_i}, y \cdot \nabla_x] = -\partial_{x_i}.$$

Hence, when ∇U is bounded, (X, Y) is hypoelliptic, as

$$\text{Span}(V_0 \cup V_1) = \mathbb{R}^d.$$

Under mild assumptions, the Langevin process admits a unique invariant probability measure given by

$$\mu_\beta(dx, dy) = \frac{e^{-\beta H(x, y)}}{\sqrt{\pi \beta^{-1}}^d Z_\beta} dx dy, \quad (1.12)$$

where Z_β is the same normalisation constant as in (1.9). Many other hypoelliptic processes exist, such as the Generalised Langevin process [168, 132], or the chains of oscillators [125].

As we will see in Section 1.3, we are not only interested in the smoothness of the law or of $P_t f$, as it is not sufficient for the study of the stochastic algorithm. Since we study Markov processes that possess an invariant measure μ , we may introduce the following Hilbert spaces:

$$L^2(\mu) = \left\{ f : E \rightarrow \mathbb{R}, \text{ measurable, } \int_E f^2 d\mu < \infty \right\},$$

or

$$H^k(\mu) = \left\{ f \in L^2(\mu), \forall \alpha \in \mathbb{N}^d, |\alpha|_1 \leq k, \int_E |\partial^\alpha f|^2 d\mu < \infty \right\}.$$

for some $k \in \mathbb{N}$. Both are Hilbert spaces, with scalar product

$$\langle f, g \rangle_{L^2(\mu)} = \int_E f g d\mu, \quad \langle f, g \rangle_{H^k(\mu)} = \sum_{\alpha \in \mathbb{N}^d, |\alpha|_1 \leq k} \int_E \partial^\alpha f \partial^\alpha g d\mu.$$

In many cases, we are interested in L^∞ bounds on $P_t f$, and Sobolev embedding combined with convergence in $H^k(\mu)$, will be the means to achieve such bounds, as discussed in Chapters 2, 3 and 4. The remainder of Section 1.2.1 will be devoted to presenting the usual methods for proving convergence in such spaces, employing functional inequalities. We will first delve into the elliptic and reversible case before introducing Gamma calculus for the study of the long-time behavior of non-elliptic processes.

The elliptic/reversible case

In order to later justify our computations, we enforce the following

Assumption 1.2.1. \mathcal{E} is a Hilbert space, the Markov process X defines a semi-group $P_t : \mathcal{E} \rightarrow \mathcal{E}$, and there exists a dense subset $\mathcal{A} \subset \mathcal{E}$ such that $\mathcal{A} \subset \mathcal{D}(L)$ and $h \in \mathcal{A} \implies h^2 \in \mathcal{A}$.

In all the spaces \mathcal{E} we will consider, we will have that \mathcal{C}_c^∞ (the set of smooth functions with compact support) is a dense subset of \mathcal{E} . Moreover, in the case of diffusions with regular

coefficients, we have $\mathcal{C}_c^\infty \subset \mathcal{D}(L)$, and hence we may think of \mathcal{A} as \mathcal{C}_c^∞ . In this section, we also suppose that the process X is reversible:

Assumption 1.2.2. μ denotes an invariant measure for the semi-group $(P_t)_{t \geq 0}$, $\mathcal{E} \subset L^2(\mu)$, and X is reversible with respect to μ , in the sense that for all $t \geq 0$, P_t is self-adjoint in $L^2(\mu)$.

Define for $h \in \mathcal{A}$ the so-called *carré du champ*

$$\Gamma(h) = \frac{1}{2} (L(h^2) - 2hLh). \quad (1.13)$$

This definition is motivated by the following formal computation:

$$\partial_t \int_E (P_t f - \mu(P_t f))^2 d\mu = 2 \int_E (P_t f - \mu(P_t f)) L P_t f d\mu - \int_E L (P_t f)^2 d\mu = -2 \int_E \Gamma(P_t f) d\mu.$$

Definition 1.2.3. We say that μ satisfies a Poincaré inequality (with respect to Γ) if there exists $\lambda > 0$ such that:

$$\lambda \int_E (h - \mu(h))^2 d\mu \leq \int_E \Gamma(h) d\mu, \quad (1.14)$$

for all $h \in \mathcal{A}$.

In the reversible case, this Poincaré inequality is related to the so-called spectral gap of the process, since λ can be taken as the greatest non-zero eigenvalue of L . Hence, it is only natural that it is related to the long time behavior of the semi-group, as shown by the following:

Proposition 1.2.3. Under Assumption 1.2.1, the existence of a Poincaré inequality is equivalent to: for all $t \geq 0$

$$\|P_t f - \mu(f)\|_{L^2(\mu)} \leq e^{-2\lambda t} \|f - \mu(f)\|_{L^2(\mu)}, \quad (1.15)$$

for all $f \in L^2(\mu)$.

Hence, Poincaré inequality gives us convergences towards equilibrium and even speed of convergence through λ . Take the example of the overdamped Langevin process (1.8). In this case:

$$\Gamma(h) = \beta^{-1} |\nabla h|^2,$$

and the stationary measure is the Gibbs measure (1.9). It can be shown that this probability measure satisfies the Poincaré inequality

$$\lambda \int_{\mathbb{R}^d} (h - \nu_\beta(h))^2 d\nu_\beta \leq \int_{\mathbb{R}^d} |\nabla h|^2 d\nu_\beta,$$

if for instance $U \in \mathcal{C}^2(\mathbb{R}^d)$ and

$$\inf |\nabla U|^2 - \Delta U > -\infty,$$

yielding exponential convergence in $L^2(\nu_\beta)$. Estimates on the Poincaré constant, and more particularly its dependency on the dimension and the temperature β^{-1} , are of great importance to analyse the speed of convergence of these Markov processes and their application to stochastic algorithms, as we will see in Section 1.3. The *carré du champs* also yields local information on the semi-group, but those will not be of interest in this thesis. Moreover, other functional inequalities exist, like the log-Sobolev and the Sobolev inequalities, which yield convergences in other spaces, as well as other properties such as hyper and ultracontractivity, see [6]. For instance, using a log-Sobolev inequality instead of a Poincaré inequality, one could prove the

convergence in entropy, where the entropy of a probability measure ν with respect to μ is defined as:

$$\text{Ent}(\nu|\mu) = \begin{cases} \int \ln\left(\frac{d\nu}{d\mu}\right) d\nu & \text{if } \nu \ll \mu, \\ +\infty & \text{else.} \end{cases}$$

This does not define a distance, but the entropy is particularly well-adapted to particle systems or high dimensional settings, as this quantity scales better than L^p distances with the dimension and is an upper bound for some Wasserstein distances, that will be defined in Section 1.2.2 (such as the total variation distance with the Pinsker inequality).

The method presented in this Section does not require reversibility, but only a Poincaré inequality (1.14). It however fails as such in the case of kinetic process. Let's consider the case of the Langevin process (1.10). Its *carré du champs* is expressed as:

$$\Gamma(h) = \gamma\beta^{-1}|\nabla_y h|^2.$$

Considering a function h that only depends on x , an inequality of the form:

$$\lambda \int_{\mathbb{R}^{2d}} (h - \mu_\beta(h))^2 d\mu_\beta \leq \int_{\mathbb{R}^{2d}} |\nabla_y h|^2 d\mu_\beta$$

cannot hold with $\lambda > 0$. According to Proposition 1.2.3, it is not possible to achieve convergence as for the overdamped Langevin process. The next section is dedicated to adapting the previously discussed method to kinetic processes.

Hypocoercivity and generalized Gamma calculus

The Langevin process is not coercive, as in Proposition 1.2.3, but is hypocoercive, a term introduced in [163].

Definition 1.2.4. *A semi-group P with invariant measure μ is said to be hypocoercive on \mathcal{E} if there exist $C > 1$ and $\lambda > 0$ such that:*

$$\|P_t f - \mu(f)\|_{\mathcal{E}} \leq C e^{-\lambda t} \|f - \mu(f)\|_{\mathcal{E}}, \quad (1.16)$$

for all $f \in \mathcal{E}$.

If $C = 1$, then we revert to the case of Section 1.2.1, and the process is simply coercive. However, when $C > 1$, this convergence is not equivalent to the Poincaré inequality with respect to the *carré du champ*. Contrary to the convergence (1.15), this property is invariant by replacing the distance by an equivalent one on \mathcal{E} . In fact, Villani developed in his famous memoir [163] a method to show hypocoercive convergence by using a modified norm. This method has later been formalized using the so-called Gamma calculus [9, 134]. Demonstrating such convergence is usually equivalent to finding the correct distance for which the semi-group is actually coercive, as we will now see. We are interested in the evolution of quantities of the form:

$$\int_E \phi(P_t f) d\mu,$$

for quadratic functionals $\phi : \mathcal{C}^\infty(\mathcal{X}) \rightarrow \mathcal{C}^\infty(\mathcal{X})$ of the form:

$$\phi(h) = |A\nabla^\alpha h|^2 = \sum_{\alpha_1 + \dots + \alpha_{2d} = \alpha} |A_{\alpha_1, \dots, \alpha_{2d}} \partial_{z_1}^{\alpha_1} \dots \partial_{z_{2d}}^{\alpha_{2d}} h|^2,$$

for some $\alpha \in \mathbb{N}$ and tensor A , as well as linear combination of such functionals. To this end, define:

$$\Gamma_{L,\phi}(h) = \frac{1}{2} (L(\phi(h)) - D_h\phi(h)Lh), \quad (1.17)$$

where $D_h\phi$ denote the differential operator of ϕ . This definition is motivated by the following formal computation:

$$\frac{d}{dt} \int_E \phi(P_t f) d\mu = - \int_E \Gamma_{L,\phi}(P_t f) d\mu, \quad (1.18)$$

which uses that μ is invariant for P_t . If we can get an inequality of the form

$$c \int_E \phi(h) d\mu \leq \int_E \Gamma_{L,\phi}(h) d\mu \quad (1.19)$$

for all smooth $h \in \mathcal{A}$, then this implies the convergence:

$$\int_E \phi(P_t f) d\mu \leq e^{-ct} \int_E \phi(f) d\mu. \quad (1.20)$$

Therefore, if $\int_E \phi(f) d\mu$ is equivalent to the L^2 or H^k distance, then our goal would be achieved. This tool is particularly well adapted for the study of quadratic functional such as the L^2 or H^k norms, due to the following identity:

Proposition 1.2.4. *If there exists $A = (A_1, \dots, A_p) : \mathcal{C}^\infty \rightarrow (\mathcal{C}^\infty)^p$ a linear operator such that $\phi(h) = |Ah|^2$, then*

$$\Gamma_{L,\phi}(h) = \Gamma_{L,2}(Ah) + Ah \cdot [L, A]h,$$

where $\Gamma_{L,2}(Ah) = \sum_{i=1}^p \Gamma(A_i h)$, Γ is the carré du champ defined in (1.13), and $[L, A] = ([L, A_1], \dots, [L, A_p])$.

Let's now see how this applies to the $L^2(\mu)$ and $H^1(\mu)$ of the Langevin process, in the case of a bounded hessian potential: $\|\nabla^2 U\|_\infty < \infty$. Let's recall that under this condition, the Langevin process admits the measure μ_β defined in (1.12) as its unique invariant measure, and its generator is given by:

$$L = y \cdot \nabla_x - \nabla U \cdot \nabla_y - \gamma y \cdot \nabla_y + \gamma \beta^{-1} \Delta_y. \quad (1.21)$$

We will show convergence in H^1 using Gamma calculus. We have:

$$[L, \nabla_x] = \nabla^2 U \nabla_y, \quad [L, \nabla_y] = -\nabla_x + \gamma \nabla_y.$$

Hence using Young inequality we have:

$$\begin{aligned} (\nabla_x - \nabla_y)g \cdot [L, \nabla_x - \nabla_y]g &= (\nabla_x - \nabla_y)g \cdot (\nabla^2 U \nabla_y + \nabla_x - \gamma \nabla_y)g \\ &\geq \frac{1}{2} |\nabla_x g|^2 - 2(1 + \gamma + \|\nabla^2 U\|_\infty)^2 |\nabla_y g|^2, \end{aligned}$$

as well as

$$\nabla_y g \cdot [L, \nabla_y]g = \nabla_y g \cdot (-\nabla_x + \gamma \nabla_y)g \geq -\frac{1}{4} |\nabla_x g|^2 - |\nabla_y g|^2.$$

Thus, with

$$\phi(h) = ch^2 + |(\nabla_x - \nabla_y)h|^2 + |\nabla_y h|^2, \quad c = \gamma^{-1} \beta \left(2 + 2(1 + \gamma + \|\nabla^2 U\|_\infty)^2 \right),$$

Proposition 1.2.4, the linearity of Γ_ϕ with respect to ϕ , as well as the positivity of Γ yield that

$$\Gamma_\phi(g) \geq c\Gamma(g) + (\nabla_x - \nabla_y)g \cdot [L, \nabla_x - \nabla_y]g + \nabla_y g \cdot [L, \nabla_y]g \geq \frac{1}{2}|\nabla g|^2. \quad (1.22)$$

The measure μ_β satisfies the Poincaré inequality

$$\lambda \int_{\mathbb{R}^{2d}} (h - \mu_\beta(h))^2 d\mu_\beta \leq \int_{\mathbb{R}^{2d}} |\nabla h|^2 d\mu_\beta,$$

for some $\lambda > 0$, which, combined with inequality (1.22), yields

$$- \int_{\mathbb{R}^{2d}} \Gamma_\phi(g) d\mu_\beta \leq -\kappa \int_{\mathbb{R}^{2d}} \phi(g) d\mu_\beta$$

for some $\kappa > 0$. This inequality, at least formally, yields the H^1 convergence:

$$\int_{\mathbb{R}^{2d}} (P_t f)^2 + |\nabla P_t f|^2 d\mu_\beta \leq C e^{-ct} \int_{\mathbb{R}^{2d}} f^2 + |\nabla f|^2 d\mu_\beta$$

for some $C, c > 0$ that can be made explicit, and all $f \in H^1(\mu)$. Actually, using an $L^2 \rightarrow H^1$ hypoelliptic regularization [81]

$$\int_{\mathbb{R}^{2d}} (P_t f)^2 + |\nabla P_t f|^2 d\mu_\beta \leq \frac{K}{t^\alpha} \int_{\mathbb{R}^{2d}} f^2 d\mu_\beta, \quad \forall t \in]0, 1]$$

for some $K, \alpha > 0$, this also yield the L^2 convergence:

$$\int_{\mathbb{R}^{2d}} (P_t f)^2 d\mu_\beta \leq C \frac{e^{-ct}}{\min(1, t)^\alpha} \int_{\mathbb{R}^{2d}} f^2 d\mu_\beta.$$

These computations can be made rigorous using the Lumer-Phillips theorem. All computations are conducted on the semi-group's generator, and this theorem, rooted in the Hille-Yoshida theory, allows us to transfer a property from the generator to the semi-group. In the case of the Langevin process, Villani's method worked thanks to the bracket condition of hypoellipticity given in Definition 1.2.2. Regardless, some processes might exhibit hypocoercive convergence without being hypoelliptic, as is the case for some kinetic PDMPs. In these case, other methods exist to show hypocoercivity, such as the ones developed in [50, 1].

This method will be employed in Chapters 2, 3 and 4, in H^k spaces, to obtain either estimates on the semi-group or on the time-marginals of the law of the process under different sets of assumptions on the process. The proof of the inequality (1.19) will consistently rely on the use of the Poincaré inequality throughout this thesis. In the case of non-quadratic ϕ , one could also use other functional inequalities such as the Log-Sobolev inequality when $\phi(h) = h \ln(h)$ represents the entropy.

1.2.2 Wasserstein distance and coupling methods

The second family of methods we are going to look at are coupling methods, based on Wasserstein distances. These distances are typically introduced within the context of optimal transport and have the advantage that they don't require *a priori* the existence of an invariant probability measure, but will in fact be used for the proof of existence of such a measure, as we will discuss later on. Moreover, they are well-suited for studying the long-term behavior of Markov processes,

thanks to their probabilistic interpretation, even in cases where the generator is not a differential operator.

The topology

Definition 1.2.5. For any two probability measures ν_1, ν_2 , we define a coupling of ν_1 and ν_2 as (X^1, X^2) such that the law of X^1 (resp. X^2) is ν_1 (resp. ν_2).

Given a distance \mathbf{d} on E , $p \in \mathbb{N}$, and $\nu_1, \nu_2 \in \mathcal{M}^1(E)$, we define the associated Wasserstein distance as follows:

$$W_{\mathbf{d},p}(\nu_1, \nu_2) = \left(\inf \{ \mathbb{E}(\mathbf{d}^p(X^1, X^2)), (X^1, X^2) \text{ coupling of } \nu_1 \text{ and } \nu_2 \} \right)^{1/p}.$$

Given a Markov semi-group P , we call a coupling of $(\nu_1 P_t)_{t \geq 0}$ and $(\nu_2 P_t)_{t \geq 0}$ a stochastic process $(X_t^1, X_t^2)_{t \geq 0}$ such that $(X_t^1)_{t \geq 0}$ and $(X_t^2)_{t \geq 0}$ are Markov processes of semi-group $(P_t)_{t \geq 0}$ and initial condition ν_1 for X^1 and ν_2 for X^2 .

When $p = 1$, it is also referred to as the Kantorovich distance. This definition yields a distance on the space:

$$\mathcal{M}_p^1(E) = \left\{ \nu \in \mathcal{M}^1(E), \int_E \mathbf{d}(x, x_0)^p \nu(dx) < \infty \right\},$$

and this space is independent of the choice of $x_0 \in E$. We will be mostly interested in the case $p = 1$ and $p = 2$. If \mathbf{d} is bounded, then all these distances are equivalent. A specific instance is when $\mathbf{d}(x, y) = 2\mathbb{1}_{x \neq y}$ and $p = 1$, leading to the recovery of the total variation distance denoted by $W_{\mathbf{d}}(\nu_1, \nu_2) = \|\nu_1 - \nu_2\|_{TV}$. The Wasserstein distances satisfy the following properties:

Proposition 1.2.5. • If (E, \mathbf{d}) is a Polish space, then $(\mathcal{M}_p^1, W_{\mathbf{d},p})$ is also a Polish space.

- In this case, there exists an optimal coupling, meaning a coupling (X^1, X^2) of ν_1 and ν_2 such that $W_{\mathbf{d}}(\nu_1, \nu_2) = \mathbb{E}(\mathbf{d}(X^1, X^2))$.
- $\|\cdot\|_{TV}$ makes $\mathcal{M}^1(E)$ complete for any set E , and there always exists an optimal coupling for this distance.

Proofs of these facts can be found in [164, Theorem 6.18 and Theorem 4.1]. These properties hold even though $(E, 2\mathbb{1}_{x \neq y})$ is not separable as soon as E is uncountable. In the sequel, we will omit the dependence on \mathbf{d} , and W_p will denote $W_{\mathbf{d},p}$. We will also refer to the law of the pair (X^1, X^2) as the optimal coupling.

Now, let's explain why the Wasserstein distance is well-suited to the study of the long-time behavior of Markov processes. The objective is to establish a coupling for all $x, y \in E$ of $\delta_x P_t$ and $\delta_y P_t$. Typically, such a coupling should ensure that $X_s^1 = X_s^2 \implies X_t^1 = X_t^2, \forall t \geq s$. When this happens, we say that the processes X^1 and X^2 have coupled at time s . Given that the Wasserstein distance is defined by an infimum, any coupling, not necessarily an optimal one, can provide an upper bound for the distance, as for all $t \geq 0$ the following inequality holds:

$$W_{\mathbf{d}}(\nu_1 P_t, \nu_2 P_t) \leq \mathbb{E}(\mathbf{d}(X_t^1, X_t^2)).$$

More precisely we have:

Proposition 1.2.6. Suppose that (E, \mathbf{d}) is a Polish space or that $\mathbf{d}(x, y) = 2\mathbb{1}_{x \neq y}$, and that there exist $t_0 > 0$, $0 < \kappa < 1$, $\alpha > 0$ such that for all $x, y \in E$, there exists two couplings, (X^x, X^y)

and (\bar{X}^x, \bar{X}^y) , of $(\delta_x P_t)$ and $(\delta_y P_t)$ such that for all $t \geq 0$, $(x, y) \mapsto (X_t^x, X_t^y)$ is measurable,

$$\mathbb{E}(\mathbf{d}(X_{t_0}^x, X_{t_0}^y)^p) \leq \kappa^p \mathbf{d}(x, y)^p, \quad (1.23)$$

and

$$\mathbb{E}(\mathbf{d}(X_t^x, X_t^y)^p) \leq \alpha^p \mathbf{d}(x, y)^p, \quad \forall t \in [0, t_0]. \quad (1.24)$$

Then the semi-group (P_t) admits a unique invariant measure μ , and we have that for all $\nu \in \mathcal{M}_p^1(E)$:

$$W_p(\nu P_t, \mu) \leq C e^{-ct} W_p(\nu, \mu),$$

for some constants $C, c > 0$ explicit in κ, α and t_0 .

Proof. Fix $\nu_1, \nu_2 \in \mathcal{M}^1(E)$, and let (X_0, Y_0) be an optimal coupling of ν_1, ν_2 . Denote $X_t = X_t^{X_0}$ and $Y_t = Y_t^{Y_0}$. (X_{t_0}, Y_{t_0}) is a coupling of $\nu_1 P_{t_0}$ and $\nu_2 P_{t_0}$, and hence using the definition of the Wasserstein distance and conditioning we get:

$$\begin{aligned} W_p^p(\nu_1 P_{t_0}, \nu_2 P_{t_0}) &\leq \mathbb{E}(\mathbf{d}(X_{t_0}, Y_{t_0})^p) = \int_{E \times E} \mathbb{E}(\mathbf{d}(X_{t_0}^x, Y_{t_0}^y)^p) \pi(dx dy) \\ &\leq \kappa^p \int_{E \times E} \mathbf{d}(x, y)^p \pi(dx, dy) = \kappa^p W_p^p(\nu_1, \nu_2). \end{aligned}$$

Thus, the application $\nu \mapsto \nu P_{t_0}$ is a contraction on the complete space \mathcal{M}_p^1 , and the Banach fixed point theorem yield that it admits a unique fixed point $\mu \in \mathcal{M}_p^1(E)$, and μ is such that

$$W_p(\nu P_{t_0}^k, \mu) \leq \kappa^k W_p(\nu, \mu).$$

An invariant measure of the semi-group is necessarily a fixed point of P_{t_0} . If there exists $t \geq 0$ such that $\mu P_t \neq \mu$, then, by the semi-group property of P , μP_t would be a second fixed point of P_{t_0} . This implies that μ is the unique invariant measure of the semi-group. Integrating Inequality (1.24) with respect to the initial condition implies that for all $t \in [0, t_0]$:

$$W_p(\nu_1 P_t, \nu_2 P_t) \leq C W_p(\nu_1, \nu_2).$$

Therefore, we may write

$$W_p(\nu P_t, \mu) = W_p(\nu P_t, \mu P_t) \leq \kappa^{\lfloor t/t_0 \rfloor} W_p(\nu P_{t - \lfloor t/t_0 \rfloor t_0}, \mu P_{t - \lfloor t/t_0 \rfloor t_0}) \leq \alpha \kappa^{\lfloor t/t_0 \rfloor} W_p(\nu, \mu)$$

which concludes the proof with $C = \alpha \kappa^{-1}$ and $c = -t_0^{-1} \ln(\kappa)$. \square

Constructing a coupling that satisfies (1.24) is typically straightforward, and the main challenges arise in building the coupling from (1.23).

A first example

Let's consider an example to illustrate how this works. Take the following SDE on \mathbb{R}^d :

$$dX_t = b(X_t)dt + dB_t, \quad (1.25)$$

where B is a Brownian motion, and b satisfies the following one-sided Lipschitz condition:

$$\exists \kappa > 0, \forall x, y \in \mathbb{R}^d, (b(x) - b(y)) \cdot (x - y) \leq -\kappa |x - y|^2. \quad (1.26)$$

This condition implies that the deterministic drift tends to bring points in space closer together. It is for example satisfied by the gradient of convex functions. Let $\mathbf{d}(x, y) = \|\cdot\|_2$ be the Euclidean norm. Fix $x, y \in \mathbb{R}^d$ and a Brownian motion B . We can then define the so-called parallel coupling:

$$X_t = x + \int_0^t b(X_s) ds + B_t, \quad Y_t = y + \int_0^t b(Y_s) ds + B_t. \quad (1.27)$$

They are both driven by the same Brownian motion. Ito's formula yields:

$$d|X_t - Y_t|_2^2 = 2(b(X_t) - b(Y_t)) \cdot (X_t - Y_t) dt \leq -2\kappa|X_t - Y_t|_2^2 dt,$$

and hence

$$\|X_t - Y_t\|_2 \leq e^{-\kappa t} \|X_0 - Y_0\|_2$$

which implies inequality (1.23). We can conclude that the SDE (1.25) defines a Markov process that admits a unique invariant measure, and that the law of this process converges exponentially fast towards this invariant measure at rate κ for the distance W_p , for all $p \geq 1$. In the case where (1.26) only holds outside a compact set, contraction in W_1 was proved in [55] for a distance \mathbf{d} equivalent to the euclidean one, using the famous reflection coupling introduced in [117]. In the case of non-elliptic processes, a mix between parallel and reflection coupling was used in [56] to prove convergence of the Langevin process (1.10). To my knowledge, it remains open to know if it is possible to construct a metric on \mathbb{R}^d and a coupling to prove the Wasserstein convergence for a process satisfying the Hörmander's bracket condition from Definition 1.2.2 and a contractivity assumption similar to (1.26) outside a compact set.

Convergence in weighted total variation and Lyapunov functions

We have shown in the previous section the convergence of the process (1.25) in Wasserstein distance W_p under a uniform one-sided Lipschitz condition on the drift. Now, we are interested in the convergence of the same process in total variation distance, i.e., considering $\mathbf{d}(x, y) = 2\mathbb{1}_{x \neq y}$. Denote the process by X^x when the initial condition is $x \in \mathbb{R}^d$, and let's suppose that b is Lipschitz continuous. Then, from Proposition 1.2.1, we get that the random variable X_t^x admits a density with respect to the Lebesgue measure, denoted by $h_t(x, \cdot)$, and the mapping $(x, y) \mapsto h_t(x, y)$ is continuous and non-negative. Actually, using controllability arguments, one can show that it is positive. Suppose we have the additional condition

$$\inf_{x, y \in \mathbb{R}^d} h_{t_0}(x, y) > 0,$$

which would hold if the diffusion was living in a compact space, like the periodic torus, or if a Sobolev inequality would hold, thus implying ultracontractivity. In that case, we would satisfy condition (1.23): the uniform creation of density implies exponential convergence towards a unique equilibrium in total variation distance. Indeed, we can construct an explicit coupling satisfying (1.23). Let's write $c = \inf_{\mathbb{R}^d \times \tilde{K}} h_{t_0}$, where \tilde{K} is a compact set of Lebesgue measure 1, and denote the Lebesgue measure by l . Notice that

$$\mathcal{L}aw(X_{t_0}^x) = (1 - c) \frac{\mathcal{L}aw(X_{t_0}^x) - cl(\cdot \cap \tilde{K})}{1 - c} + cl(\cdot \cap \tilde{K}).$$

Now, let's define random variables as follows:

- Z is a random variable with law $l(\cdot \cap \tilde{K})$,
- B is a Bernoulli random variable with parameter c ,
- For all $x \in \mathbb{R}^d$, Z^x is a random variable with law $\frac{\mathcal{L}aw(X_{t_0}^x) - c l(\cdot \cap \tilde{K})}{1-c}$.

Then, the law of the random variable

$$X^x = \mathbb{1}_{B=1}Z + \mathbb{1}_{B=0}Z^x$$

is indeed $\delta_x P_{t_0}$, and we have

$$\|\delta_x P_{t_0} - \delta_y P_{t_0}\|_{TV} \leq 2\mathbb{P}(X^x \neq X^y) \leq 2\mathbb{P}(B=0) = 2(1-c) = (1-c)\|\delta_x - \delta_y\|_{TV}$$

for all $x, y \in \mathbb{R}^d$, corresponding to (1.23). More generally, a condition

$$\forall x \in E, \mathbb{P}_x(X_{t_0} \in \cdot) \geq c\theta, \quad (1.28)$$

for some probability measure $\theta \in \mathcal{M}^1$, called a Doeblin condition, yields condition (1.23), and hence convergence in total variation distance. However, when the state space is not compact, the condition (1.28) might not hold uniformly on E . In this case, we need the existence of a so-called Lyapunov function. In many cases of interest, the process goes back to a compact set on which such an inequality holds.

Definition 1.2.6. *A function $V : E \rightarrow [1, \infty)$ is called a Lyapunov function if V has compact level sets and there exist $C > 0$ and $0 < \alpha < 1$ such that:*

$$\mathbb{E}_x(V(X_{t_0})) \leq (1-\alpha)V(x) + \alpha C, \quad (1.29)$$

for some $t_0 > 0$.

Informally speaking, the existence of a Lyapunov function is equivalent to the fact that the process returns exponentially fast to compact sets. The usual way to prove the existence of a Lyapunov function is to use the generator characterisation: (1.29) is implied by the fact that $V \in \mathcal{D}(L)$ and:

$$LV \leq -cV + C,$$

for some $C, c > 0$. Suppose that the one-sided Lipschitz condition holds for the drift, but only 'at infinity': there exists some compact set $K \subset \mathbb{R}^d$ such that:

$$\forall x \in \mathbb{R}^d \setminus K, b(x) \cdot x \leq -\kappa\|x\|_2.$$

Then, if $V(x) = x^2 + 1$, we have:

$$LV = -2b(x) \cdot x + 2d \leq -2\kappa V(x) + 2(\kappa + d),$$

and hence V is a Lyapunov function. Now, let's write

$$\mathbf{d}_{V,\beta}(x, y) = 2\mathbb{1}_{x \neq y}(1 + \beta V(x) + \beta V(y)).$$

The addition of a Lyapunov function to a Doeblin condition yields a Harris-type theorem, which corresponds to the following result:

Proposition 1.2.7. *Suppose that V is a Lyapunov function satisfying (1.29), and that there exists a probability measure θ such that for all $x \in \{V < C'\}$,*

$$\mathbb{P}_x(X_{t_0} \in \cdot) \geq c\theta,$$

for some $C' > 2C$ and $c > 0$. Then there exists an explicit $\beta > 0$ such that $\nu \mapsto \nu P_{t_0}$ is a contraction in the space $(\mathcal{M}^1(E), W_{d_V, \beta, 1})$, and all conclusions of Proposition 1.2.6 hold. Moreover, we have the total variation convergence:

$$\|\nu P_t - \mu\|_{TV} \leq D e^{-dt} \int V(x) \nu(dx),$$

for some $D, d > 0$.

This kind of method first sprung from the work of Meyn and Tweedie, see [128]. Proof of this statement and variations can be found in [52, 79].

Particle systems

In this thesis, we primarily apply coupling methods to mean-field particle systems. For a given vector $\mathbf{x} = (x_1, \dots, x_N) \in E^N$, we define its empirical measure as:

$$\pi(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N \delta_{x_i}.$$

It is a probability measure that counts the number of point (x_i) in any given set. A mean field particle system is a Markov process $\mathbf{X} = (X^1, \dots, X^N)$ with state space E^N , where N is the number of particles, such that each particle X^i only interacts with the other through their empirical measure $\pi(\mathbf{X}_t)$. In Section 1.3, we will introduce the so-called Fleming-Viot process, which is an instance of mean field particle system used for sampling. Another widely studied system is the famous McKean-Vlasov particle system:

$$dX_t^i = -\nabla U(X_t^i) - \frac{1}{N} \sum_{j=1}^N \nabla W(X_t^i - X_t^j) dt + dB_t. \quad (1.30)$$

This kind of process is interesting because it models systems made up of interacting agents.

Definition 1.2.7. *We say that a (finite) sequence of random variable $(X_i)_{1 \leq i \leq N}$ is exchangeable if for all permutation $\sigma : \llbracket 1, N \rrbracket \rightarrow \llbracket 1, N \rrbracket$, $(X_{\sigma(i)})_{1 \leq i \leq N}$ is equal in law to $(X_i)_{1 \leq i \leq N}$.*

In particular, if (X_i) is exchangeable, then X_i and X_j have the same laws for all i, j . The next proposition gives us the convergence of the empirical measure of independent random variables:

Proposition 1.2.8 ([62]). *If (Z_i) is a sequence of independent random variables with common law ν with moments of order $q > 0$:*

$$\int_{\mathbb{R}^d} x^q \nu(dx) < \infty.$$

Then for all $1 < p < q$, the following convergence holds in W_p distance :

$$\pi\left((Z_i)_{1 \leq i \leq N}\right) = \frac{1}{N} \sum_{i=1}^N \delta_{Z_i} \xrightarrow[N \rightarrow \infty]{} \nu,$$

where the Wasserstein distance is relative to any norm on \mathbb{R}^d .

One interesting feature of such mean field systems is that they satisfy the so-called mean field limit: the particles interacting through their empirical measure are not independent but define an exchangeable system. Therefore, one may hope that as N goes to infinity, the convergence of the empirical measure towards their common law remains true, as soon as it is true at the initial time. This is called propagation of chaos, and would yield that as the number of particles goes to infinity, instead of seeing the interaction with all others, each particle only sees a deterministic averaged interaction which corresponds to their common law. Hence, they would become independent, and converge towards a non-linear process (in example (1.30), the McKean-Vlasov process). For such processes, the goal in Chapters 6 and 7 will be to show that the particle system converges towards an equilibrium, at a rate that is independent of the number of particles, see Section 1.3.3. To this end, we need a distance that scales well with the number of particles, and which is close to the distance at hand. For convergences in total variation distances, we define:

$$\mathbf{d}_N(\mathbf{x}, \mathbf{y}) = \frac{1}{N} \sum_{i=1}^N \mathbf{1}_{x_i \neq y_i}$$

or in the case where one needs a Lyapunov function:

$$\mathbf{d}_N(\mathbf{x}, \mathbf{y}) = \frac{1}{N} \sum_{i=1}^N \mathbf{1}_{x_i \neq y_i} (1 + \beta V(x_i) + \beta V(y_i)).$$

The following lemma is the main motivation behind those distances:

Proposition 1.2.9. *Let $\nu^N P_t^N$ be the law of the particle system \mathbf{X}_t , and denote by $\nu^{k,N}$ the k -first particles marginal. Suppose that \mathbf{X}_0 is exchangeable, and that there exist $C, c > 0$ such that*

$$W_{\mathbf{d}_N}(\nu^N P_t^N, \mu^N) \leq C e^{-ct} W_{\mathbf{d}_N}(\nu^N, \mu^N).$$

Then for all $k \in \llbracket 1, N \rrbracket$, we have:

$$\|(\nu^N P_t^N)^k - \mu^{k,N}\|_{TV} \leq \frac{k}{N} C e^{-ct} W_{\mathbf{d}_N}(\nu^N, \mu^N).$$

Proof. A mean field particle system at time $t \geq 0$ is exchangeable as soon as its initial condition is. Additionally, if ν_1 and ν_2 are two exchangeable probability measures on E^N , by denoting ν_1^k , ν_2^k their k particles marginal, we have:

$$\|\nu_1^k - \nu_2^k\|_{TV} \leq \frac{k}{N} W_{\mathbf{d}_N}(\nu_1, \nu_2).$$

□

Such distances were employed in [38] for a Fleming-Viot process and in [133] for general processes with mean-field jump interaction. A discrete measure cannot converge in total variation distance towards a measure with density, making the total variation distance unsuitable for the mean field limit, where one wants to show the convergence of the empirical measure. To achieve long-time convergence and uniform in-time propagation of chaos, a distance close to the W_1

distance in \mathbb{R}^d must be used. For instance, the distance:

$$\mathbf{d}_N(\mathbf{x}, \mathbf{y}) = \frac{1}{N} \sum_{i=1}^N |x_i - y_i|,$$

was used in [76, 118].

1.3 Stochastic algorithms and contributions of this thesis

Now, let's delve into the presentation of some MCMC-type algorithms. The theoretical investigation of these algorithms is rooted in the analysis of the long-time behavior of certain Markov processes, as discussed in Section 1.2. We will explore three types of algorithms, corresponding to the three parts of the thesis: the sampling of Gibbs measures, stochastic optimization, and the sampling of quasi-stationary measures using Fleming-Viot particle systems.

1.3.1 Sampling Gibbs measures

The first type of algorithm involves sampling Gibbs measures. Many physical systems can be described by a Hamiltonian (or energy) of the form:

$$H(x, y) = U(x) + \frac{1}{2}|y|^2, \quad (1.31)$$

where $U : \mathbb{R}^d \rightarrow \mathbb{R}_+$ (or $U : \mathbb{T}^d \rightarrow \mathbb{R}_+$, where \mathbb{T}^d is the d -dimensional torus) is a potential function, and $|y|^2/2$ represents the kinetic energy. When the dimension d is large, obtaining the exact evolution of the system becomes infeasible, and a statistical description must be employed. In statistical physics, for systems with fixed temperature $T = \beta^{-1} > 0$ and size, but that can exchange energy, the system is characterized by the Gibbs measure (1.12). The probability for the system to be in a state $(x, y) \in \mathbb{R}^{2d}$ solely depends on its energy and we recall that it is given by

$$\mu_\beta(dx, dy) = \frac{e^{-\beta H(x, y)}}{\sqrt{\pi \beta^{-1}}^d Z_\beta} dx dy.$$

One goal of molecular dynamic is to compute macroscopic quantities of physical systems defined by averages of the form

$$\mu_\beta(f) := \mathbb{E}(f(X, Y)), \quad (X, Y) \sim \mu_\beta, \quad (1.32)$$

for some function $f : \mathbb{R}^d \rightarrow \mathbb{R}$. One important example in chemistry is a system of $N \gg 1$ particles with van der Waals interaction, which corresponds to a noble gas. In this case, $d = 3N$ is of the order of $\mathcal{N}_A \approx 10^{23}$, and $x = (x_1, \dots, x_N)$ represents the positions of the particles. For a more in-depth introduction to molecular dynamics, refer to [161], as well as [111] for a mathematical perspective. Sampling high-dimensional Gibbs measures is not exclusive to statistical physics; it is also of paramount importance in computational statistics and machine learning. For instance, suppose given independent and identically distributed samples $(X_i, Y_i)_i$ from an unknown probability measure μ^* on $\mathbb{R}^d \times \mathbb{R}$. We are interested in the best predictor f^* of Y knowing X :

$$f^* \in \arg \min \mathbb{E} \left((Y_1 - f(X_1))^2 \right).$$

The solution to this problem is given by $f^*(x) = \mathbb{E}(Y|X = x)$, which is not accessible in practice. If we assume that f^* can be efficiently approximated by a linear functional, then given a matrix

θ , and writing $U(\theta) = \mathbb{E}(\|Y - \theta X\|^2)$, a random variable whose law is the Gibbs measure

$$\nu_\beta(d\theta) = \frac{e^{-\beta U(\theta)}}{Z_\beta} d\theta,$$

or its expectancy, are estimators of the solution, see [114, 98]. In this case, and many others, there is no kinetic energy, and we are only interested in the space variable marginal ν_β , also referred to as Gibbs measure, of the previously defined Gibbs measure μ_β .

The tasks involved in sampling such probability measures have three aspects:

1. **Designing a Markov Process:** The first task is to design a Markov process X that has the targeted probability measure as its unique invariant state and is ergodic. The rate of convergence of this Markov process should be as high as possible, and especially it should not approach 0 too rapidly as the dimension d goes to infinity.
2. **Choosing a Discretization Scheme:** A discretization scheme X^δ for the Markov process needs to be chosen so that it can be implemented on a computer. Some processes are easier to discretize than others, but in most cases, this introduces bias. This bias must be considered in both the choice of the process and its numerical scheme.
3. **Monte-Carlo Method for Approximation:** Finally, a Monte-Carlo method is needed to approximate the expectations of the numerical scheme. If the target is the invariant measure μ and the numerical scheme admits an invariant measure μ^δ , then the ergodic property

$$\lim_{T \rightarrow \infty} \frac{1}{T} \sum_{i=1}^T f(X_i^\delta) = \mu^\delta(f), \text{ almost surely,}$$

can be used. The error is then given by the bias of the invariant measure, and by the fact that $T \in \mathbb{N}$ is finite. Another solution, that allows also the computation of $\mathbb{E}(f(X_t))$ for finite $t \geq 0$, is to compute a large number $M \in \mathbb{N}$ of independent realisations of $X_{[t/\delta]}^\delta$, say $X_{[t/\delta]}^{\delta,i}$, and use that fact that under some integrability assumption:

$$\lim_{M \rightarrow \infty} \frac{1}{M} \sum_{i=1}^M f(X_{[t/\delta]}^{\delta,i}) = \mathbb{E}(f(X_t)), \text{ almost surely.}$$

This second Monte Carlo introduces three types of errors. The first error is finite time error, arising from the fact that we can only access $\mathbb{E}(f(X_t))$ for finite $t \geq 0$. The second error is the Monte-Carlo error, stemming from the approximation of $\mathbb{E}(f(X_t))$ (namely M is finite), and the third error results from the bias in the numerical scheme, where $\mathbb{E}(f(X_t^\delta)) \neq \mathbb{E}(f(X_t))$. The total error can typically be expressed in the form::

$$\mathbb{E} \left(\left| \frac{1}{M} \sum_{i=1}^M f(X_i^\delta) - \mu_\beta(f) \right| \right) \leq C \left(e^{-ct} + \frac{1}{\sqrt{M}} + \delta^\alpha \right).$$

The Monte Carlo error could potentially be improved by using other estimators of $\mathbb{E}(f(X_t))$ from the numerical scheme, such as Multilevel Monte Carlo methods (refer to [68]). However, the focus in the first two chapters of this thesis will be on the first and third errors.

There are many choice for the process used in the sampling, as we will see now. The most

commonly used process for sampling from ν_β is the overdamped Langevin process:

$$dX_t = -\nabla U(X_t)dt + \sqrt{2\beta^{-1}}dB_t, \quad (1.33)$$

where B is a Brownian motion, thus making X a diffusion process, see [110, 112] for its use in stochastic algorithms.

Assuming mild conditions on U , such as $U \in \mathcal{C}^\infty$, ∇U Lipschitz continuous, and satisfying

$$(\nabla U(x) - \nabla U(y)) \cdot (x - y) \leq -c|x - y|^2$$

for all $x, y \in \mathbb{R}^d \setminus K$, where K is some compact set and $c > 0$, it can be shown, using the results from Section 1.2, that this process is ergodic with respect to ν_β . The specific type of convergence depends on the assumptions about U and the methods used.

The Euler-Maruyama scheme is a well-known discretization method for Langevin-type processes. It reads here:

$$X_{n+1}^\delta = X_n^\delta - \delta \nabla U(X_n^\delta) + \sqrt{2\beta^{-1}\delta}G_n$$

where $(G_n)_n = (B_{(n+1)\delta} - B_{n\delta})_n$ a family of independent normal random variable. This discretization leads to the Unadjusted Langevin Algorithm (ULA). If ∇U is Lipschitz continuous, it can be demonstrated that this numerical scheme converges strongly (in the sense of pathwise) and weakly with a convergence order of 1.

Definition 1.3.1. *A numerical scheme is said to converges strongly with rate of convergence α if for all $T > 0$, there exists $C > 0$ such that for all δ small enough:*

$$\sup_{0 \leq n \leq T/\delta} \mathbb{E} (|X_n^\delta - X_{n\delta}|) \leq C\delta^\alpha.$$

A numerical scheme is said to converges weakly with rate of convergence α if for all $t \geq 0$, and f in a suitable class of function, there exists $C > 0$ such that:

$$|\mathbb{E} (f(X_n^\delta)) - \mathbb{E} (f(X_t))| \leq C\delta^\alpha,$$

where $n\delta = t$.

In general, the weak and strong order of convergence are not the same, as in the case of multiplicative noise where the strong order is 1/2. However, for the purposes of this thesis, only weak convergence is considered since the goal is the computation of averages. Proofs for weak convergence often rely on estimates of the semi-group, such as:

$$|\partial^\alpha P_t f(x)| \leq C(1 + |x|^k), \quad (1.34)$$

for regular enough f and $|\alpha|_1 < \alpha_{max}$, along with moment bounds on the numerical scheme, see [156] for instance in the case of the ULA. It can get intricate as soon as the drift is not Lipschitz continuous as in [123] where it is shown that the explicit Euler scheme might not be ergodic for non-globally Lipschitz vector field. See also [88] for the study of the failure of the Euler-Maruyama scheme. In such cases, alternative schemes need to be employed, as discussed in [78, 87, 89, 90, 30]. Discretization introduces bias in the invariant measure, which can be mitigated using a general method called metropolization. For example, in the case of the Euler scheme for the over-damped Langevin dynamics, the Metropolis Adjusted Langevin Algorithm (MALA) is:

- $\bar{X}_{n+1}^\delta = X_n^\delta - \delta \nabla U(X_n^\delta) + \sqrt{2\beta^{-1}\delta}G_n$

- Let U be uniform on $[0, 1]$.
- If $U \leq \min(1, e^{\beta(U(X_n^\delta) - U(\bar{X}_{n+1}^\delta))})$, then $X_{n+1}^\delta = \bar{X}_{n+1}^\delta$, else $X_{n+1}^\delta = X_n^\delta$.

This is the so-called Metropolis Adjusted Langevin Algorithm (MALA), and it is known to admit ν_β as its invariant measure. Other schemes, such as the Milstein scheme [145, Chapter 10], can be employed to achieve better orders of convergence. Implicit numerical schemes are another option, but they may not be well-suited for high-dimensional settings. The well-posedness of an implicit numerical scheme is not guaranteed, and even if it were, it would likely be numerically costly in practice.

A general class of processes are kinetic processes, which are characterized by the equations

$$dX_t = Y_t dt,$$

where X is the position, and noise only acts on the speed Y . Kinetic processes can be utilized for sampling from the measure ν_β using only its position variable. They are expected to exhibit better convergence rates than elliptic diffusions, displaying a ballistic behavior rather than the diffusive behavior of reversible processes.

To establish estimates on the semi-groups, similar to (1.34), necessary for proving weak convergence, hypocoercive methods, as discussed in Section 1.2.1, must be employed. One of the most physically relevant kinetic processes is the underdamped Langevin process, which models the movement of a particle in a potential U while in contact with a heat bath at temperature $T = \beta^{-1} > 0$. We recall that it solves:

$$\begin{cases} dX_t = Y_t dt, \\ dY_t = -\nabla U(X_t) dt - \gamma Y_t dt + \sqrt{2\gamma\beta^{-1}} dB_t. \end{cases}$$

Under mild assumptions, this process is ergodic with respect to μ_β , allowing for the sampling of the full Gibbs measure. A straightforward Euler-Maruyama scheme can be used for this process, but explicit splitting schemes are commonly employed in Molecular Dynamics simulations, better suited for Hamiltonian dynamics, see [107].

Another family of kinetic processes includes kinetic Piecewise Deterministic Markov Processes. PDMPs have the advantage that they can be simulated exactly, eliminating bias. In general, such processes admit $\nu_\beta \otimes \pi$ as steady states, where π is a probability measure on the state space of the speed variable, see [138, 52]. An example of a kinetic PDMP is the Bouncy-Particle sampler, with a generator given by

$$\begin{aligned} Lf(x, y) &= y \cdot \nabla_x f + (v \cdot \nabla U(x))_+ (f(x, R(x, y)) - f(x, y)) + \lambda \int_{\mathbb{R}^d} (f(x, y') - f(x, y)) \frac{e^{-v'^2/2}}{(2\pi)^{d/2}} dv', \end{aligned}$$

where $\lambda > 0$ is a refreshment parameter and $R(x, y) = y - 2\nabla U(x) \cdot v \nabla U(x) / |\nabla U(x)|^2$. The first jump part imposes the Gibbs measure μ_β as an invariant measure, and the refreshment is introduced for ergodicity. To study the long time behavior of PDMP's, the method developed in [163] is not adapted, as the *carré du champ* is not of gradient type. However other method can be applied, see [50, 1] for hypocoercivity, as well as coupling method described in Section 1.2.2.

There are many other processes used for sampling from a Gibbs measure. For instance, one can mention the Hamiltonian Monte Carlo (HMC) method [69, 26]. In this method, a trajectory

(X_t, Y_t) evolves using the Hamiltonian dynamics

$$\begin{cases} dX_t = Y_t dt, \\ dY_t = -\nabla U(X_t) dt, \end{cases}$$

and every time T , Y is re-sampled independently from the past according to a $\mathcal{N}(0, \beta I_d)$ distribution. See also [27] for a review of various usable methods.

Contributions In Part I of this thesis, the focus will be on the weak error expansion of numerical schemes, also known as weak backward error analysis, for kinetic processes. This involves searching for series expansions in weak convergences, denoted as

$$\mathbb{E}_z(f(X_n^\delta)) = \mathbb{E}_z(f(X_t)) + C_1(t)\delta^\alpha + \dots + C_k(t)\delta^{\alpha+k} + O(\delta^{\alpha+k+1}),$$

for all $k \in \mathbb{N}$, where $n\delta = t$. More particularly, we are interested in cases where the constants C_p , as well as the rest, are bounded in time, leading to uniform weak convergence over time. This expansion then also applies to the bias of the invariant measure. The analysis involves estimates such as

$$\partial^\alpha P_t f(x, y) \leq C e^{-ct} (1 + |x|^k + |y|^k),$$

for function satisfying $\mu_\beta(f) = 0$. The weak error expansion of numerical schemes was initially proven and numerically studied by Talay and Tubaro in [158]. Their work primarily focuses on the Euler-Maruyama and Milstein schemes for Elliptic SDEs with globally Lipschitz continuous coefficients. Talay also proved similar expansions for Hamiltonian systems with polynomial growth at infinity in [157], although using an implicit Euler scheme. Further studies on these expansions can be found in [41, 101, 100]. For explicit numerical schemes for the Langevin process with bounded potentials on the torus, refer to [107], and for Langevin processes with more general kinetic energies, see [153]. Uniform convergence in time of a numerical scheme is also explored in [3].

Chapter 2 is devoted to the sampling of Gibbs measure using the Langevin process in the case of a singular potential, as in the case of N particles within a confining potential and subject to Lennard-Jones interactions. Explicit numerical schemes are known to exhibit instability when the drift of the stochastic differential equation lacks Lipschitz continuity [123]. To address the issue of singularity, a novel numerical scheme that avoids instability phenomena and can be applied even in high-dimensional settings is proposed. Employing hypocoercive method adapted to the singular case as in [10], estimates on the semi-group of (1.10) are proven and used to show uniform in time weak error expansion of this new numerical scheme, as well as at stationary.

The most expensive part when simulating the process (1.10) is the computation of ∇U . A common approach is to substitute this gradient with a stochastic version. The goal of Chapter 3 is to explore an alternative solution. The idea is to break down the potential as $\nabla U = \sum_{i=0}^K F_i$, where F_0 represents the cheap to compute part (corresponding to the short range interaction in a gas of particles). We then consider the process:

$$\begin{cases} dX_t = Y_t dt, \\ dY_t = -F_0(X_t) dt - \gamma Y_t dt + \sqrt{2\gamma\beta^{-1}} dB_t, \end{cases}$$

and the process jumps at rate λ_i according to some jump kernel q_i depending on F_i in a way that ensures that the equilibrium measure of the process is indeed the Gibbs measure. This is a mix between diffusion and piecewise deterministic Markov process, with the latter being a type of Markov process known for its advantageous simulation properties. This study also draws upon hypocoercive methods.

Perspectives: Firstly, another process employed for sampling purposes in molecular dynamics is the generalized Langevin process [168]. It is a hypocoercive process exhibiting a higher degree of degeneracy than kinetic processes. It would be valuable to extend the computation in Sobolev spaces of any order for such a process to establish the weak convergence of numerical schemes. Additionally, exploring out-of-equilibrium processes is intriguing. When the gradient ∇U in the Langevin process (1.10) is replaced by a general force F , the invariant measure is not explicit and may not satisfy a Poincaré inequality. Despite this, it remains important to efficiently sample such measures. Lastly, in the context of sampling Gibbs measures, a criterion for efficiency is the variance of the Monte Carlo estimator. This aspect could be further studied through a central limit theorem for the occupation measure process of the two processes analyzed in Chapters 2 and 3.

1.3.2 Optimisation

Part II of this thesis delves into a problem closely related to the sampling of Gibbs measure: the optimization of non-convex functions. The focus is on a function, called the objective function in optimization but referred to as the potential in the thesis, $U : \mathbb{R}^d \rightarrow \mathbb{R}$, which is bounded from below. The goal is to address the problem of finding the minimum (or the minima) of U over \mathbb{R}^d . In various applications, non-convex potentials with multiple local minima, not necessarily confined within a compact set, are of interest. For example, in the context of Molecular Dynamics, U may represent the energy of a configuration of a physical system, and the minima correspond to its metastable states. In computational statistics, U could represent minus the logarithm of the posterior probability, and its minima indicate the maximum likelihood. A well-known benchmark problem for non-convex optimization discussed in this thesis is the mixture of Gaussian distributions. If (X_i) is a data set consisting of Gaussian variable with means $\Sigma_i \theta$, then the maximal likelihood is given by the minimum of a potential that takes the form

$$U(\theta) = \ln \left(\sum_{i=1}^n a_i \exp \left(-\lambda_i (\theta - \Sigma_i^{-1} X_i)^2 \right) \right). \quad (1.35)$$

When dealing with a convex U , standard gradient descent or its many variants are often sufficient for finding the minimum. However, the challenge arises in the case of non-convex potentials, as typical gradient descent algorithms tend to converge to local minima. One approach would be to initiate multiple gradient descents from random initial points, but the basin of attraction for global minima is usually of lower dimension compared to the ambient space. As a result, the probability of starting in this set is quite low. Additionally, in high-dimensional settings, an exhaustive search is impossible. To overcome these challenges, new paradigms that takes into account the geometry of U are needed to explore the space. The goal is to devise algorithms that impose minimal assumptions on U , typically requiring

$$U \in \mathcal{C}^1(\mathbb{R}^d), \quad \lim_{\|x\| \rightarrow \infty} U(x) = +\infty.$$

However, these assumptions may not be sufficient for the proposed algorithms.

There are various methods for non-convex optimization, including the utilization of mean-field particle systems like (1.30) for optimizing neural networks [86, 67] or genetic algorithms based on Fleming-Viot-type particle systems, as discussed in Section 1.3.3, see [148]. However, in this thesis, we will focus on two specific solutions for this optimization problem. The first one

is provided by simulated annealing, based on the observation that, under mild assumptions,

$$\nu_\beta \left(U > \min_{\mathbb{R}^d} U + \varepsilon \right) \xrightarrow{\beta \rightarrow \infty} 0,$$

for all $\varepsilon > 0$, where ν_β is the Gibbs measure given in (1.9). This implies that if X is an ergodic Markov process with invariant measure ν_β , and if β is large enough, X will spend most of its times in the vicinity of the global minima. The simulated annealing algorithm involves gradually increasing β over time. Given a generator L_β which admits ν_β as its invariant measure for all $t \geq 0$, and a cooling schedule $\beta_t \xrightarrow{t \rightarrow \infty} \infty$, the goal is to design an inhomogeneous Markov process X_t with generator L_{β_t} . If β increases slowly enough, the law of X_t will be close to its instantaneous equilibrium ν_{β_t} , and X will converge in probability towards the set of global minima of U . The faster the temperature goes to 0, the more the Gibbs measure will charge the minimum. However, if β increases too fast, the process might become trapped in the vicinity of a local minimum with positive probability, leading to algorithm failure. This transition is known to occur with a logarithmic schedule: if $\beta_t = \ln(1+t)/c$ and the process is based on the overdamped Langevin process:

$$dX_t = -\nabla U(X_t)dt + \sqrt{2\beta_t^{-1}}dB_t, \quad (1.36)$$

then under mild assumption on U (see below), convergence holds for $c > c^*$ and fails for $c < c^*$, where c^* is an explicit constant known as the largest energy barrier of the potential

$$c^* = \sup_{x_1, x_2} c(x_1, x_2)$$

with

$$c(x_1, x_2) = \inf \left\{ \max_{0 \leq t \leq 1} U(\xi(t)) - U(x_1) - U(x_2) \right\}$$

where the infimum runs over $\{\xi \in \mathcal{C}([0, 1], \mathbb{R}^d), \xi(0) = x_1, \xi(1) = x_2\}$.

The phase transition is attributed to metastability, a crucial phenomenon in the study of low-temperature processes, among other things. Let's revisit the process with fixed temperature (1.8), and consider a domain $D \subset \mathbb{R}^d$ corresponding to the basin of attraction for the gradient descent from a point $x_0 \in \mathbb{R}^d$. We are concerned with the first exit time from the domain:

$$\tau = \inf \{t \geq 0, X_t \notin D\}.$$

This problem was investigated in [65], revealing that τ is of the order $e^{\beta(\min_{\partial D} U - \min_D U)}$. When the temperature β^{-1} is zero, the process behaves as a simple gradient descent, and it never leaves D . However, over an extended period, the introduced noise causes the process to move away from the vicinity of local minima. The speed of convergence of the law of X_t towards its equilibrium μ_β is related to the pace at which it visits space. The longer it takes to exit the basin of attraction of local minima, the slower the convergence becomes. This can be quantified using *PDE* and functional inequality as described in Section 1.2.1. Since c^* is the minimal energy elevation required to transition from any local minimum (or even any point), to a global minimum, $e^{\beta c^*}$ represents the order of the time needed to explore space. The Poincaré inequality, introduced in Definition 1.2.3, is one way to quantify this phenomenon.

Proposition 1.3.1 ([83, 126]). *Under the assumption that either $U : \mathbb{T}^d \rightarrow \mathbb{R}_+$ or $U : \mathbb{R}^d \rightarrow \mathbb{R}_+$*

and

$$\liminf_{|x| \rightarrow \infty} |\nabla U(x)| > 0, \quad \inf_{\mathbb{R}^d} |\nabla U|^2 - \Delta U > -\infty,$$

ν_β satisfies a Poincaré inequality

$$\lambda(\beta) \int_{\mathbb{R}^d} f^2 d\nu_\beta \leq \int_{\mathbb{R}^d} |\nabla f|^2 d\nu_\beta,$$

for all $f \in C^1$, $\int f d\nu_\beta = 0$, and $\lambda(\beta)$ satisfies

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(\lambda(\beta)) = -c^*.$$

Combined with Proposition 1.2.3, this yields that the speed of convergence is of order $e^{\beta c^*}$, which is exponential bad if $c^* > 0$. This situation occurs when U possesses multiple local minima. In the context of simulated annealing, understanding metastability and exit times is crucial for selecting appropriate cooling schedules that balance exploration and exploitation. The objective is to avoid becoming trapped in local minima while still converging to the global minimum as the temperature decreases. This factor will be decisive in the convergence of simulated annealing (1.36). The proof idea is usually the same. In the case of U defined on the periodic torus \mathbb{T}^d , it proceeds as follows. Let h_t be the density of X_t with respect to ν_{β_t} . Assuming that $h_t \in L^2(\nu_{\beta_t})$, we have:

$$\mathbb{P}(U(X_t) > \min U + \varepsilon) \leq \|h_t\|_{L^2(\nu_{\beta_t})} (\nu_{\beta_t}(U > \min U + \varepsilon))^{1/2}. \quad (1.37)$$

If we can show that $t \mapsto \|h_t\|_{L^2(\nu_{\beta_t})}$ is bounded, then we would obtain the desired result. Formally we have:

$$\begin{aligned} \partial_t \|h_t - 1\|_{L^2(\nu_{\beta_t})}^2 &= -\beta_t \int_{\mathbb{T}^d} |\nabla h_t|^2 d\nu_{\beta_t} + \beta_t' \int_{\mathbb{R}^d} (h_t - 1)^2 U d\nu_{\beta_t} \\ &\leq -\beta_t \lambda(\beta_t) \int_{\mathbb{T}^d} (h_t - 1)^2 d\nu_{\beta_t} + \beta_t' \|U\|_\infty \int_{\mathbb{T}^d} (h_t - 1)^2 d\nu_{\beta_t}. \end{aligned}$$

In this simple case where U is bounded (because continuous on a compact set), this computation combined with the estimate on λ from Proposition 1.3.1 indicates that if $\beta_t = \frac{\ln(1+t)}{c}$, then $\|h_t\|_{L^2(\nu_{\beta_t})}$ remains bounded as soon as $c > c^*$. To get the correct rate of convergence, one must actually replace the L^2 norm of the density in (1.37) by an L^∞ norm and use the Sobolev inequality. Proof of the convergence of the overdamped Langevin simulated annealing for slow logarithmic cooling schedule and of the non-convergence for fast logarithmic cooling schedule was first established by Holley, Kusuoaka and Strook [84, 83], using Sobolev inequalities, for a potential U on a compact manifold. The case of \mathbb{R}^n has been studied by Chiang, Hwang and Sheu [37], Royer [150] and Miclo [129], under restrictive conditions on the behavior at infinity of U , in particular $|\nabla U| \rightarrow +\infty$ at infinity. These conditions are related to the functional inequalities used in these works, in particular spectral gap and Nelson hypercontractivity inequalities. The question of reducing these assumptions in order to consider slowly-growing potentials has been addressed by Zitt in [171], essentially by replacing spectral gap inequalities by weaker functional inequalities. The results of Zitt apply for instance if, outside some ball, $U(x) = |x|^\alpha$ with $\alpha \in (0, 1)$. More recently, Fournier and Tardif in [64] and with Monmarché in [63] have been interested in somehow minimal conditions on the growth of U at infinity. In [63], they established that, for coercive potentials in the sense that $x \cdot \nabla U(x) \geq 0$ for $|x|$ large enough, there is a phase

transition for $U_\alpha(x) = \alpha \ln(1 + \ln(1 + |x|^2))$ at some value α_* of α (depending on the cooling schedule β and the dimension), i.e. there is convergence if $\alpha > \alpha_*$ and non-convergence if $\alpha < \alpha_*$, which is related to the transient properties of Bessel processes. More generally, convergence of the annealing algorithm is also proven in [63] under conditions that allow arbitrarily slow growth. In [64], the convergence of the simulated annealing is established as soon as $\lim_{|x| \rightarrow \infty} U(x) = \infty$ and $\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)} dx < \infty$ for some $\alpha_0 > 0$. Although it doesn't cover all the cases of [63] (notice indeed that the condition is not met for U_α for any $\alpha > 0$), this is a very simple and mild condition. One of the main differences of [64, 63] with respect to previous works is that the question of the recurrence of the process is treated separately from the question of convergence in probability to the minimum of U . Indeed, once recurrence is proven, it is essentially sufficient to use the known results of convergence in the compact case to conclude. Notice that, unfortunately, this localization argument does not provide a rate of convergence as did previous works. Note as well that the idea that the behavior of U at infinity is not so important already appears in [37, 150] (see in particular [37, Lemma 6.4]) where it is proven that it is sufficient (under the conditions enforced in these works) to prove the result in the case where $U(x) = |x|^4$ for $|x|$ large enough.

On the other hand, Monmarché studied in [137] the simulated annealing based on the kinetic Langevin process:

$$\begin{cases} dX_t = Y_t dt \\ dY_t = -\nabla U(X_t) dt - \beta_t Y_t dt + \sqrt{2} dB_t. \end{cases}$$

The use of this non reversible process is motivated by its better convergence properties with respect to the overdamped process, as discussed in Section 1.3.1, although, in the regime $\beta \rightarrow +\infty$, it doesn't reduce the critical value of c in the logarithmic regime. Convergence of the kinetic simulated annealing is established in [137] for slow logarithmic cooling schedules similar to the overdamped case, under restrictive conditions on U , namely U is essentially quadratic at infinity, and the Hessian of U is bounded. The proof is similar to the overdamped Langevin case except that establishing quantitative longtime convergence estimates (at a fixed β) for the process toward its equilibrium rely on so-called hypocoercive methods presented in 1.2.1. The arguments of [137] have been adapted to Generalized Langevin processes in [31]. This simulated algorithm can also be understood as a deterministic dynamics that converges towards local minima, to which we added a noise that goes to zero with time. The same can thus be done with process that does not admit the Gibbs measure as an equilibrium as in [23].

Contribution: Chapter 4 of this thesis is based on an article published in *Electronic Journal of Probability* [95]. The goal was to combine the works [137] and [64] to show convergence of the kinetic Langevin simulated annealing for potential under minimal conditions on the growth of U at infinity when $c > c^*$. We showed as well failure of the algorithm when $c < c^*$ using hypocoercivity methods in Sobolev spaces H^k , which seems to be a novel result for kinetic processes. Indeed, unlike the elliptic case, it remains an open problem to show that Sobolev inequality implies ultracontractivity, which was the main tool in the work [84, 83].

The previously mentioned Freidlin-Wentzell theory [65] also provides insights into the behavior of low-temperature diffusion processes, suggesting that such processes move from one potential well to another by passing through index-1 saddle points. One strategy for escaping the domain of attraction (for gradient descent) of a local minimum would hence be to actively search for saddle points. Building on this understanding, Chapter 5, which is based on an article published in *Statistics and computing* [96], we introduced a novel process for both optimisation and saddle point search in [96]. We conducted a numerical study of this new process on basic examples from both statistics and Molecular Dynamics, such as the Gaussian mixture (1.35), as well as addressed fundamental theoretical questions.

Let's motivate further this last contribution. In Molecular Dynamic, index-1 saddle points

are also of interest, as if the local minima of the energy represent the metastable states, they represent the transition pathways between metastable states of a physical system. However, saddle point search remains a less standard topic than optimisation, especially in probability. A first class of methods, based on reaction paths, requires the knowledge of two local minimizers, and then finds a path of minimal elevation between them, which passes through a saddle point see e.g. [70, 53]. A second class of methods, considered e.g. in [54, 121, 66, 115, 151, 17, 75] and references within and which will be the one used in the definition of the process of Chapter 5, relies on local walkers, analogous of the gradient descent for optimization, i.e. solutions of some ODEs for which saddle points of U are stable equilibrium. Given some $x \in \mathbb{R}^d$, write:

$$\lambda_1(x) \leq \lambda_2(x) \leq \dots \leq \lambda_d(x)$$

for the ordered eigenvalues of $\nabla^2 U(x)$, and suppose that we are given $v_1(x), \dots, v_d(x) \in \mathbb{R}^d$ such that $v_i(x)$ is an eigenvector of $\nabla^2 U(x)$ associated to $\lambda_i(x)$ (in other words, when the eigenvalues are not all simple, we assume that we have an arbitrary rule to select a given eigenbasis, for instance we take the basis obtained as the limit of the Jacobi algorithm). The idealised saddle dynamic (ISD) is the solution of

$$\dot{x}_t = - (I - 2v_1(x_t)v_1(x_t)^T) \nabla U(x_t). \quad (1.38)$$

In other words, x_t follows a gradient descent, except in the direction $v_1(x_t)$ where a reflection is performed, i.e. the process follows a gradient ascent in this direction. Notice that in general $x \mapsto v_1(x)$ is not continuous so the existence of this process is unclear and may be restricted to some parts of the space or to a finite time interval. One could also see a saddle point as a minimum of the function $x \mapsto |\nabla U(x)|^2$ or variants, which was done in [51, 19]. By introducing noise into the dynamic (1.38), we define a new process for locating index-1 saddle points. Subsequently, by alternately switching between this process and a noisy gradient descent (specifically, the overdamped Langevin process 1.8), we formulate a new process for optimization.

Perspectives: It would be of interest to show convergence (or non-convergence) for simulated annealing based on other non-reversible processes, such as annealed piecewise deterministic Markov process (e.g., the Zig-Zag process or Bouncy Particle Sampler), as they offer certain simulation advantages, or non-conservative overdamped Langevin process. This last example may prove useful in the context of this last switched process. Several open questions also remain for this switched process: how long does it take to exit from a well in the low temperature limit? What about the speed of convergence towards its invariant measure? What is the limit of the invariant measure when $\varepsilon \rightarrow 0$? What would be the long-term behavior of an annealed version of this process?

1.3.3 A particle approximation for quasi-stationary distributions

The third and final type of algorithm involves sampling the quasi-stationary distribution using the Fleming-Viot process. Let's first motivate this purpose. In Molecular Dynamic, it is of interest to sample state-to-state dynamics. Assuming that we can partition space into metastable subsets of a given Markov process X through a mapping $S : \mathbb{R}^d \rightarrow \mathbb{N}$, the goal is to efficiently compute a trajectory $S(X_t)$. However, by definition, exiting a metastable state takes a very long time. To accelerate such exit, various algorithms, collectively known as kinetic Monte Carlo (kMC) methods, have been developed. One such algorithm is the parallel replica algorithm [104], which relies on the sampling of a quasi-stationary distribution (QSD). In all generality, it is defined as follow:

Definition 1.3.2. *Given a Markov process X living in a domain D and a stopping time τ , a QSD is a probability measure μ that satisfies:*

$$\mathbb{P}_\mu(X_t \in \cdot | \tau > t) = \mu,$$

for all $t \geq 0$.

This definition is similar to that of the stationary measure, and like stationary measures, QSDs describe the long-term behavior of the process but are conditioned on the fact that $\tau > t$. In kMC, this stopping time corresponds to the exit time of a metastable domain D :

$$\tau_{\partial D} = \inf \{t \geq 0, X_t \notin D\}, \quad (1.39)$$

where D is an open set. In many cases, it can be shown that there exists a unique QSD $\mu \in \mathcal{M}^1(D)$, and

$$\forall \nu \in \mathcal{M}^1(D), \lim_{t \rightarrow \infty} \mathbb{P}_\nu(X_t \in \cdot | \tau > t) = \mu.$$

In metastable cases, this convergence is faster than the exit time of the domain D , and hence, for some intermediate time scale, the law of X is described by the QSD. Therefore, QSDs are another valuable tool for the study of metastability, in addition to the study of constants in functional inequalities, as seen in Proposition 1.3.1. Moreover, it can be shown that:

Proposition 1.3.2. *If μ is a QSD, then there exists $\alpha > 0$ such that:*

$$\forall t \geq 0; \mathbb{P}_\mu(\tau > t) = e^{-\alpha t}.$$

This arises from the fact that a QSD is an eigenvector of a certain operator, and α is thus an eigenvalue. This property is actually an equivalence in many cases, see [104, Proposition 4]. The idea behind the parallel replica algorithm is to wait for some time for the law of the process to reach its QSD, and then replace the process with N independent processes $(X^i)_{1 \leq i \leq N}$, all starting from the QSD. Denote

$$\tau_1^N = \inf \{t \geq 0, \exists i \in \llbracket 1, N \rrbracket, X_t^i \notin D\},$$

and let I_1^N be the index of the particle that exited the domain at time τ_1^N . The property of the QSD implies that $(\tau_1^N, X_{\tau_1^N}^{I_1^N})$ is equal in law to $(\tau/N, X_\tau)$, where X is started from the QSD. This implies that we can sample an exit event exactly in a time N times smaller, and the error is simply introduced by approximating the law of X with the QSD.

However, the conditioning introduces a non-linearity in the evolution of $\mathbb{P}(X_t \in \cdot | \tau > t)$, which adds complexity to the sampling process and introduces new phenomena compared to the study of stationary distributions. For instance, a linear combination of QSDs is not necessarily a QSD, implying that there might be a finite but greater than one number of QSDs (which is not possible for stationary measures). Before delving into the sampling methods, let's explore killed processes further.

Stopping times, also called killing times, are usually of two types: the so-called soft-killing and hard-killing. Hard-killing corresponds to the exit of a domain, and is usually challenging to study. Given some domain $D \subset E$, it is given by (1.39). On the other hand, soft-killing is a more regular case, and given some death rate $\lambda : E \rightarrow \mathbb{R}_+$ and an exponential random variable E_λ with parameter 1, we define the killing time as:

$$\tau_\lambda = \inf \left\{ t \geq 0, E_\lambda \leq \int_0^t \lambda(X_s) ds \right\}.$$

Using τ as a general killing time, a killed process defines a non-conservative semi-group by:

$$P_t f(x) = \mathbb{E}(f(X_t) \mathbb{1}_{\tau > t}).$$

Similar to the conservative Markov semi-group, P_t is solution to a PDE. If the process is killed outside a domain D , then $P_t f$ is the solution to the PDE with Dirichlet condition:

$$\begin{cases} \partial_t v = Lv, \\ v(0, \cdot) = f, \\ v|_{\partial D} = 0, \end{cases} \quad (1.40)$$

for f in a suitable class of function, and where L is the generator of the underlying Markov process. In the case of soft-killing, the semi-group is the solution to:

$$\begin{cases} \partial_t v = Lv - \lambda v, \\ v(0, \cdot) = f. \end{cases} \quad (1.41)$$

In any case, the considerations on long-time behavior of Markov process can be extended to killed processes. The QSD is a left-eigenvector of this semi-group. In the case where the process is symmetric with respect to some reference measure μ , the QSD admits a density with respect to this measure which is a right eigenvectors of the semi-group. Usual spectral gap is now defined as the difference between the first and second eigenvalues, which gives the rate of convergences towards the QSD, and the first eigenvalue is the killing rate from Proposition 1.3.2. The soft-killing case is linked with Feynman-Kac semi-group, as we have the following equality:

$$P_t f(x) = \mathbb{E}_x \left(f(X_t) e^{-\int_0^t \lambda(X_s) ds} \right).$$

The sampling of QSD is thus of interest in simulating the ground states of Schrödinger's operator. For further references on the study of QSDs, see [35, 47, 36, 32, 7, 60, 8] and references within.

In a manner akin to McKean-Vlasov diffusions (1.30), a mean-field particle system \mathbf{X} , known as the Fleming-Viot process, can be used to sample the QSD. Informally, it operates as follows: each of the $N \in \mathbb{N}$ particles evolves independently, following the same dynamics as X , until one of them is killed. The killed process then selects another particle uniformly at random, branches into it, and subsequently evolves independently of the others from this new position. More rigorously: fix some initial condition $\mu \in \mathcal{M}^1(D^N)$. Let $(I_n^i)_{1 \leq i \leq N, n \in \mathbb{N}}$ be a family of independent random variables, where for $1 \leq i \leq N$, I_n^i is uniform on $\{1, \dots, N\} \setminus \{i\}$. Let $\mathbf{X}_0 = (X_0^1, \dots, X_0^N)$ be distributed according to μ , and (\bar{X}^i) be a family of independent Markov processes following the same dynamic as X , with $\bar{X}_0^i = X_0^i$. Set

$$\tau_1 = \min_i \tau_1^i,$$

where τ_1^i is the killing time of \bar{X}^i . Then, denote by i_1 the index of the particle which died at time τ_1 . It is uniquely defined almost surely if, for example, the death time has a density on \mathbb{R}_+ , so that the probability that two particles hit the boundary at the same time is zero (this is true in most cases of interest). For $i \neq i_1$, $0 \leq t \leq \tau_1$, or $i = i_1$ and $1 \leq t < \tau_1$, simply let:

$$X_t^i = \bar{X}_t^i \quad \text{and} \quad X_{\tau_1}^{i_1} = \bar{X}_{\tau_1}^{i_1}.$$

This defines the process between times 0 and τ_1 . The process is then defined on (τ_1, ∞) by

induction: if the process is defined up to time τ_{n-1} , we define it between time τ_{n-1} and τ_n in the same way, with \mathbf{X}_0 replaced by $\mathbf{X}_{\tau_{n-1}}$, i_1 by i_n the index of the particle that hits ∂D at time τ_n , and $I_1^{i_0}$ by $I_n^{i_n}$. Thus, $(\tau_n)_n$ is the sequence of branching times of the process.

Under mild assumption, the process $\mathbf{X} = (X^1, \dots, X^N)$ is well-defined and does not explode in finite time, in the sense that $\sup_n \tau_n = \infty$ almost surely. This holds true immediately in the soft-killing case as long as $\|\lambda\|_\infty < \infty$. Refer to [166, Theorem 2.1] and [14, 15] for diffusions killed at the boundary of a domain.

If X is a Markov process with generator L , killed at rate λ , then the Fleming-Viot process is a Markov process with generator:

$$\mathcal{L}f = \sum_{i=1}^N \left(L_i f + \frac{\lambda(x_i)}{N-1} \sum_{j \neq i} (f(\mathbf{x}^{i,j}) - f(\mathbf{x})) \right),$$

for $f : E^N \rightarrow \mathbb{R} \in \mathcal{D}(L)$, where $L_i f = L(x_i \mapsto f(x_1, \dots, x_N))$ and $\mathbf{x}_k^{i,j} = \mathbf{x}_k$ if $k \neq j$ and $\mathbf{x}_j^{i,j} = \mathbf{x}_i$. A martingale formulation for a hard killed process is more challenging to define and can be found in [71, Proposition 1].

Fleming-Viot processes were first introduced in the work of Moran [139], in the study of population genetics models. Their application to the approximation of a QSD dates back to [25], where the authors study the case of a Brownian motion in a rectangle. They were interested in the following convergence, commonly known as propagation of chaos, which can be shown in many cases:

$$\lim_{N \rightarrow \infty} \frac{1}{N} \sum_{i=1}^N f(X_t^i) = \mathbb{P}(X_t \in \cdot | \tau > t), \quad (1.42)$$

for f in a suitable class of functions, under certain assumptions on the initial conditions, thus affirming that the process may be used for sampling purposes in the case of conditioned process. Since then, many results have been proven in different cases and for various questions, including long-time convergence, propagation of chaos, and existence of the Fleming-Viot process.

In the case of a process in a countable state space, the study began with [59]. The Fleming-Viot process is well defined here as soon as the death rate is bounded, and the authors have shown, under several conditions, the uniqueness of the QSD, convergence toward this QSD, the ergodicity of the Fleming-Viot process, and the propagation of chaos for finite time and at equilibrium. In [73], the authors improved the propagation of chaos with a quantitative rate, introducing the π -return process. For processes in a finite state space, the propagation of chaos is proven for all times and for the stationary measure, with a stronger convergence in [5], and the convergence as $N \rightarrow \infty$ was refined with a central limit theorem in [108].

In the case of processes in a general space, numerous results are available. Finite-time propagation of chaos is addressed in [24, 71, 165, 45], with central limit theorems as $N \rightarrow \infty$ in [29, 48]. Then, uniform-in-time propagation of chaos and long-time convergence are established in [46, 44, 149]. The long-time convergence is established when the underlying process is a Brownian motion in [25].

Other methods of approximating a QSD have been developed in discrete and continuous cases in [12, 13, 11], based on self-interacting processes

In cases where multiple QSDs exist, one of them is defined as the minimal and corresponds to the greatest associated eigenvalue. The associated Fleming-Viot process is usually still an irreducible Markov process and hence possesses a unique invariant measure. It is expected that this invariant measure converges toward the minimal QSD, but this remains open in many cases. This problem has been addressed in [34, 72, 160].

Contributions: Part III of the thesis is dedicated to the study of the Fleming-Viot process. For practical purposes, when the objective is to compute averages against the QSD, we are interested in bounds of the form

$$\mathbf{d}(\pi_t, \mu) \leq C \left(\frac{1}{N^\alpha} + e^{-ct} \right),$$

for some distance \mathbf{d} on the set of probability measure, where π is the empirical measure of the particle system, and μ the target distribution. Such bounds allow for the separate choice of the number of particles and the time to achieve a specific level of error. To this end, Chapters 6 and 7 prove such bounds by establishing exponential ergodicity of the Fleming-Viot system at a rate independent of N in the sense that there exist $C, c > 0$ independent of N such that for all $t \geq 0$:

$$\|\nu P_t^N - \mu^N\|_{TV} \leq NCe^{-ct}, \quad (1.43)$$

where P^N is the semi-group of the Fleming-Viot system with N particle, and μ^N its invariant measure. The scaling in N in this convergence is what one would obtain in the case of a vector comprised of N independent processes.

Chapter 6, based on a paper published in *ESAIM: Probability and Statistics* [94], is concerned with the soft-killing case, where a numerical scheme for the system is also proposed. Chapter 7 studies the hard-killing regime for the overdamped Langevin process (1.8) in a metastable domain. Both works are based on the coupling method presented in Section 1.2.2. These works use a perturbation approach where the interaction is assumed to be small enough with respect to the mixing properties of the underlying Markov process, corresponding to the metastable regime, notably for kMC. On the other hand, Chapter 8 deals with a Fleming-Viot process based on a non-metastable system, namely for which killing occurs on a faster time scale than convergence to (quasi-)stationarity. In the simplest case of a countable state space, we show that in the limit where the minimum of the killing rate goes to infinity, instead of converging towards a deterministic measure, the empirical measure process converges towards a dynamic in the set of Dirac measures.

Perspectives: It would be of interest to construct a coupling that implies exponential ergodicity (1.43) outside of the case where mixing is faster than killing. This could be achieved by studying the variance of the particle system, as Chapter 8 suggests that in cases where the death rate is high, the empirical measure is close to a Dirac, indicating that the particles are close to one another.

Additionally, exploring whether exponential ergodicity, independent of N , remains true when the first eigenvalue is smaller than the spectral gap would be valuable. Studying scenarios where mixing might not occur in the diffusion process but could emerge through killing and re-sampling is also intriguing. This is relevant to situations resembling Schrödinger operators that arise in quantum physics, which are operators of the form $\Delta + V$, where V is a confining potential.

Another interesting question concerns the sampling of an exit event using the Fleming-Viot process. Starting from the QSD, the exit time of a domain follows an exponential distribution, independent of the event's location. The parallel replica algorithm relies on sampling such a random variable when the initial condition is the QSD. However, with the Fleming-Viot process, there is a bias in the sampling, as we can only access its stationary measure. Under this invariant measure, and with a finite number of particles, correlations exist between them, which are expected to go to 0 as N goes to infinity. This raises crucial questions for practitioners: if τ^N is the first time a particle is killed in the Fleming-Viot process, what is the limiting behavior of $(N\tau_1^N, X_{\tau_1^N})$? Given that the Fleming-Viot process enables the sampling of several killing events, does this result in a sequence of inter-event times $N(\tau_k^N - \tau_{k-1}^N)$ that converges to a

Poisson process?

Part I

Sampling Gibbs measures

Chapter 2

Weak error expansion of a numerical scheme with rejection for singular Langevin process

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Abstract : We show expansion *à la Talay-Tubaro* of a numerical scheme with rejection for the Langevin process in the case of a singular potential. In order to achieve this, we provide estimates on the associated semi-group of the process. The class of admissible potentials includes the Lennard-Jones interaction with confinement, which is an important potential in molecular dynamics and served as the primary motivation for this study.

2.1 Introduction

As explained in Section 1.3.1, we are interested here in the sampling of the Gibbs measure

$$\mu_\beta(dx, dy) = \frac{e^{-\beta H(x,y)}}{Z} dx dy, \quad (2.1)$$

where

$$H(x, y) = U(x) + \frac{1}{2}|y|^2, \quad (2.2)$$

$U : \mathbb{R}^d \rightarrow \mathbb{R}_+$ (or $U : \mathbb{T}^d \rightarrow \mathbb{R}_+$, where \mathbb{T}^d is the d -dimensional torus) is a potential function, $|y|^2/2$ represents the kinetic energy, and Z is a normalization constant. One important example in chemistry is a system of $N \gg 1$ particles with van der Waals interaction, which corresponds to a noble gas. In this case, $d = 3N$, and $x = (x_1, \dots, x_N)$ represents the positions of the particles. The potential can be written as

$$U(x) = \sum_{i=1}^N U_c(x_i) + \sum_{1 \leq i \neq j \leq N} U_i(|x_i - x_j|),$$

where $U_c : \mathbb{R}^{3N} \rightarrow \mathbb{R}_+$ is a confining potential and for $r \in \mathbb{R}^3$,

$$U_i(r) = 4 \left(\frac{1}{|r|^{12}} - \frac{1}{|r|^6} \right).$$

The interaction part U_i is commonly known as the Lennard-Jones potential. In the case where the gas is confined in a volume D , one could then get its pressure by computing the average

$$P = \mu_\beta(f_P), \quad f_P(x, y) = \frac{1}{3|D|} \sum_{i=1}^N \left(\frac{y_i^2}{m} - x_i \cdot \nabla_{x_i} U(x) \right),$$

where $m > 0$ is the mass of a particle. What makes this example interesting is the presence of singularities in the potential, as it can take infinite value, and the fact that the function f_P is not locally integrable.

For non-singular potentials, there are numerous numerical schemes available to simulated from the Langevin process

$$\begin{cases} dX_t = Y_t dt, \\ dY_t = -\nabla U(X_t) dt - \gamma Y_t dt + \sqrt{2\gamma\beta^{-1}} dB_t, \end{cases} \quad (2.3)$$

The goal here is to adapt such a scheme and prove a series expansion in the weak convergence for singular potential, focusing on the following one:

$$\begin{cases} \bar{X}_{n+1} = \bar{X}_n + \mathbb{1}_{E_\delta(\bar{X}_n, \bar{Y}_n, G_n) \in \mathcal{H}_{\delta, \ell}} \delta \bar{Y}_{n+1}, \\ \bar{Y}_{n+1} = \bar{Y}_n + \mathbb{1}_{E_\delta(\bar{X}_n, \bar{Y}_n, G_n) \in \mathcal{H}_{\delta, \ell}} \left(-\delta \nabla U(\bar{X}_n) - \delta \gamma \bar{Y}_n + \sqrt{2\gamma\beta^{-1}} \delta G_n \right) \end{cases} \quad (2.4)$$

for some time step $\delta > 0$, where (G_n) is a family of independent standard Gaussian random variable, and where for a small fixed parameter $\ell > 0$,

$$\mathcal{H}_{\delta, \ell} = \{ \phi \leq \delta^{-\ell} \}, \quad (2.5)$$

with

$$\phi(x, y) = H(x, y) + 4d\gamma\beta^{-1} \frac{y \cdot \nabla U(x)}{1 + |\nabla U(x)|^2}, \quad (2.6)$$

and

$$E_\delta(x, y, g) = \left(x + \delta \left(y - \delta \nabla U(x) - \delta \gamma y + \sqrt{2\gamma\beta^{-1}\delta}g \right), y - \delta \nabla U(x) - \delta \gamma y + \sqrt{2\gamma\beta^{-1}\delta}g \right).$$

The definition of ϕ stems from the fact that, under our assumptions, for all $b < \beta$, $e^{b\phi}$ is a Lyapunov function for the Langevin process (2.3) (see Proposition 2.3.3 below), as well as for this numerical scheme (as proved in Lemma 2.4.2). Hence, this numerical scheme is a version with rejection of the following (first-order) splitting scheme

$$\begin{cases} \tilde{X}_{n+1} = \tilde{X}_n + \delta \tilde{Y}_{n+1}, \\ \tilde{Y}_{n+1} = \tilde{Y}_n - \delta \nabla U(\tilde{X}_n) - \delta \gamma \tilde{Y}_n + \sqrt{2\gamma\beta^{-1}\delta}G_n, \end{cases} \quad (2.7)$$

but we only accept a step of the scheme if its Lyapunov function doesn't exceed some threshold depending on the time step. We could have considered a simple Euler-Maruyama scheme, but if the initial condition satisfies $U(X_0 + \delta Y_0) = \infty$, then the chain would not be well defined. The splitting scheme (2.7) is the simplest numerical scheme that is well-defined with probability 1 for all initial conditions, and under a one-sided Lipschitz condition on U , it can be shown that this Markov chain is ergodic. However, there is another problem, which is that even if the numerical scheme is almost-surely well defined, \tilde{X}_n has a density bounded below by the Lebesgue measure on all compact sets. Hence, if f is not locally integrable, then :

$$\mathbb{E}(f(\tilde{X}_n)) = \infty, \quad \forall n \geq 1.$$

This is also the case for all splitting schemes, and it poses two problems. Firstly, it restricts us to consider averages only against bounded functions, which excludes the computation of important quantities such as the mean energy for the Lennard-Jones potential or the pressure of noble gases. Secondly, it prevents the construction of a Lyapunov function, which is a critical step in the proof of weak convergence for numerical schemes. To address these issues, we introduced the numerical Scheme (2.4), which has better integrability properties, see Section 2.4. Any scheme used for bounded smooth potential (e.g. splitting schemes) can be adapted in a similar manner (namely with rejection) for singular potentials. We study this specific first-order splitting scheme for simplicity. In the context of singular potentials in high-dimensional spaces, an implicit scheme may be ill-defined, and in any case would have a prohibitive numerical cost. Hence, we consider only explicit schemes. Another possible numerical scheme would have been to use rejection at a threshold depending only on the energy, i.e. replacing $\{\phi \leq \delta^{-\ell}\}$ by $\{H \leq \delta^{-\ell}\}$. However, since the Hamiltonian is not a Lyapunov function of the Langevin process, it is not clear that this numerical scheme admits $e^{b\phi}$ as a Lyapunov function, and hence satisfies the integrability property needed for the proofs. Notice in particular that ∇U is already computed for the drift, hence no supplementary computations are needed to check if ϕ is low enough. While in practice, averages are often computed using schemes without rejection, there are cases where rejection could lead to better results. The discussion in Section 2.2.2 likely elaborates further on this aspect.

There are two approaches for showing the convergence of a numerical scheme towards the continuous process. The first one is strong convergence, which focuses on the convergence of trajectories. However, since our goal is the computation of averages, we are interested in weak convergence. For $f : \mathbb{R}^d \rightarrow \mathbb{R}$ in a suitable class of functions and $t \geq 0$, we aim to show that:

$$\lim_{\delta \rightarrow 0} \mathbb{E}(f(\bar{X}_n)) = \mathbb{E}(f(X_t)),$$

where $n = \lfloor t/\delta \rfloor$. Our objective is to get a series expansion of this convergence, commonly known as expansion *à la Talay-Tubaro*, from the seminal work [158]. Write (P_t) for the semi-group of the Langevin process (2.3) defined for regular and integrable enough function by:

$$P_t f(x, y) = \mathbb{E}_{(x, y)}(f(X_t, Y_t)).$$

Methods to show weak convergence and series expansion of such convergence rely on estimates on $P_t f$ and its derivatives, typically of the form: for $f : \mathbb{R}^d \rightarrow \mathbb{R}$, which grows at most polynomially at infinity (as well as its derivative of all orders), for all multi-index $\alpha \in \mathbb{N}^{2d}$, there exists $C, k > 0$ such that:

$$|\partial^\alpha P_t f(x, y)| \leq C(1 + |x|^k + |y|^k).$$

Such estimates cannot hold in the singular setting. Therefore, the primary objective of this work is to establish equivalent estimates in the singular setting, which will be addressed in Section 2.3. Those estimates will then enable us to prove in Section 2.4 an expansion *à la Talay-Tubaro* for the numerical scheme (2.4), as well as for its invariant measure. In Section 2.2, we will present the assumptions, theorems, and comparisons with existing works.

2.2 Mathematical setting and results

2.2.1 Assumptions and mains results

Fix a potential $U : \mathbb{R}^d \rightarrow [0, \infty]$ and write

$$\mathcal{D} = \{x \in \mathbb{R}^d, U(x) < \infty\}, \quad \mathcal{X} = \mathcal{D} \times \mathbb{R}^d, \quad (2.8)$$

for the domain of definition of the process (X, Y) solution to equation (2.3). In all of this work, we will write $z = (x, y) \in \mathcal{X}$ for the global variable, and $|\cdot|$ for the l^2 -norm on \mathbb{R}^d . For any Banach space \mathcal{B} , let $\mathcal{C}^\infty(\mathcal{B}, \mathbb{R})$ denote the set of smooth functions from \mathcal{B} to \mathbb{R} , $\mathcal{C}_b^\infty(\mathcal{B}, \mathbb{R})$ the set of bounded smooth functions, and $\mathcal{C}_c^\infty(\mathcal{B}, \mathbb{R})$ the set of smooth functions with compact support. Let $\mathcal{M}^1(\mathbb{R}^{2d})$ denote the set of probability measures on \mathbb{R}^{2d} . We work under several sets of assumptions. First:

Assumption 2.2.1. • $U \in \mathcal{C}^\infty(\mathcal{D}, \mathbb{R}_+)$.

- \mathcal{D} is connected and the set:

$$\mathcal{D}_n = \{x \in \mathbb{R}^d, U(x) < n\}$$

is bounded for all $n \in \mathbb{N}$.

- U defines a Gibbs measure at temperature β :

$$\int_{\mathcal{D}} e^{-\beta U(x)} dx < \infty.$$

Assumption 2.2.2. • The following limit holds:

$$\lim_{x \rightarrow \mathcal{D}^c} \frac{|\nabla^2 U(x)|}{|\nabla U(x)|^2} = 0.$$

- There exists $c_0, c_\infty, d_0, d_\infty > 0$, $\eta_0 \in \mathbb{R} \setminus [-1, 0]$, $\eta_\infty > 1$ such that:

$$c_\infty U^{2 - \frac{2}{\eta_\infty}} + d_\infty \leq |\nabla U|^2 \leq c_0 U^{2 + \frac{2}{\eta_0}} + d_0.$$

Assumption 2.2.3. For all $\alpha \in \mathbb{N}^d$, there exist $C_\alpha > 0$, $k_\alpha \in \mathbb{N}$ such that

$$|\partial^\alpha U| \leq U^{k_\alpha} + C_\alpha.$$

Let $\mathcal{P}(U)$ denote the set of admissible functions for our theorems:

$$\mathcal{P}(U) = \{f \in C^\infty(\mathcal{X}, \mathbb{R}) \mid \forall \alpha \in \mathbb{N}^{2d}, \exists C, c > 0, c < \beta, |\partial^\alpha f| \leq C e^{cH}\}.$$

The first theorem gives the estimates on the semi-group necessary for the proof of weak convergence.

Theorem 2.2.1. Suppose Assumptions 2.2.1, 2.2.2 and 2.2.3. Then for all $f \in \mathcal{P}(U)$, and all multi-index $\alpha \in \mathbb{N}^{2d}$, there exist $C, q > 0$, $b \in (\beta(1 - \frac{1}{2d}), \beta)$, such that for all $t > 0$, $z \in \mathcal{X}$

$$|\partial^\alpha (P_t f - \mu_\beta(f))(z)| \leq C e^{-qt} e^{bH(z)}.$$

This theorem allows for the proof of the two following theorems:

Theorem 2.2.2. Suppose Assumption 2.2.1, 2.2.2 and 2.2.3. Then there exists $l_0 > 0$ such that for all $0 < \ell < l_0$, $f \in \mathcal{P}(U)$, and $t \geq 0$, there exists a family $(C_i(t))_i$ of explicit real numbers such that for all $k \in \mathbb{N}$:

$$\mathbb{E}_z(f(\bar{Z}_n)) = \mathbb{E}_z(f(Z_t)) + C_1(t)\delta + \dots + C_k(t)\delta^k + O(\delta^{k+1}),$$

where $(\bar{Z}_n)_n = (\bar{X}_n, \bar{Y}_n)_n$ is the numerical scheme defined in (2.4), $n\delta = t$, and $O(\delta^{k+1})$ is uniform in t .

Theorem 2.2.3. Suppose Assumption 2.2.1, 2.2.2 and 2.2.3. Then there exists $\delta_0, \ell_0 > 0$ such that for all $0 < \delta < \delta_0$, $0 < \ell < \ell_0$, the numerical scheme defined in (2.4) admits an unique invariant measure $\mu_{\beta, \delta} \in \mathcal{M}^1(\mathbb{R}^{2d})$. For all $f \in \mathcal{P}(U)$, there exists $C, c > 0$ such that for all $z \in \mathcal{H}_{\delta, \ell}$:

$$|\mathbb{E}_z(f(\bar{Z}_n)) - \mu_{\beta, \delta}(f)| \leq C e^{-cn}.$$

Moreover, there exists a family $(\tilde{C}_i)_i$ of explicit real numbers such that for all $k \in \mathbb{N}$:

$$\mu_{\beta, \delta}(f) = \mu_\beta(f) + \tilde{C}_1\delta + \dots + \tilde{C}_k\delta^k + O(\delta^{k+1}).$$

Let's comment on those assumptions and theorems. Assumptions 2.2.1 and 2.2.2 are derived from [10], on which this work is based. As explained in their work, Assumption 2.2.1 is the minimal requirement to ensure the pathwise well-posedness of the process (2.3), as well as for the Gibbs measure to be well-defined and a stationary measure of the Langevin process. Assumption 2.2.2 differs slightly from the one in [10], as they suppose that there exists $\kappa > 0$ such that for all $v \in \mathbb{R}^d$

$$|\nabla^2 U(x)v| \leq \frac{\beta}{16d} |\nabla U(x)|^2 |v| + \kappa |v|, \quad (2.9)$$

which would allow potentials that exhibit logarithmic singularities. Here, we forbid those potentials, following the assumption stated in [82]. This assumption plays a vital role in the construction of a Lyapunov function for both the continuous-time process and the numerical scheme. We

need a Lyapunov function of order e^{bH} for any $b < \beta$, which cannot be achieved under (2.9). In this case, it would be possible that the bounds on the semi-group given by Theorem 2.2.1 are not in $L^1(\mathcal{L}aw(\bar{Z}_n))$. Since the proof of theorem 2.2.1 relies on computation in Sobolev spaces, and the use of Sobolev embedding, as in [170, 95], we need an additional assumption on the derivatives of the potential of all orders in order to carry out the computation. However, the Villani-type condition presented in [170] is not satisfied by singular potentials, as in the H^1 case from [10]. Therefore, we impose Assumption 2.2.3. This set of assumptions encompasses any repulsive interaction that exhibits a sufficiently rapid explosion (at least algebraic), such as Lennard-Jones interaction, and Coulomb interaction as soon as the particles are living in \mathbb{R}^q for $q \geq 3$, coupled with an additional confinement potential. However, it's important to note that 2-dimensional Coulomb interactions ($U_i(r) \propto \ln(r)$) do not satisfy these assumptions.

It is well-established in numerical probability that the proof of weak convergence relies on estimates of the kind given by Theorem 2.2.1. The proof of this theorem is based on Gamma calculus, see Section 1.2.1. This enables us to make series expansion at any order of the error induced by the numerical scheme at each step, with a remaining term of the form $\delta^k \mathbb{E} \left(e^{bH(\bar{Z}_n)} \right)$. This would be infinite in the case of a numerical scheme without any rejection mechanism like (2.7), but we will show that in the case of the numerical scheme (2.4), there is, under our assumptions, as in the continuous setting, a Lyapunov function of this order, uniformly over small time step. In particular, we may apply the method developed in [158] to get weak convergence as well as expansion *à la Talay-Tubaro* for this numerical scheme. It can be noticed from the proofs that the constants $(C_k(t))_k$ and $(\tilde{C}_k(t))_k$ are independent of $\ell > 0$, and can be expressed in the same way as if we considered the numerical scheme (2.7) with a regular potential, as in [107]. For instance, we have the following formula:

$$C_1(t) = \int_0^t \mathbb{E}_z (\psi(s, Z_{t-s})) ds,$$

where

$$\begin{aligned} \psi(t, z) = & (\nabla U + \gamma y) \cdot (\nabla_y / 2 - \nabla_x) P_t f + \frac{1}{2} \partial_t^2 P_t f - \frac{1}{2} y \cdot \nabla_x \partial_t P_t f + \frac{1}{2} (\nabla U + \gamma y) \cdot \nabla_y^2 y (\nabla U + \gamma y) \\ & - \frac{1}{2} y \cdot \nabla_{x,y}^2 (\nabla U + \gamma y) + \gamma \beta^{-1} \sum_{i=1}^d \partial_{x_i} \partial_{y_i} P_t f - \frac{2}{3} \gamma \beta^{-1} \partial_t \Delta_y P_t f \\ & - \frac{7}{12} \gamma \beta^{-1} (\nabla U + \gamma y) \cdot \nabla_y \Delta_y P_t f + \frac{1}{3} \gamma \beta^{-1} y \cdot \nabla_x \Delta_y P_t f \\ & + \frac{1}{2} (\gamma \beta^{-1})^2 \sum_{i=1}^d \partial_{y_i}^4 P_t f + \frac{1}{6} (\gamma \beta^{-1})^2 \sum_{i \neq j=1}^d \partial_{y_i}^2 \partial_{y_j}^2 P_t f. \end{aligned}$$

Besides, a corollary of Theorem 2.2.2 is the uniform in time weak convergence of the process. For a given $f \in \mathcal{P}(U)$, and $z \in \mathbb{R}^{2d}$, there exists $C > 0$ such that for all $t \geq 0$, $n\delta = t$:

$$|\mathbb{E}_z(f(\bar{Z}_n)) - \mathbb{E}_z(f(Z_t))| \leq C\delta.$$

Theorems 2.2.2 and 2.2.3 are also motivated by the following fact:

$$2\mathbb{E} \left(f \left(Z_{2n}^{\delta/2} \right) \right) - \mathbb{E} \left(f \left(Z_n^\delta \right) \right) = \mathbb{E} \left(f \left(Z_t \right) \right) - \frac{C_2}{2} \delta^2 + O(\delta^3),$$

which yields a better order convergence. With arbitrary order expansion, it is possible to get any

order of convergence using a combination of $\left(\mathbb{E}\left(f\left(Z_{2^k n}^{\delta/2^k}\right)\right)\right)$. This is the so-called Romberg-Richardson interpolation. For numerical experiments on this improvement, see the work of Talay and Tubaro [158].

2.2.2 Comparison between numerical scheme with and without rejection

In practice, numerical studies often utilize splitting schemes with no rejection on the bounded torus. If the potential is defined on $\mathbb{T}^d = (\mathbb{R}/\mathbb{Z})^d$, then the Langevin process (2.3) would be defined on $\mathbb{T}^d \times \mathbb{R}^d$. All proofs would still be valid, preserving the theorems' validity. As discussed in the introduction, for the numerical scheme (2.7), it is not possible to take the expectation of unbounded functions, and an invariant probability measure may not exist. Additionally, it also remains an open problem as to whether finite time weak expansion would still hold under our assumptions for bounded functions and numerical schemes without rejection. Regarding the use of schemes without rejection in practical applications, it is justified by the fact that the continuous process does not reach the singularities. For any fixed time $T > 0$, one can select a time step $\delta > 0$ small enough so that the numerical scheme without rejection does not get close to the singularities, and the computation of averages would yield reasonable results. However, for a fixed δ , the scheme would approach arbitrarily close to the singularity in large time, leading to abnormally large steps. Whereas with the rejection mechanism, it is possible to choose larger time steps, resulting in a more computationally efficient process, and avoiding the issue of getting too close to the singularities. This advantage of the rejection mechanism makes it a preferable choice in certain practical scenarios, such as in the following 1-dimensional toy model:

$$U(x) = \frac{1}{x} + x^2,$$

for which we conducted the following numerical experiment: fix $\beta^{-1} = 15$, $\gamma = 1$, and a final time $T = 15000$. Define the empirical averages by

$$n \mapsto S_n = \frac{1}{n} \sum_{k=0}^{n-1} U(Y_k),$$

where $Y_k = \bar{X}_k$ or $Y_k = \tilde{X}_k$. For different values of δ , we simulate $K = 1000$ copies S^i of $S_{\lfloor T/\delta \rfloor}$. We plot the evolution of the proportion of copies that have more than 1% error:

$$\delta \mapsto \frac{1}{K} \sum_{i=1}^K \mathbb{1}_{S^i \notin [0.99\mu_\beta(U), 1.01\mu_\beta(U)]},$$

where we estimated $\mu_\beta(U)$ using *Wolfram Alpha*. We get the result in Figure 2.1.

We can observe that for very small δ , the scheme without rejection produces satisfactory results. Nonetheless, there exists an interval of values of δ where the scheme with rejection significantly outperforms the other. The proportion of failures does not converge to 0 because of the error stemming from insufficiently long simulation times. For values of δ that aren't small enough, the energy threshold cannot, to prevent explosion, be set high enough to ensure the convergence of the empirical averages to a value close to $\mu_\beta(U)$ (≈ 9.035). This behavior is illustrated in Figure 2.2, where we display a typical trajectory for both cases, with $\delta = 10^{-2}$.

For smaller β , the explosion phenomenon would be even more prominent because the variance of the Gaussian distribution is proportional to $\gamma\delta\beta^{-1}$. As β decreases, the variance increases,

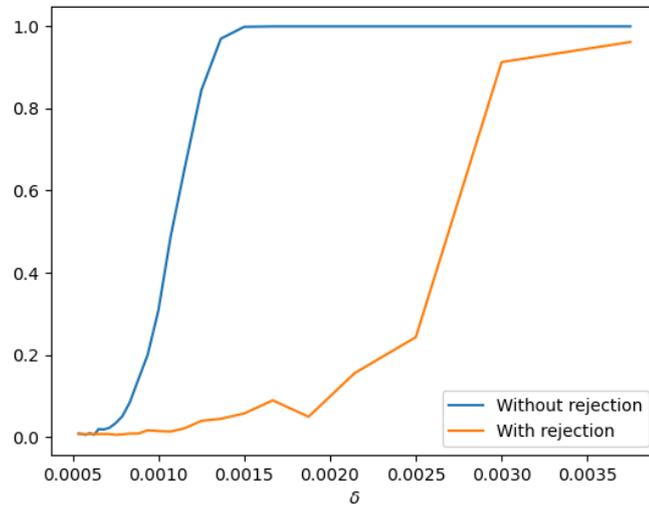
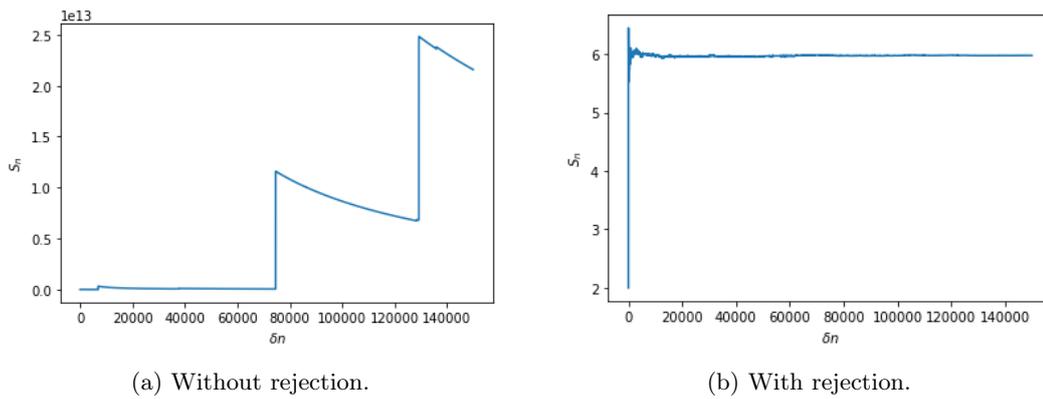


Figure 2.1: Failure probability.



(a) Without rejection.

(b) With rejection.

Figure 2.2: $n \mapsto S_n$, $\delta = 10^{-2}$.

making the numerical scheme more susceptible to divergent behavior and explosions in the trajectories. Hence, a smaller β exacerbates the challenge of handling the singularities and maintaining stable and accurate numerical computations. This unstable behavior could also arise in the case of a metastable process. The metastability imposes long simulation times, which could prove longer than the time needed for the numerical scheme to visit the singularities. The conclusion of this experiment/discussion is that the use of the rejection mechanism in practical applications may help to avoid divergent behavior and explosions, leading to more stable and accurate results.

An alternative approach to address the singularities is to employ a Metropolis-adjusted scheme, as the one presented in [136]. Similarly to our scheme, Metropolis-adjusted algorithms tend to reject transitions going too close to singularities, but the difference is that they also reject moves in low-energy regions, where the process spends most of its time. For the toy model discussed in this section, such a scheme exhibits remarkably high performance, with a success rate exceeding 99% for all considered time steps. However, in high-dimensional settings, Metropolis-adjusted schemes often result in numerous rejections and exhibit suboptimal performance. As a result, they are typically not used in the realms of molecular dynamics or statistics, even in the case of regular potentials.

2.3 Proof of Theorem 2.2.1

The proof of Theorem 2.2.1 relies on Sobolev embedding, and H^k -estimates. Similar results have been established for Langevin processes and close to quadratic potentials, in the sense that there exists $0 < m \leq M$ such that $mI_d \leq \nabla^2 U \leq MI_d$, where I_d stands for the identity matrix of size d , in [157]. Here we will use a method previously employed in [170, 95]. For a given $f \in \mathcal{P}(U)$, our goal is to show bound of the form:

$$\int_{\mathcal{X}} |\partial^\alpha (P_t f e^{-bH})|^2 dz \leq C e^{-qt},$$

for some $0 < b < \beta$ and all $\alpha \in \mathbb{N}^{2d}$. Sobolev embedding would then yield Theorem 2.2.1. To do so, we define a norm $\|\cdot\|_k$ that dominates the H^k -Sobolev norm, but such that $t \mapsto \|P_t f - \mu_\beta(f)\|_k$ converges exponentially fast to 0. However, contrary to the cited work, we need to take into account the singular potential by using a Lyapunov function. It was shown in [10] that the Langevin process (2.3) admits a family of Lyapunov functions $(V_{0,\bar{b}})$ such that for all $0 < \bar{b} < \beta/(2d)$, $\varepsilon > 0$:

$$C^{-1} e^{(1-\varepsilon)\bar{b}H} < V_{0,\bar{b}} < C e^{(1+\varepsilon)\bar{b}H},$$

see [10, Equation 5.2] for its exact definition and Proposition 2.3.3 below for its main properties. Thanks to this family of Lyapunov functions, we may now define our modified Sobolev norms. Let $\nabla_x^l \nabla_y^p h$ denote the vector of all derivative of h of order l on x and p on y :

$$\nabla_x^l \nabla_y^p h = \{ \partial_x^{\alpha_1} \partial_y^{\alpha_2} h \mid |\alpha_1| = l, |\alpha_2| = p \},$$

and its norm

$$|\nabla_x^l \nabla_y^p h|^2 = \sum_{|\alpha_1|=l; |\alpha_2|=p} |\partial_x^{\alpha_1} \partial_y^{\alpha_2} h|^2.$$

Fix $0 < \bar{b} < \beta/(2d)$, and $k \in \mathbb{N}^*$. Write $V = V_{0,\bar{b}}^{1/k}$, and for $p \in \llbracket 1, k \rrbracket$, $W_p = V^p + \lambda$, for some $\lambda > 0$. For $h \in \mathcal{C}^\infty(\mathcal{X}, \mathbb{R})$, denote:

$$\begin{aligned} \|h\|_{mH^{r,k},\bar{b}}^2 &= \int_{\mathcal{X}} h^2 W_k d\mu_\beta \\ &+ \int_{\mathcal{X}} \sum_{p=1}^r \left(\sum_{i=0}^{p-1} \omega_{i,p} |\nabla_x^i \nabla_y^{p-i} h|^2 + \omega_{p,p} |(\nabla_x^p - \xi \nabla_x^{p-1} \nabla_y) h|^2 \right) (1 + \varepsilon_p W_{k-p}) d\mu_\beta, \end{aligned} \quad (2.10)$$

where $(\omega_{i,p})$ and (ε_p) are two families of positive parameters to be fixed later, and $\xi = \frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{4} + 1}$. The exact value of ξ does not matter, as the important term is the scalar product $\nabla_x^p \cdot \nabla_x^{p-1} \nabla_y$. However this expression allows for simplified computation, see inequality (2.21). For the sequel of this work, we will drop the dependence in \bar{b} in the definition of the norm and simply write $\|\cdot\|_{mH^{r,k}}$. Write:

$$mH^k = \{h \in \mathcal{L}^2(\mathcal{X}, \mathbb{R}), \quad \|h\|_{mH^{k,k}} < \infty\}.$$

The goal is to show that for $f \in \mathcal{P}(U)$, we may chose \bar{b} such that $\|P_t f - \mu_\beta(f)\|_{mH^{r,k}}$ decreases exponentially fast along the dynamic.

Theorem 2.3.1. *Under Assumptions 2.2.1, 2.2.2 and 2.2.3, for all $f \in \mathcal{P}(U)$, $k \in \mathbb{N}$, there exists $0 < \bar{b} < \beta/(2d)$ such that for all $t \geq 0$, $P_t f \in mH^k$, and we have that there is $q_k > 0$ such that:*

$$\|P_t f - \mu_\beta(f)\|_{mH^{k,k}} \leq e^{-q_k t} \|f\|_{mH^{k,k}}. \quad (2.11)$$

This section will be mostly about the proof of this theorem, which relies on Gamma calculus, as presented in 1.2.1. We start by proving H^1 convergence in Section 2.3.1, which serves as an initial case for an induction argument which will prove Theorem 2.3.1 in Section 2.3.2. Finally, Theorem 2.2.1 will be proven in Section 2.3.3.

In the sequel, we denote by L the generator of the process (2.3) given by

$$L = y \cdot \nabla_x - \nabla U \cdot \nabla_y - \gamma y \cdot \nabla_y + \gamma \beta^{-1} \Delta_y, \quad (2.12)$$

and by L^* its adjoint in $L^2(\mu_\beta)$, given by:

$$L^* = -y \cdot \nabla_x + \nabla U \cdot \nabla_y - \gamma y \cdot \nabla_y + \gamma \beta^{-1} \Delta_y.$$

Recall the definition of the generalized *carré du champ*

$$\Gamma_\phi(h) = \frac{1}{2} (L(\phi(h)) - D_h \phi(h) Lh), \quad (2.13)$$

where $\phi : \mathcal{C}^\infty(\mathcal{X}) \rightarrow \mathcal{C}^\infty(\mathcal{X})$ and $D_h \phi$ denote the differential operator of ϕ . Recall also the Proposition that allows for the computations of this generalized *carré du champ*.

Proposition 2.3.1. *If there exists $A = (A_1, \dots, A_p) : \mathcal{C}^\infty \rightarrow (\mathcal{C}^\infty)^p$ a linear operator such that $\phi(h) = |Ah|^2$, then*

$$\Gamma_{L,\phi}(h) = \Gamma_{L,2}(Ah) + Ah \cdot [L, A]h,$$

where $\Gamma_{L,2}(Ah) = \sum_{i=1}^p \Gamma(A_i h)$, $\Gamma(h) = \Gamma_{L,h^2}(h)$, and $[L, A] = ([L, A_1], \dots, [L, A_p])$.

2.3.1 H^1 -setting

We now adapt the introduction to the singular case, as done in [10], to serve as the initialization of our induction argument. However, the modified H^1 -norm used in the cited work does not contain any Lyapunov function in the \dot{H}^1 part (i.e. the term with derivative of order 1), and we need some for the induction. Hence we use a slightly different norm, given in (2.10), which becomes for $r = 1$:

$$\|h\|_{mH^{1,k}} = \int_{\mathcal{X}} (h^2 W_k + \omega (|\nabla_y h|^2 + |(\nabla_x - \xi \nabla_y)h|^2) (1 + \varepsilon W_{k-1})) d\mu_\beta, \quad (2.14)$$

where $\xi = \frac{\gamma}{2} + \sqrt{\frac{\gamma^2}{4} + 1}$, and $\varepsilon > 0$, will be determined later. As in [10], we need a local Poincaré inequality:

Proposition 2.3.2. *For all compact set $K \subset \mathcal{X}$, μ_β satisfies a Poincaré inequality on K : there exists $\rho > 0$ such that for all $f \in C^\infty(\mathcal{X}, \mathbb{R})$:*

$$\int_K f^2 d\mu_\beta \leq \rho \int_K |\nabla f|^2 d\mu_\beta + \frac{1}{\mu_\beta(K)} \left(\int_K f d\mu_\beta \right)^2. \quad (2.15)$$

Proof. Proof of such inequality can be found in [6]. \square

The functions W and V satisfy the following properties, which are described in [10, Theorem 4.15]:

Proposition 2.3.3. *Under Assumptions 2.2.1 and 2.2.2, for all $\bar{b} > 0$, all $k \in \mathbb{N}$, there exists $V_{0,\bar{b}} : \mathcal{X} \rightarrow [1, \infty)$ such that if $V = V_{0,\bar{b}}^{1/k}$, $W_p = V^p + \lambda$ for some $\lambda > 0$, $V : \mathcal{X} \rightarrow [1, \infty)$ is \mathcal{C}^2 , and there exist $\alpha, \sigma > 0$, $J \subset \mathcal{X}$ such that:*

- For all $\varepsilon > 0$, there exists $C > 0$ such that

$$C^{-1} e^{(1-\varepsilon)\bar{b}H} < V < C e^{(1+\varepsilon)\bar{b}H}. \quad (2.16)$$

- J is compact, connected, and for all $p \in [1, k]$:

$$L^* V^p \leq -\alpha \frac{p}{k} V^p + \sigma \mathbb{1}_J.$$

- For all $p \in \llbracket 1, k \rrbracket$, $g \in C_b^\infty(\mathcal{X}, \mathbb{R})$, we have that $LgW_p, gL^*W_p \in L^1(\mu_\beta)$ and

$$\int_{\mathcal{X}} LgW_p d\mu_\beta = \int_{\mathcal{X}} gL^*W_p d\mu_\beta.$$

- $\forall (x, y) \in \mathbf{X}$,

$$V^k(x, y) \geq \frac{2\sigma\mu_\beta(J^c)}{\alpha\mu_\beta(J)}. \quad (2.17)$$

- $\forall (x, y) \in \mathbf{X}, v \in \mathbb{R}^d$,

$$W_k(x, y)|v|^2 \geq \beta(\sigma\rho' + 1) \left(\left(\frac{1}{2} + \frac{2}{\gamma^2} \right) |v|^2 + \frac{1}{2\gamma^2} |\nabla^2 U v|^2 \right), \quad (2.18)$$

where

$$\rho' = 4(1 + \xi^2)\rho/\gamma, \quad (2.19)$$

and ρ is the constant from the Poincaré inequality on J .

In particular, (2.16) yields that $\lim_{H \rightarrow \infty} V = \infty$, and (2.17) that the set J is not so large. In order to study the evolution of the norm (2.14) along the trajectories, we use Gamma calculus. All computations will be performed on functions $h : \mathcal{X} \rightarrow \mathbb{R}$ such that

$$\int_{\mathcal{X}} h d\mu_\beta = 0. \quad (2.20)$$

Recall the definition (2.13) of Γ_ϕ . We have

$$[L, \nabla_x] = \nabla^2 U \nabla_y, \quad [L, \nabla_y] = -\nabla_x + \gamma \nabla_y.$$

Hence from Proposition 2.3.1 we get that:

$$\Gamma_{|\nabla_y \cdot|^2}(h) \geq \gamma \beta^{-1} |\nabla_y^2 h|^2 - \nabla_y h \cdot (\nabla_x - \xi \nabla_y) h + (\gamma - \xi) |\nabla_y h|^2,$$

and:

$$\begin{aligned} \Gamma_{|(\nabla_x - \xi \nabla_y) \cdot|^2}(h) &\geq \gamma \beta^{-1} |(\nabla_x \nabla_y - \xi \nabla_y^2) h|^2 + \xi |(\nabla_x - \xi \nabla_y) h|^2 \\ &\quad + \xi(\xi - \gamma) \nabla_y h \cdot (\nabla_x - \xi \nabla_y) h + \nabla^2 U \nabla_y h \cdot (\nabla_x - \xi \nabla_y) h. \end{aligned}$$

Finally, with our choice of ξ and $\phi(h) = |\nabla_y h|^2 + |(\nabla_x - \xi \nabla_y) h|^2$, one gets:

$$\begin{aligned} \Gamma_\phi(h) &= \Gamma_{|\nabla_y \cdot|^2}(h) + \Gamma_{|(\nabla_x - \xi \nabla_y) \cdot|^2}(h) \\ &\geq \gamma \beta^{-1} |\nabla_y^2 h|^2 + \gamma \beta^{-1} |(\nabla_x \nabla_y - \xi \nabla_y^2) h|^2 \\ &\quad + \gamma |(\nabla_x - \xi \nabla_y) h|^2 - \frac{2}{\gamma} |\nabla_y h|^2 + \nabla^2 U \nabla_y h \cdot (\nabla_x - \xi \nabla_y) h. \end{aligned}$$

Young inequality then yields:

$$\Gamma_\phi(h) \geq \gamma \beta^{-1} |\nabla_y^2 h|^2 + \gamma \beta^{-1} |(\nabla_x \nabla_y - \xi \nabla_y^2) h|^2 + \frac{\gamma}{2} |(\nabla_x - \xi \nabla_y) h|^2 - \mathcal{R}(x, \nabla_y h), \quad (2.21)$$

where

$$\mathcal{R}(x, v) = \frac{2}{\gamma} |v|^2 + \frac{|\nabla^2 U v|^2}{2\gamma}.$$

Write:

$$H(t) = \|P_t f - \int_{\mathcal{X}} f d\mu_\beta\|_{mH^{1,k}}.$$

Because of the Lyapunov function, we have additional terms in the derivative of H in comparison to the regular case. This formally reads:

$$\begin{aligned} H'(t) &= \int_{\mathcal{X}} ((P_t f)^2 L^* W_k - \gamma \beta^{-1} |\nabla_y P_t f|^2 W_k) d\mu_\beta \\ &\quad + \omega \varepsilon \int_{\mathcal{X}} (|\nabla_y P_t f|^2 + |(\nabla_x - \xi \nabla_y) P_t f|^2) L^* W_{k-1} d\mu_\beta \end{aligned}$$

$$- \omega \int_{\mathcal{X}} (\Gamma_{|\nabla_y \cdot|^2}(P_t f) + \Gamma_{|\nabla_x - \xi \nabla_y \cdot|^2}(P_t f)) (1 + \varepsilon W_{k-1}) d\mu_\beta.$$

Hence to conclude in the H^1 setting, we need a control on the additional terms. This is the object of the next lemma, which is also the initialisation of the induction argument used in the next section for the H^k setting:

Lemma 2.3.1. *For all $k \in \mathbb{N}^*$, under Assumptions 2.2.1 and 2.2.2, there exist $q, \omega, \varepsilon > 0$ such that:*

$$\begin{aligned} & \int_{\mathcal{X}} (h^2 L^* W_k - \gamma \beta^{-1} |\nabla_y h|^2 W_k) d\mu_\beta \\ & \quad + \omega \varepsilon \int_{\mathcal{X}} (|\nabla_y h|^2 + |(\nabla_x - \xi \nabla_y) h|^2) L^* W_{k-1} d\mu_\beta \\ & \quad - \omega \int_{\mathcal{X}} (\Gamma_{|\nabla_y \cdot|^2}(h) + \Gamma_{|\nabla_x - \xi \nabla_y \cdot|^2}(h)) (1 + \varepsilon W_{k-1}) d\mu_\beta \\ & \leq -q \left(\|h\|_{mH^{1,k}} + \int_{\mathcal{X}} W_{k-1} (|\nabla_y^2 h|^2 + |\nabla_x \nabla_y h|^2) d\mu_\beta \right), \end{aligned} \quad (2.22)$$

for all $h \in C_b^\infty(\mathcal{X}, \mathbb{R})$.

Notice that in contrast to inequality (4.8) of [10], we keep the higher order derivative for the induction, see Section 2.3.2.

Proof. We first treat the L^2 -term using the Lyapunov property of V :

$$\int_{\mathcal{X}} h^2 L^* W_k d\mu_\beta \leq -\frac{\alpha}{1+\lambda} \int_{\mathcal{X}} h^2 W_k d\mu_\beta + \sigma \int_J h^2 d\mu_\beta.$$

Using Cauchy-Schwarz inequality, inequality (2.17) and that h satisfies (2.20), one gets

$$\left(\int_J h d\mu_\beta \right)^2 = \left(\int_{J^c} h d\mu_\beta \right)^2 \leq \mu_\beta(J^c) \int_{\mathcal{X}} h^2 d\mu_\beta \leq \frac{\alpha \mu_\beta(J)}{2\sigma(1+\lambda)} \int_{\mathcal{X}} h^2 W_k d\mu_\beta.$$

The local Poincaré inequality (2.15) on J can then be written as follow:

$$\begin{aligned} \sigma \int_J h^2 d\mu_\beta & \leq \sigma \rho' \frac{\gamma}{2} \int_J (|\nabla_x - \xi \nabla_y h|^2 + |\nabla_y h|^2) d\mu_\beta + \frac{\sigma}{\mu_\beta(J)} \left(\int_J h d\mu_\beta \right)^2 \\ & \leq \sigma \rho' \int_{\mathcal{X}} \frac{\gamma}{2} |\nabla_x - \xi \nabla_y h|^2 - \mathcal{R}(x, \nabla_y h) + \mathcal{R}(x, \nabla_y h) + |\nabla_y h|^2 d\mu_\beta \\ & \quad + \frac{\alpha}{2(1+\lambda)} \int_{\mathcal{X}} h^2 W_k d\mu_\beta, \end{aligned}$$

where ρ' was defined in (2.19). Using inequality (2.18), we get:

$$\int_{\mathcal{X}} \mathcal{R}(x, \nabla_y h) + \frac{\gamma}{2} |\nabla_y h|^2 d\mu_\beta \leq \frac{\gamma \beta^{-1}}{\sigma \rho' + 1} \int_{\mathcal{X}} |\nabla_y h|^2 W_k d\mu_\beta.$$

We also have from inequality (2.21):

$$\int_{\mathcal{X}} \frac{\gamma}{2} |\nabla_x - c \nabla_y h|^2 - \mathcal{R}(x, \nabla_y h) d\mu_\beta \leq \int_{\mathcal{X}} \Gamma_{|\nabla_y \cdot|^2}(h) + \Gamma_{|\nabla_x - c \nabla_y \cdot|^2}(h) d\mu_\beta.$$

We treat the second line of (2.22) using the Lyapunov property as follow:

$$\begin{aligned}
& \int_{\mathcal{X}} (|\nabla_y h|^2 L^* W_{k-1} + |(\nabla_x - \xi \nabla_y) h|^2 L^* W_{k-1}) d\mu_\beta \\
& \leq \int_{\mathcal{X}} (|\nabla_y h|^2 + |(\nabla_x - \xi \nabla_y) h|^2) \sigma \mathbb{1}_J d\mu_\beta \\
& \leq \frac{2\sigma}{\gamma} \int_{\mathcal{X}} \left(\frac{\gamma}{2} |\nabla_y h|^2 + \mathcal{R}(x, \nabla_y h) + \frac{\gamma}{2} |(\nabla_x - \xi \nabla_y) h|^2 - \mathcal{R}(x, \nabla_y h) \right) d\mu_\beta \\
& \leq \frac{2\sigma}{\beta(1 + \sigma\rho')} \int_{\mathcal{X}} |\nabla_y h|^2 W_k d\mu_\beta + \frac{2\sigma}{\gamma} \int_{\mathcal{X}} \Gamma_{|\nabla_y \cdot|^2}(h) + \Gamma_{|(\nabla_x - \xi \nabla_y) \cdot|^2}(h) d\mu_\beta.
\end{aligned}$$

Next, the ε -term of the third line is bounded thanks to (2.21) as follow:

$$\begin{aligned}
& - \int_{\mathcal{X}} (\Gamma_{|\nabla_y \cdot|^2}(h) + \Gamma_{|(\nabla_x - \xi \nabla_y) \cdot|^2}(h)) W_{k-1} d\mu_\beta \\
& \leq -\gamma\beta^{-1} \int_{\mathcal{X}} (|\nabla_y^2 h|^2 + |(\nabla_x \nabla_y - \xi \nabla_y) h|^2) W_{k-1} d\mu_\beta \\
& \quad - \frac{\gamma}{2} \int_{\mathcal{X}} |(\nabla_x - \xi \nabla_y) h|^2 W_{k-1} d\mu_\beta + \int_{\mathcal{X}} \mathcal{R}(x, \nabla_y h) W_{k-1} d\mu_\beta.
\end{aligned}$$

Thanks to Assumption 2.2.2 we get that there is $C > 0$ such that $|\nabla^2 U| \leq CV$. This yields that

$$\begin{aligned}
\mathcal{R}(x, \nabla_y h) W_{k-1} & \leq C' (|\nabla_y h|^2 + |\nabla^2 U \nabla_y h|^2) W_{k-1} \\
& \leq C'' (|\nabla_y h|^2 + |\nabla_y h|^2 V^{1/(k-1)}) W_{k-1} \leq \kappa |\nabla_y h|^2 W_k
\end{aligned}$$

and:

$$\begin{aligned}
& - \int_{\mathcal{X}} (\Gamma_{|\nabla_y \cdot|^2}(h) + \Gamma_{|(\nabla_x - \xi \nabla_y) \cdot|^2}(h)) W_{k-1} d\mu_\beta \\
& \leq -\gamma\beta^{-1} \int_{\mathcal{X}} (|\nabla_y^2 h|^2 + |\nabla_x \nabla_y h|^2) W_{k-1} d\mu_\beta \\
& \quad - \frac{\gamma}{2} \int_{\mathcal{X}} |(\nabla_x - \xi \nabla_y) h|^2 W_{k-1} d\mu_\beta + \kappa \int_{\mathcal{X}} |\nabla_y h|^2 W_k d\mu_\beta.
\end{aligned}$$

We then get the following upper bound for the left-hand side of equation (2.22):

$$\begin{aligned}
& - \frac{\alpha}{2(1 + \lambda)} \int_{\mathcal{X}} h^2 W_k d\mu_\beta \\
& \quad - \left(\gamma\beta^{-1} - \frac{2\varepsilon\sigma\beta^{-1}}{\sigma\rho' + 1} - \kappa\varepsilon\omega \right) \int_{\mathcal{X}} |\nabla_y h|^2 W_k d\mu_\beta \\
& \quad - \varepsilon\omega\gamma\beta^{-1} \int_{\mathcal{X}} (|\nabla_y^2 h|^2 + |\nabla_x \nabla_y h|^2) W_{k-1} d\mu_\beta \\
& \quad + \left(\frac{2\sigma\varepsilon\omega}{\gamma} + \sigma\rho' - \omega \right) \int_{\mathcal{X}} \Gamma_{|\nabla_y \cdot|^2}(h) + \Gamma_{|(\nabla_x - \xi \nabla_y) \cdot|^2}(h) d\mu_\beta \\
& \quad - \frac{\gamma\varepsilon\omega}{2} \int_{\mathcal{X}} |(\nabla_x - \xi \nabla_y) h|^2 W_{k-1} d\mu_\beta.
\end{aligned}$$

Taking $\omega > \sigma\rho'$, ε small enough so that the second and fourth terms of the previous bounds are negative, and using the fact that $W_{k-1} \leq W_k$ (because $V \geq 1$) then concludes the proof. \square

Removing the second order terms, Lemma 2.3.1 formally yields:

$$H'(t) \leq -qH(t),$$

for some $q > 0$. Since $W_k \geq 1$ for all $k > 0$, this would imply convergence in H^1 -norm

$$\|P_t f - \mu_\beta(f)\|_{H^1} \leq C e^{-qt} \|f - \mu_\beta(f)\|_{mH^{1,k}},$$

for some $C > 0$. This is only a formal computation, which we will justify in the proof of Theorem 2.3.1.

2.3.2 H^k -setting

Building upon the result of the previous section, we may now perform computations in higher-order Sobolev spaces. From those computations arise derivatives of U of arbitrary orders, hence we now need to assume Assumption 2.2.3. Since the Lyapunov function satisfies $V = e^{bH+o(H)}$, for some $0 < b < \beta$, this assumption implies: for all $\alpha \in \mathbb{N}^d$, there exists $\kappa_\alpha > 0$ such that

$$|\partial^\alpha U| \leq \kappa_\alpha V. \quad (2.23)$$

Recall the definition of the modified Sobolev norm from (2.10), fix some $r \in \llbracket 1, k \rrbracket$, and write:

$$H_{r,k}(t) = \|P_t f - \int_{\mathcal{X}} f d\mu_\beta\|_{mH^{r,k}}.$$

We formally have:

$$\begin{aligned} H'_{r,k}(t) &= \int_{\mathcal{X}} \left((P_t f)^2 L^* W_k - \gamma \beta^{-1} |\nabla_y P_t f|^2 W_k \right) d\mu_\beta \\ &\quad + \int_{\mathcal{X}} \sum_{p=1}^r \varepsilon_p \left(\sum_{i=0}^{p-1} \omega_{i,p} |\nabla_x^i \nabla_y^{p-i} P_t f|^2 + \omega_p |(\nabla_x^p - \xi \nabla_x^{p-1} \nabla_y) P_t f|^2 \right) L^* W_{k-p} d\mu_\beta \\ &\quad - \int_{\mathcal{X}} \sum_{p=1}^r \left(\sum_{i=0}^{p-1} \omega_{i,p} \Gamma_{i,p-i}(P_t f) + \omega_p \Gamma_p(P_t f) \right) (1 + \varepsilon_p W_{k-p}) d\mu_\beta \end{aligned} \quad (2.24)$$

where we wrote:

$$\Gamma_{l,p} = \Gamma_{|\nabla_x^l \nabla_y^p|^2},$$

and

$$\Gamma_p = \Gamma_{|(\nabla_x^p - \xi \nabla_x^{p-1} \nabla_y)|^2}$$

for any $l, p \in \mathbb{N} \times \mathbb{N}^*$. As in the previous section, we need to bound this derivative. This bound is obtained through an induction principle on $r \in \llbracket 1, k \rrbracket$, and the repetitive use of Proposition 2.3.1. First we compute:

$$[L, \nabla_x^l \nabla_y^p] = \gamma \nabla_x^l \nabla_y^p - \mathbb{1}_{p \geq 1} \nabla_x^{l+1} \nabla_y^{p-1} + \sum_{i=1}^l \binom{l}{i} \nabla^{i+1} U \otimes \nabla_x^{l-i} \nabla_y^p,$$

where the terms in the sum as to be understood as:

$$\left| \frac{l}{i} \right| \nabla^{i+1} U \otimes \nabla_x^{l-i} \nabla_y^p = \left(\sum_{j=1}^d \sum_{k_s \leq l_s} \prod_{s=1}^d \binom{l_s}{k_s} \partial_{x_j} \partial^{k_s} U \partial_{y_j} \partial_x^{l-k} \partial_y^{p+1} \right)_{\sum l_j = l, \sum p_j = p}.$$

Using Proposition 2.3.1, we get that:

$$\Gamma_{l,p}(h) = \Gamma(\nabla_x^l \nabla_y^p h) + \nabla_x^l \nabla_y^p h \cdot [L, \nabla_x^l \nabla_y^p] h.$$

If $p \geq 2$, we may then bound below using inequality (2.23):

$$\Gamma_{l,p}(h) \geq \gamma \beta^{-1} |\nabla_x^l \nabla_y^{p+1} h|^2 - \theta_{l,p} \left(|\nabla_x^l \nabla_y^p h|^2 + V \sum_{i=1}^l |\nabla_x^{l-i} \nabla_y^{p+1} h|^2 \right) - \frac{1}{4\gamma} |\nabla_x^{l+1} \nabla_y^{p-1}|^2, \quad (2.25)$$

for some $\theta_{l,p} \geq 0$. If $p = 1$, there is a term $|\nabla_x^{l+1} h|^2$ in the commutator, which will be problematic, as we cannot control it by induction using the derivative of the lower-order terms. In order to take care of it, we fix a small parameter $\eta_l > 0$, use the inequality $a \cdot b \leq |a|^2/(2\eta) + \eta|b|^2/2$ and we bound below again using inequality (2.23):

$$\Gamma_{l,1}(h) \geq \gamma \beta^{-1} |\nabla_x^l \nabla_y^2 h|^2 - \theta_{l,1} \left(|\nabla_x^l \nabla_y^1 h|^2 + V \sum_{i=1}^l |\nabla_x^{l-i} \nabla_y^2 h|^2 \right) - \eta_l |\nabla_x^{l+1} - \xi \nabla_x^l \nabla_y| h|^2. \quad (2.26)$$

As usual in hypocoercive computations for kinetic processes, the derivative of a Sobolev norm of order p will lack in its derivative a term of the form $|\nabla_x^p h|^2$. It will be the derivative of the cross term $\nabla_x^p h \cdot \nabla_x^{p-1} \nabla_y$ in $|(\nabla_x^p - c \nabla_x^{p-1} \nabla_y) h|^2$ that will give us this missing derivative. Indeed, using that $\xi \geq \gamma$ and inequality (2.23), one has:

$$\begin{aligned} \nabla_x^p h \cdot [L, -\xi \nabla_x^{p-1} \nabla_y] h &= \xi \nabla_x^p h \cdot \left(\nabla_x^p - \gamma \nabla_x^{p-1} \nabla_y - \sum_{i=1}^p \left| \frac{p}{i} \right| \nabla^{i+1} U \otimes \nabla_x^{p-i} \nabla_y \right) h \\ &\geq \frac{\gamma}{2} |\nabla_x^p h|^2 - CV \left(\sum_{l=1}^p |\nabla_x^{p-l} \nabla_y h|^2 + \sum_{l=1}^{p-1} |\nabla_x^{p-1-l} \nabla_y^2 h|^2 \right). \end{aligned} \quad (2.27)$$

We also have that

$$|(\nabla_y \nabla_x^p - \xi \nabla_x^{p-1} \nabla_y^2) h|^2 \geq \frac{1}{2} |\nabla_x^p \nabla_y h|^2 - \frac{1}{2} \xi |\nabla_x^{p-1} \nabla_y^2 h|^2$$

Hence after rearranging the terms, Proposition 2.3.1 again yields:

$$\begin{aligned} \Gamma_p(h) &\geq \\ &\frac{\gamma \beta^{-1}}{2} |\nabla_x^p \nabla_y h|^2 + \frac{\gamma}{2} |(\nabla_x^p - \xi \nabla_x^{p-1} \nabla_y) h|^2 - \theta_{p,0} V \left(\sum_{l=1}^p |\nabla_x^{p-l} \nabla_y h|^2 + \sum_{l=0}^{p-1} |\nabla_x^{p-1-l} \nabla_y^2 h|^2 \right), \end{aligned} \quad (2.28)$$

for some $\theta_{p,0} > 0$. Thanks to those different lower bounds, we will be able to prove the next lemma which is the central part of this section.

Lemma 2.3.2. *Fix $k \in \mathbb{N}^*$. There exists $(\omega_{i,p})_{1 \leq i \leq p \leq k}$, $(\varepsilon_p)_{1 \leq p \leq k}$, all positive, such that for all $r \in \llbracket 1, k \rrbracket$, there exists $q_r > 0$ such that for all $h \in \mathcal{C}_b^\infty(\mathcal{X}, \mathbb{R})$:*

$$\begin{aligned}
& \int_{\mathcal{X}} (h^2 L^* W_k - \gamma \beta^{-1} |\nabla_y h|^2 W_k) d\mu_\beta \\
& + \int_{\mathcal{X}} \sum_{p=1}^r \varepsilon_p \left(\sum_{i=0}^{p-1} \omega_{i,p} |\nabla_x^i \nabla_y^{p-i} h|^2 + \omega_p |(\nabla_x^p - \xi \nabla_x^{p-1} \nabla_y) h|^2 \right) L^* W_{k-p} d\mu_\beta \\
& - \int_{\mathcal{X}} \sum_{p=1}^r \left(\sum_{i=0}^{p-1} \omega_{i,p} \Gamma_{i,p-i}(h) + \omega_p \Gamma_p(h) \right) (1 + \varepsilon_p W_{k-p}) d\mu_\beta \\
& \leq -q_r \left(\|h\|_{mH^{r,k}} + \int_{\mathcal{X}} \sum_{i=0}^r |\nabla_x^i \nabla_y^{r+1-i} h|^2 W_{k-r} d\mu_\beta \right). \tag{2.29}
\end{aligned}$$

Proof. The proof is done by induction. The case $r = 1$ corresponds to Lemma 2.3.1. Let $r \in \llbracket 1, k \rrbracket$, and we suppose the inequality (2.29) true for such an r . To prove the result at rank $r + 1$, we want to bound:

$$\begin{aligned}
& -q_r \int_{\mathcal{X}} \left(h^2 W_k + \sum_{1 \leq i+j \leq r, j \geq 1} |\nabla_x^i \nabla_y^j h|^2 W_{k-(i+j)} + \sum_{i=1}^r |(\nabla_x^i - \xi \nabla_x^{i-1} \nabla_y) h|^2 W_{k-i} \right) d\mu_\beta \\
& -q_r \int_{\mathcal{X}} \sum_{i=0}^r |\nabla_x^i \nabla_y^{r+1-i} h|^2 W_{k-r} d\mu_\beta \\
& + \varepsilon_{r+1} \int_{\mathcal{X}} \left(\sum_{i=0}^r \omega_{i,r+1} |\nabla_x^i \nabla_y^{r+1-i} h|^2 + \omega_{r+1} |(\nabla_x^{r+1} - \xi \nabla_x^r \nabla_y) h|^2 \right) L^* W_{k-(r+1)} d\mu_\beta \\
& - \int_{\mathcal{X}} \left(\sum_{i=0}^r \omega_{i,r+1} \Gamma_{i,r+1-i}(h) + \omega_{r+1} \Gamma_{r+1}(h) \right) (1 + \varepsilon_{r+1} W_{k-(r+1)}) d\mu_\beta.
\end{aligned}$$

First we bound using the Lyapunov property:

$$|\nabla_x^i \nabla_y^{r+1-i} h|^2 L^* W_{k-(r+1)} \leq \sigma |\nabla_x^i \nabla_y^{r+1-i} h|^2.$$

The goal now is to check that for any order of derivative, we may chose ε_{r+1} , $(\omega_{i,r+1})$ and (ω_{r+1}) such that inequality (2.29) holds true with $(r + 1)$ instead of r . To this end, we will use the inequality (2.25), (2.26) and (2.28) on the Γ 's. The term of order $r + 2$ of derivatives is:

$$-\gamma \beta^{-1} \int_{\mathcal{X}} \left(\sum_{i=0}^r \omega_{i,r+1} |\nabla_x^i \nabla_y^{r+2-i} h|^2 + \frac{\omega_{r+1}}{2} |(\nabla_x^{r+1} \nabla_y - \xi \nabla_x^r \nabla_y^2) h|^2 (1 + \varepsilon_{r+1} W_{k-(r+1)}) \right) d\mu_\beta,$$

which is already what we were looking for. This does not impose any condition on the coefficient, except the positivity of the (ω) . The derivative of order $r + 1$ in x which was missing from the rank r , is:

$$\int_{\mathcal{X}} \left(\varepsilon_{r+1} \omega_{r+1} \sigma - \frac{\gamma \omega_{r+1}}{2} (1 + \varepsilon_{r+1} W_{k-(r+1)}) + \eta_r \omega_{r,r+1} (1 + \varepsilon_{r+1} W_{k-(r+1)}) \right) |(\nabla_x^{r+1} - \xi \nabla_x^r \nabla_y) h|^2 d\mu_\beta.$$

We choose $\eta_r = \frac{\gamma \omega_{r+1}}{8 \omega_{r,r+1}}$, and $0 < \varepsilon_{r+1} < \frac{\gamma}{8\sigma}$, so that we are left with:

$$-\frac{\gamma \omega_{r+1}}{4} \int_{\mathcal{X}} |(\nabla_x^{r+1} - \xi \nabla_x^r \nabla_y) h|^2 (1 + \varepsilon_{r+1} W_{k-(r+1)}) d\mu_\beta.$$

For the other terms of order $r+1$, fix some $i \in \llbracket 0, r \rrbracket$. The term in $|\nabla_x^i \nabla_y^{r+1-i} h|^2$ is:

$$\int_{\mathcal{X}} (-q_r W_{k-r} + \sigma \varepsilon_{r+1} \omega_{i,r+1} + (\omega_{i,r+1} \theta_{i,r+1-i} + \omega_{i+1,r+1} (1/(4\gamma) + \theta_{i+1,r+1-(i+1)} V))) (1 + \varepsilon_{r+1} W_{k-(r+1)}) |\nabla_x^i \nabla_y^j h|^2 d\mu_\beta.$$

Using that $VW_{k-(r+1)} \leq W_{k-r}(1+\lambda)$, we may choose the $(\omega_{i,r+1})$ small enough so that this last quantity is less than:

$$-\frac{q_r}{2} \int_{\mathcal{X}} W_{k-r} |\nabla_x^i \nabla_y^j h|^2 d\mu_\beta.$$

The lower order terms are treated in the same way, and this concludes the induction and the proof. \square

Proof of Theorem 2.3.1. Instead of trying to justify the derivative (2.24), we apply a semi-group argument. Our goal is to apply Lumer-Phillips theorem to the operator $L + (q_k/2)I$, where I denotes the identity operator of mH^k . This theorem can be stated as follows: an operator A on a Hilbert space generates a contraction semi-group if and only if it is maximally dissipative, see [169, Chapter IX, p.250]. Fix $0 < \bar{b} < \beta/(2d)$ and $k \in \mathbb{N}$. mH^k is a Hilbert space, with scalar product

$$\begin{aligned} \langle f, g \rangle_{mH^k}^2 &= \int_{\mathcal{X}} fg W_k d\mu_\beta \\ &+ \int_{\mathcal{X}} \sum_{p=1}^k \left(\sum_{i=0}^{p-1} \omega_{i,p} \nabla_x^i \nabla_y^{p-i} f \cdot \nabla_x^i \nabla_y^{p-i} g + \omega_{p,p} (\nabla_x^p - \xi \nabla_x^{p-1} \nabla_y) f \cdot (\nabla_x^p - \xi \nabla_x^{p-1} \nabla_y) g \right) \\ &\quad (1 + \varepsilon_p W_{k-p}) d\mu_\beta. \end{aligned}$$

Lemma 2.3.2 and a density argument yield that the operator $L + (q_k/2)I$, is dissipative:

$$\forall h \in D(L), \langle (L + (q_k/2)I)h, h \rangle_{mH^k} \leq 0,$$

where $D(L)$ denote the domain of L in mH^k defined by:

$$f \in \mathcal{D}(L), g = Lf \Leftrightarrow f \in mH^k, \lim_{t \rightarrow 0} \left\| \frac{P_t f - f}{t} - g \right\|_{mH^k} = 0.$$

We are left to show that $L + qI$, for some $q < q_k/2$, is surjective. Fix $q < q_k/2$. Thanks to Lemma 2.3.2, we have that

$$\Lambda : (f, g) \mapsto \langle -(L + qI)f, g \rangle_{mH^k}$$

is coercive and continuous from $(mH^k)^2$ to \mathbb{R} , as long as $k \geq 2$. Hence, we may apply Lax-

Milgram theorem to get that for all $g \in mH^k$, there exists $f \in mH^k$ such that for all $h \in mH^k$, we have:

$$\langle -(L + qI)f, h \rangle_{mH^k} = \langle -g, h \rangle_{mH^k},$$

which implies that f is a solution to the equation

$$(L + qI)f = g,$$

and $L + (q_k/2)I$ is maximally dissipative. Lumer-Phillips theorem then yields that the semi-group generated by $L + q_k/2$ is a contraction on mH^k : for all $f \in mH^k$

$$\|e^{q_k t/2} P_t f\|_{mH^k} \leq \|f\|_{mH^k}.$$

For all $f \in \mathcal{P}(U)$, we may fix $\bar{b} > 0$ small enough so that $f \in mH^k$, and this concludes the proof. \square

2.3.3 Proof of Theorem 2.2.1

The proof of Theorem 2.2.1, based on Theorem 2.3.1, uses the Lyapunov structure of V .

Proof of theorem 2.2.1. Fix some $f \in \mathcal{P}(U)$. Thanks to Proposition 2.3.3, we may fix the parameter \bar{b} from the Lyapunov function such that $\|f\|_{mH^k} < \infty$. For all $k \in \mathbb{N}$, we can apply Theorem 2.3.1 to get some $C > 0$ such that:

$$\|P_t f\|_{mH^k} \leq C e^{-q_k t}.$$

Fix $0 < b < \beta$, $C, \varepsilon > 0$ such that $e^{(\beta - (1 - \varepsilon)b)H} \leq C V_0$, for some $C > 0$. Thanks to Assumption 2.2.3, we may write for all $\alpha \in \mathbb{N}^{2d}$:

$$\begin{aligned} \int_{\mathcal{X}} |\partial^\alpha (P_t f e^{-bH})|^2 &\leq C \sum_{|\sigma| \leq |\alpha|} \int_{\mathcal{X}} |\partial^\sigma P_t f|^2 |\partial^{\alpha - \sigma} e^{-bH}|^2 \\ &\leq C' \sum_{|\sigma| \leq |\alpha|} \int_{\mathcal{X}} |\partial^\sigma P_t f|^2 e^{-(1 - \varepsilon)bH} \\ &= C' \sum_{|\sigma| \leq |\alpha|} \int_{\mathcal{X}} |\partial^\sigma P_t f|^2 e^{(\beta - (1 - \varepsilon)b)H} e^{-\beta H} \\ &\leq C'' \|P_t f\|_{mH^{|\alpha|}} \\ &\leq C'' e^{-q|\alpha|t}. \end{aligned}$$

We conclude with Sobolev embedding. \square

2.4 Weak error expansion

The main ingredient in the proof of a Talay-Tubaro expansion for a numerical scheme (or even simply weak convergence) are the estimates given in Theorem 2.2.1. It allows to control the error (in law) made by each step of the numerical scheme, uniformly in time. Hence we are now able to prove Theorem 2.2.2 and Theorem 2.2.3. This section is divided into two parts. The first one proves the existence of a Lyapunov function of order e^{bH} , for all $0 < b < \beta$, as well as Theorem 2.2.2, about finite time expansion of the numerical scheme (2.4). The second part shows

the existence of a unique stationary measure for the numerical scheme, as well as Theorem 2.2.3 for the Talay-Tubaro expansion of this stationary measure.

2.4.1 Finite-time expansion for the numerical scheme with rejection

The reason why we are interested in the scheme (2.4) instead of the scheme (2.7) is Lemma 2.4.2. To bound the error made by the numerical scheme, and hence to prove Theorem 2.2.2, we need uniform in $n \in \mathbb{N}$ and $\delta > 0$ integrability. To get this integrability, we show that the Lyapunov structure of the continuous process described in [82] still holds after discretization. This comes from the rejection mechanism that prevents the scheme from seeing the part of space where the gradient of the potential and its derivatives are too big compared to δ , which is a neighborhood of the singularities and of infinity. Recall the definition of $\mathcal{H}_{\delta,\ell}$ from (2.5), and denote $\zeta = 4d\gamma\beta^{-1}$. To prove Lemma 2.4.2, we first need to introduce a regularized version of the potential \hat{U} and a modified kinetic energy \hat{W} , along with a numerical scheme corresponding to the counterpart of the scheme (2.7) for the new Hamiltonian $\hat{H}(x, y) = \hat{U}(x) + \hat{W}(y)$. A comparison between this new numerical scheme with the previously considered one will lead to the result.

Lemma 2.4.1. *Under Assumptions 2.2.1 and 2.2.2, there exist $\delta_0, \ell_0 > 0$ such that for all $0 < \delta < \delta_0$ and $0 < \ell < \ell_0$, there exist*

$$\hat{U}, \hat{W} : \mathbb{R}^d \rightarrow \mathbb{R}_+$$

satisfying

- \hat{U} and \hat{W} are bounded.
- $\hat{U} = U, \hat{W} = |\cdot|^2/2$ on $\mathcal{H}_{\delta,\ell}$.
- For all $(x, y) \in \mathcal{H}_{\delta,\ell}^c$

$$\hat{\phi}(x, y) = \hat{U}(x) + \hat{W}(y) + \zeta \frac{\nabla \hat{W} \cdot \nabla \hat{U}(x)}{1 + |\nabla \hat{U}(x)|^2} \geq 1/\delta^\ell.$$

- For all $\alpha \in \mathbb{N}^{2d}, 1 \leq |\alpha|_1 \leq 4$, there exists $C_\alpha > 0, \ell_\alpha < 1/2$ such that:

$$|\partial^\alpha \hat{U}|, |\partial^\alpha \hat{W}| \leq \frac{C_\alpha}{\delta^{\ell_\alpha}}. \quad (2.30)$$

Proof. For all $0 < \ell < 1, 0 < \delta < 1$, fix a smooth, increasing and concave function

$$g_{\delta,\ell} : \mathbb{R}_+ \rightarrow \mathbb{R}_+$$

such that

$$g_{\delta,\ell}(t) = t, \forall t \in [0, 4\delta^{-\ell}]; \quad g'_{\delta,\ell}(t) \leq \frac{2(4\delta^{-\ell})^2}{t^2}, \quad |g_{\delta,\ell}^{(p)}(t)| \leq \frac{C}{t^{p+1}}, \quad \forall t \geq 4\delta^{-\ell}, p \in \llbracket 2, 4 \rrbracket,$$

for some $C > 0$. Then define

$$\hat{U} = g_{\delta,\ell}(U), \quad \hat{W} = g_{\delta,\ell}(|\cdot|^2/2).$$

Let's show that \hat{U} and \hat{W} satisfy the desired conditions. First, the conditions on $g_{\delta,\ell}$ yield that

$$g_{\delta,\ell} \leq 4\delta^{-\ell} + \int_{4\delta^{-\ell}}^{\infty} \frac{2(4\delta^{-\ell})^2}{t^2} dt = 12\delta^{-\ell},$$

so that \hat{U} and \hat{W} are bounded. For all $(x, y) \in \mathcal{H}_{\delta,\ell}$, we have using Young's inequality:

$$\delta^{-\ell} \geq U(x) + \frac{|y|^2}{2} + \zeta \frac{y \cdot \nabla U(x)}{1 + |\nabla U(x)|^2} \geq \frac{1}{2}H(x, y) - \zeta^2,$$

so that $H \leq 2\delta^{-\ell} + 2\zeta^2$. As soon as $\delta^{-\ell} \geq \zeta^2$, we have that for all $(x, y) \in \mathcal{H}_{\delta,\ell}$, $U(x) \leq 4\delta^{-\ell}$ and $|y|^2/2 < 4\delta^{-\ell}$, yielding $\hat{U}(x), \hat{W}(y) = U(x), |y|^2/2$ and the second point.

The definition of the modified kinetic energy implies that $\nabla \hat{W}(y) = g'_{\delta,\ell}(|y|^2/2)y$, and the conditions on $g_{\delta,\ell}$ then yield

$$\sup_{y \in \mathbb{R}^d} |\nabla \hat{W}(y)| \leq \max \left(\sqrt{8\delta^{-\ell}}, \sup_{s \geq \sqrt{8\delta^{-\ell}}} g'(s)s \right) \leq 16\delta^{-\ell/2}.$$

To prove the third point of the lemma, we distinguish two cases: if $(x, y) \notin \mathcal{H}_{\delta,\ell}$ satisfies $U(x) < 4\delta^{-\ell}$ and $|y|^2/2 < 4\delta^{-\ell}$, then $\hat{\phi}(x, y) = \phi(x, y) \geq \delta^{-\ell}$ by definition of $\mathcal{H}_{\delta,\ell}$. If $U(x) > 4\delta^{-\ell}$ or $|y|^2/2 > 4\delta^{-\ell}$, we have

$$\hat{\phi}(x, y) \geq 4\delta^{-\ell} - 16\zeta\delta^{-\ell/2} \geq \delta^{-\ell},$$

for δ small enough depending on $\ell > 0$. The last point is a direct consequence of the conditions imposed on $g_{\delta,\ell}$ and the definitions of \hat{U} and \hat{W} . \square

We are now able to prove:

Lemma 2.4.2. *Under Assumptions 2.2.1 and 2.2.2, there exist $\delta_0, \ell_0 > 0$ such that for all $0 < b < \beta$, there exists $V_b : \mathcal{X} \rightarrow \mathbb{R}_+$ such that:*

- $\inf_{\mathcal{X}} V_b > 0$.
- For all $\varepsilon > 0$, there exists $C > 0$ such that

$$C^{-1}e^{(1-\varepsilon)bH} \leq V_b \leq Ce^{(1+\varepsilon)bH}.$$

- There exists $\alpha, K > 0$ such that for all $0 < \delta < \delta_0$, $0 < \ell < \ell_0$, $(x, y) \in \mathcal{H}_{\delta,\ell}$:

$$\mathbb{E}_{(x,y)} (V_b(\bar{X}_1, \bar{Y}_1)) \leq (1 - \alpha\delta)V_b(x, y) + \alpha\delta K.$$

Proof. Fix $0 < b < \beta$ and write:

$$V_b(x, y) = \exp(b\phi(x, y)), \quad \hat{V}_b(x, y) = \exp\left(b\hat{\phi}(x, y)\right),$$

where ϕ was defined in (2.6) and $\hat{\phi}$ in Lemma 2.4.1. It is different from the Lyapunov function of [82] in that we need in the denominator of ϕ the term $1 + |\nabla U(x)|^2$ instead of $|\nabla U(x)|^2$. However, the proof written in [82] can be immediately adapted to cover the case we consider, and it yields that there exists a compact set $K_1 \subset \mathbb{R}^{2d}$ such that for all $(x, y) \notin K_1$:

$$\frac{LV_b(x, y)}{V_b(x, y)} \leq -c, \tag{2.31}$$

where L is the generator defined in (2.12). For any $\varepsilon > 0$, we have

$$\left| \zeta \frac{y \cdot \nabla U(x)}{1 + |\nabla U(x)|^2} \right| \leq \varepsilon |y|^2 / 2 + \frac{\zeta^2}{2\varepsilon} \times \frac{|\nabla U(x)|^2}{1 + |\nabla U(x)|^2} \leq \varepsilon H + C,$$

for some $C > 0$, and this implies the first two points. Now all that remains to do to show the third point is to show that inequality (2.31) remains true for the numerical scheme, as it stays in the region of space where $U = O(\delta^{-\ell})$. Recall the definition of \hat{U} and \hat{W} from Lemma 2.4.1. We introduce the following numerical scheme, counterpart of the scheme (2.7) for the Hamiltonian \hat{H} :

$$\begin{cases} \hat{X}_{n+1} = \hat{X}_n + \delta \nabla \hat{W}(Y_n), \\ \hat{Y}_{n+1} = \hat{Y}_n - \delta \nabla \hat{U}(\hat{X}_n) - \delta \gamma \nabla \hat{W}(\hat{Y}_{n+1}) + \sqrt{2\gamma\beta^{-1}\delta} G_n, \end{cases} \quad (2.32)$$

where (G_n) is the same family of Gaussian random variable as in the definition of the scheme (2.4). On the event $\{(\bar{X}_1, \bar{Y}_1) \neq (\hat{X}_1, \hat{Y}_1)\}$, the step of (\bar{X}_1, \bar{Y}_1) was rejected, $(\hat{X}_1, \hat{Y}_1) \notin \mathcal{H}_{\delta, \ell}$, and we have using the third point of Lemma 2.4.1

$$\hat{V}_b(\bar{X}_1, \bar{Y}_1) = \hat{V}_b(x, y) \leq e^{b\delta^{-\ell}} \leq \hat{V}_b(\hat{X}_1, \hat{Y}_1). \quad (2.33)$$

Suppose we have $K > 0$, and $0 < \alpha < 1$ both independent of δ such that:

$$\mathbb{E}_{(x, y)} \left(\hat{V}_b(\hat{X}_1, \hat{Y}_1) \right) \leq (1 - \alpha\delta) \hat{V}_b(x, y) + \alpha\delta K,$$

for all $(x, y) \in \mathcal{H}_{\delta, \ell}$. Then, using that for all $(x, y) \in \mathcal{H}_{\delta, \ell}$, $V_b(x, y) = \hat{V}_b(x, y)$, and inequality (2.33), we would have for all $(x, y) \in \mathcal{H}_{\delta, \ell}$:

$$\begin{aligned} \mathbb{E}_{(x, y)} (V_b(\bar{X}_1, \bar{Y}_1)) &= \mathbb{E} \left(\hat{V}_b(\bar{X}_1, \bar{Y}_1) \right) \leq \mathbb{E} \left(\hat{V}_b(\hat{X}_1, \hat{Y}_1) \right) \\ &\leq (1 - \alpha\delta) \hat{V}_b(x, y) + \alpha\delta K = (1 - \alpha\delta) V_b(x, y) + \alpha\delta K. \end{aligned}$$

Thus we only have to show that the Lyapunov structure holds (partially) true for the regularized numerical scheme (2.32). In the sequel of this proof, the notation $o(\delta)$ will denote a quantity uniform in $(x, y) \in \mathbb{R}^{2d}$:

$$f_\delta(x, y) = o(\delta) \Leftrightarrow \lim_{\delta \rightarrow 0} \sup_{(x, y) \in \mathbb{R}^{2d}} \frac{|f_\delta(x, y)|}{\delta} = 0.$$

We have:

$$\begin{aligned} \hat{V}_b(\hat{X}_1, \hat{Y}_1) - \hat{V}_b(x, y) &= \hat{V}_b(x, y) \left(\hat{\phi}(\hat{X}_1, \hat{Y}_1) - \hat{\phi}(x, y) \right) \\ &+ \frac{1}{2} \hat{V}_b(x, y) \left(\hat{\phi}(\hat{X}_1, \hat{Y}_1) - \hat{\phi}(x, y) \right)^2 + \hat{V}_b(x, y) \sum_{p \geq 3} \frac{1}{p!} \left(\hat{\phi}(\hat{X}_1, \hat{Y}_1) - \hat{\phi}(x, y) \right)^p. \end{aligned}$$

A Taylor expansion on $\hat{\phi}$ yields that there exists $(\theta_1, \theta_2) \in \mathbb{R}^{2d}$, random, such that:

$$\hat{\phi}(\hat{Z}_1) = \hat{\phi}(z) + (\hat{Z}_1 - z) \cdot \nabla \hat{\phi}(z) + \frac{1}{2} \nabla^2 \hat{\phi}(z) (\hat{Z}_1 - z)^{\circ 2} + \frac{1}{6} \nabla^3 \hat{\phi}(\theta_1, \theta_2) (\hat{Z}_1 - z)^{\circ 3}, \quad (2.34)$$

where $z = (x, y)$ and $\hat{Z}_1 = (\hat{X}_1, \hat{Y}_1)$. Condition (2.30) yields that for $p \in \{1, 2\}$:

$$\mathbb{E} \left(\left(\nabla^3 \hat{\phi}(\theta_1, \theta_2) (\hat{Z}_1 - z)^{\circ 3} \right)^p \right) = o(\delta).$$

Moreover, we have

$$(\hat{Z}_1 - z) \cdot \nabla \hat{\phi}(z) = \delta \nabla \hat{W}(y) \cdot \nabla_x \hat{\phi} - \delta \nabla \hat{U}(x) \cdot \nabla_y \hat{\phi} - \delta \gamma \nabla \hat{W}(y) \cdot \nabla_y \hat{\phi} + \sqrt{2\gamma\beta^{-1}\delta} G_1 \cdot \nabla_y \hat{\phi}(x, y),$$

and

$$\frac{1}{2} \nabla^2 \hat{\phi}(z) (\hat{Z}_1 - z)^{\circ 2} = \gamma \beta^{-1} \delta G_1 \cdot \nabla_y^2 \hat{\phi}(x, y) G_1 + o(\delta).$$

Thus, taking the expectation of equation (2.34) yields

$$\begin{aligned} \mathbb{E} \left(\hat{\phi}(\hat{X}_1, \hat{Y}_1) - \hat{\phi}(x, y) \right) \\ = \delta \nabla \hat{W}(y) \cdot \nabla_x \hat{\phi} - \delta \nabla \hat{U}(x) \cdot \nabla_y \hat{\phi} - \delta \gamma \nabla \hat{W}(y) \cdot \nabla_y \hat{\phi} + \delta \gamma \beta^{-1} \Delta_y \hat{\phi} + o(\delta), \end{aligned}$$

as well as

$$\mathbb{E} \left(\left(\hat{\phi}(\hat{X}_1, \hat{Y}_1) - \hat{\phi}(x, y) \right)^2 \right) = 2\delta \gamma \beta^{-1} |\nabla_y \hat{\phi}|^2 + o(\delta).$$

In the same spirit, the bounds (2.30) and equation (2.34) yield:

$$\begin{aligned} \mathbb{E} \left(\left(\hat{\phi}(\hat{X}_1, \hat{Y}_1) - \hat{\phi}(x, y) \right)^p \right) &\leq \sum_{\substack{k=0 \\ k \text{ odd}}}^p \binom{p}{k} (C\sqrt{\delta})^k \frac{k!}{2^{k/2}(k/2)!} (C\delta^{1-1/\ell})^{p-k} \\ &\leq C^p \sqrt{\delta}^p p! \sum_{\substack{k=0 \\ k \text{ odd}}}^p \frac{1}{(p-k)!(k/2)!2^{k/2}} \\ &\leq C(C\delta)^{p/2} p!. \end{aligned}$$

Hence for $\delta < C^{-1}$:

$$\mathbb{E} \left(\sum_{p \geq 3} \frac{1}{p!} \left(\hat{\phi}(\hat{X}_1, \hat{Y}_1) - \hat{\phi}(x, y) \right)^p \right) \leq C \frac{(C\delta)^{3/2}}{1 - C\delta} = o(\delta).$$

Finally, using that $\hat{U} = U$ and $\hat{W} = |\cdot|^2/2$ on $\mathcal{H}_{\delta, \ell}$, we get that for all $(x, y) \in \mathcal{H}_{\delta, \ell}$:

$$\mathbb{E}_{(x, y)} \left(\hat{V}_b(\hat{X}_1, \hat{Y}_1) \right) - \hat{V}_b(x, y) = \hat{V}_b(x, y) \left(\delta \frac{LV_b(x, y)}{V_b(x, y)} + o(\delta) \right), \quad (2.35)$$

where $o(\delta)$ is uniform in (x, y) . Hence, from equation (2.31), we have $\delta_0 > 0$ such that for all $(x, y) \in \mathcal{H}_{\delta, \ell} \setminus K_1$, $\delta < \delta_0$:

$$\mathbb{E}_{(x, y)} \left(\hat{V}_b(\hat{X}_1, \hat{Y}_1) \right) \leq (1 - \alpha\delta) V_b(x, y),$$

for some $\alpha > 0$. The map LV_b/V_b is continuous on the compact set K_1 , hence is bounded, and

inequality (2.35) yields that there exists $C > 0$ such that for $(x, y) \in K_1$:

$$\mathbb{E}_{(x,y)} \left(\hat{V}_b(\hat{X}_1, \hat{Y}_1) \right) \leq V_b(x, y) + C\delta$$

which concludes the proof. \square

This Lyapunov structure has an immediate corollary: the numerical scheme will stay away from the singularities uniformly on δ , even though its forbidden area is a level set depending on δ .

Corollary 2.4.1. *Under Assumptions 2.2.1 and 2.2.2, there exist $\delta_0, \ell_0 > 0$ such that for all $0 < b < \beta$, $0 < \ell < \ell_0$, $z \in \mathcal{X}$:*

$$\sup_{0 < \delta < \delta_0} \sup_{n \in \mathbb{N}} \mathbb{E}_z \left(e^{bH(\bar{Z}_n)} \right) < \infty.$$

Moreover, for all $z \in \mathcal{X}$, there exists $C, c > 0$ such that for all $a > 0$, $0 < \delta < \delta_0$, $0 < \ell < \ell_0$ and $n \in \mathbb{N}$:

$$\mathbb{P}_z \left(H(\bar{Z}_n) \geq a \right) \leq Ce^{-ca}.$$

Proof. Fix $b < b' < \beta$. The second Lyapunov property of Lemma 2.4.2 implies that:

$$\mathbb{E}_z \left(e^{bH(\bar{X}_n, \bar{Y}_n)} \right) \leq C \mathbb{E}_z \left(V_{b'}(\bar{X}_n, \bar{Y}_n) \right),$$

for some $C > 0$, whereas an induction argument using the third property yields

$$\mathbb{E}_z \left(V_{b'}(\bar{X}_n, \bar{Y}_n) \right) \leq \max(V_{b'}(x, y), K).$$

Both inequality combined then gives the first point of the Corollary. The second point is a direct application of Markov inequality. \square

The next lemma will allow us to do series expansion of $P_t(\bar{Z}_n)$ to prove Theorem 2.2.2. We write for $z_1, z_2 \in \mathbb{R}^{2d}$, $[z_1, z_2] = \{tz_1 + (1-t)z_2, t \in [0, 1]\}$.

Lemma 2.4.3. *For all $\kappa > 0$, there exists $C, \delta_0 > 0$ such that for all $0 < \delta < \delta_0$, $z_1, z_2 \in \{H \leq \kappa \ln 1/\delta\}$, and $|z_1 - z_2| \leq \delta^{\frac{2}{3}}$, all $z \in [z_1, z_2]$:*

$$H(z) \leq H(z_1) + C$$

Proof. Fix $z_1, z_2 \in \{H \leq \kappa \ln 1/\delta\}$, such that $|z_1 - z_2| \leq \delta^{\frac{2}{3}}$. We have that $[z_1, z_2] \subset B(z_1, \delta^{\frac{2}{3}})$. We first show that

$$B(z_1, \delta^{\frac{2}{3}}) \subset \{H \leq \kappa' \ln 1/\delta\},$$

for some $\kappa' > 0$. To this end, fix $z \in B(z_1, \delta^{\frac{2}{3}})$, and write for $0 \leq s \leq 1$:

$$\varphi(s) = U(z_1 + s(z - z_1)).$$

Thanks to Assumption 2.2.1, we have that φ is finite and smooth for $s < s_0$ small enough. We show at the same time that we may have $s_0 = 1$ and that $\varphi(1) \leq \kappa' \ln(1/\delta)$. We have:

$$\varphi'(s) = \nabla U(z_1 + s(z - z_1)) \cdot (z - z_1)$$

$$\leq |\nabla U(z_1 + s(z - z_1))| |z - z_1| \leq \delta^{\frac{2}{3}} \sqrt{c_0 \varphi^{2 + \frac{2}{\eta_0}} + d_0} \leq \delta^{\frac{2}{3}} \sqrt{c_0} \left(\varphi + \left(\frac{d_0}{c_0} \right)^{\frac{\eta_0}{2 + 2\eta_0}} \right)^{1 + \frac{1}{\eta_0}}.$$

Hence there is $c_1, c_2 > 0$ independent of z_1, z and δ such that for $s \leq s_0$:

$$\frac{\varphi'(s)}{(\varphi + c_2)^{1 + \frac{1}{\eta_0}}} \leq c_1 \delta^{\frac{2}{3}}.$$

Integrating this last inequation yields:

$$\frac{\eta_0}{(\varphi(s) + c_2)^{1/\eta_0}} \geq \frac{\eta_0}{(\varphi(0) + c_2)^{1/\eta_0}} - c_1 \delta^{\frac{2}{3}} s.$$

Whether $\eta_0 < 0$ or $\eta_0 > 1$, because $\varphi(0) \leq \kappa \ln(1/\delta)$, we have that there exists $\delta_0, \kappa' > 0$ such that for all $0 < \delta < \delta_0$, $\varphi(1) \leq \kappa' \ln(1/\delta)$. Hence using Assumption 2.2.2 again, we have that

$$\forall z \in \mathcal{B}(z_1, \delta^{\frac{2}{3}}), |\nabla U(z)| \leq \kappa'' (\ln(1/\delta))^{1 + \frac{1}{\eta_0}},$$

for some $\kappa'' > 0$. Using a Taylor expansion on φ , we get that for all $z_1 \in \{H \leq \kappa \ln 1/\delta\}$ and $z \in B(z_1, \delta^{\frac{2}{3}})$:

$$U(z) \leq U(z_1) + \kappa'' \delta^{\frac{2}{3}} (\ln 1/\delta)^{\frac{1}{\eta_0}},$$

and this concludes the proof with $C = \sup_{0 < \delta < \delta_0} \kappa'' \delta^{\frac{2}{3}} (\ln 1/\delta)^{\frac{1}{\eta_0}}$. \square

Proof of theorem 2.2.2. As in [158], we only prove the case $k = 1$ for simplicity, since for $k > 1$, the proof is the same. Fix some function $f \in \mathcal{P}(U)$, and write $u(t, x, y) = P_t f(x, y)$. Recall that u is solution to:

$$\begin{cases} \partial_t u = Lu, \\ u(t = 0, \cdot) = f, \end{cases} \quad (2.36)$$

where L is the generator defined by (2.12). For the sequel of the proof, fix $t > 0$. For all $n \in \mathbb{N}$, $\delta > 0$ is such that $n\delta = t$. We can write the total error made by the numerical scheme as:

$$\begin{aligned} \mathbb{E}_z (f(\bar{Z}_n)) - \mathbb{E}_z (f(Z_t)) &= \mathbb{E}_z (u(0, \bar{Z}_n) - u(n\delta, z)) \\ &= \sum_{p=0}^{n-1} \mathbb{E}_z (u(p\delta, \bar{Z}_{n-p}) - u((p+1)\delta, \bar{Z}_{n-(p+1)})). \end{aligned}$$

To make a series expansion of the expectations in the sum, we need to distinguish between three cases. Fix some $\kappa > 0$ to be determined later, $n, p \in \mathbb{N}$, $p \leq n$, and denote:

$$\begin{aligned} \mathcal{A}_1 &= \left\{ Z_{n-p}, Z_{n-(p+1)} \in \{H \leq \kappa \ln(1/\delta)\}, |Z_{n-p} - Z_{n-(p+1)}| \leq \delta^{2/3} \right\}, \\ \mathcal{A}_2 &= \left\{ Z_{n-p}, Z_{n-(p+1)} \in \{H \leq \kappa \ln(1/\delta)\}, |Z_{n-p} - Z_{n-(p+1)}| \geq \delta^{2/3} \right\}, \\ \mathcal{A}_3 &= \{Z_{n-p} \notin \{H \leq \kappa \ln(1/\delta)\}\} \cup \{Z_{n-(p+1)} \notin \{H \leq \kappa \ln(1/\delta)\}\}. \end{aligned}$$

The event \mathcal{A}_1 is the event on which we may do a series expansion of

$$u(p\delta, \bar{Z}_{n-p}) - u((p+1)\delta, \bar{Z}_{n-(p+1)}),$$

thanks to Lemma 2.4.3. Let's first show that the two other event have very low probability as δ goes to 0. Theorem 2.2.1 yields the existence of some $0 < b < \beta$, $C, q > 0$ such that:

$$|u - \int_{\mathcal{X}} f d\mu_\beta| \leq C e^{-qt} e^{bH}.$$

Fix $q_1, q_2 \geq 1$ such that

$$1/q_1 + 1/q_2 = 1, \quad bq_1 < \beta.$$

Using Holder inequality we get:

$$\begin{aligned} & |\mathbb{E}_z ((u(p\delta, \bar{Z}_{n-p}) - u((p+1)\delta, \bar{Z}_{n-(p+1)})) \mathbb{1}_{\mathcal{A}_2})| \\ & \leq C e^{-qp\delta} \left(\left(\mathbb{E}_z \left(e^{bq_1 H(\bar{Z}_{n-p})} \right) \right)^{1/q_1} + \left(\mathbb{E}_z \left(e^{bq_1 \bar{H}(Z_{n-(p+1)})} \right) \right)^{1/q_1} \right) (\mathbb{P}(\mathcal{A}_2))^{1/q_2}. \end{aligned}$$

On the event $\{H(\bar{Z}_{n-(p+1)}) \leq \kappa \ln(1/\delta)\}$, there is some $c > 0$ such that

$$|\nabla U(\bar{X}_{n-(p+1)})| + |Y_{n-(p+1)}| \leq C(\ln(1/\delta))^c$$

and

$$|\bar{Z}_{n-k} - \bar{Z}_{n-(k+1)}| \leq C\delta \ln(1/\delta)^c + \sqrt{\delta} |G|$$

where G is a standard Gaussian random variable. Hence for δ small enough, there is $c, C > 0$ such that:

$$\mathbb{P}(\mathcal{A}_2) \leq \mathbb{P}(G \geq c\delta^{1/6}) \leq C e^{-c\delta^{1/6}},$$

and finally

$$|\mathbb{E}_z ((u(p\delta, \bar{Z}_{n-p}) - u((p+1)\delta, \bar{Z}_{n-(p+1)})) \mathbb{1}_{\mathcal{A}_2})| \leq C e^{-c\delta^{1/6}}.$$

Next, using Holder's inequality again:

$$\begin{aligned} & \mathbb{E}_z ((u(p\delta, \bar{Z}_{n-p}) - u((p+1)\delta, \bar{Z}_{n-(p+1)})) \mathbb{1}_{\mathcal{A}_3}) \\ & \leq C e^{-qp\delta} \left(\left(\mathbb{E} \left(e^{bq_1 H(\bar{Z}_{n-p})} \right) \right)^{1/q_1} + \left(\mathbb{E} \left(e^{bq_1 \bar{H}(Z_{n-(p+1)})} \right) \right)^{1/q_1} \right) (\mathbb{P}(\mathcal{A}_3))^{1/q_2}. \end{aligned}$$

Fix $b' < \beta$. We have, using Markov inequality:

$$\mathbb{P}(\mathcal{A}_3) \leq 2 \sup_n \mathbb{P} \left(e^{b'H(Z_n)} \geq e^{-b'\kappa \ln(1/\delta)} \right) \leq 2 \sup_n \mathbb{E} (e^{b'H(Z_n)}) \delta^{b'\kappa} = C \delta^{b'\kappa}.$$

We can now fix $\kappa > 3q_2/b'$ to get that:

$$\mathbb{E}_z ((u(p\delta, \bar{Z}_{n-p}) - u((p+1)\delta, \bar{Z}_{n-(p+1)})) \mathbb{1}_{\mathcal{A}_3}) = O(\delta^3).$$

On the event \mathcal{A}_1 , we may use Lemma 2.4.3 to make a series expansion of u . For $0 \leq s \leq 1$, write

$$\varphi(s) = u((p+1-s)\delta, \bar{Z}_{n-(p+1)} + s(\bar{Z}_{n-p} - \bar{Z}_{n-(p+1)})).$$

Then:

$$(\varphi(1) - \varphi(0)) \mathbb{1}_{\mathcal{A}_1} = \left(\sum_{r=1}^5 \frac{\varphi^{(r)}(0)}{r!} + \frac{\varphi^{(6)}(\theta)}{6!} \right) \mathbb{1}_{\mathcal{A}_1},$$

for some $0 \leq \theta \leq 1$. Theorem 2.2.1 yields that there is $C > 0$, $0 < b < \beta$ such that:

$$|\varphi^{(6)}(\theta)| \mathbb{1}_{\mathcal{A}_1} \leq C \left(\delta^3 G^6 + \delta^{7/2} G^5 \ln(1/\delta) + \dots + \delta^6 (\ln(1/\delta))^6 \right) e^{bH(\bar{Z})} \mathbb{1}_{\mathcal{A}_1}$$

for some $\bar{Z} \in [\bar{Z}_{n-p}, \bar{Z}_{n-(p+1)}]$. However, Lemma 2.4.3 also yields that

$$H(\bar{Z}) \mathbb{1}_{\mathcal{A}_1} \leq H(\bar{Z}_{n-p}) + C.$$

Hence, Holder's inequality yields:

$$\mathbb{E} \left(|\varphi^{(6)}(\theta)| \mathbb{1}_{\mathcal{A}_1} \right) \leq C \delta^3 \sup_n \mathbb{E} \left(e^{q_1 b H(\bar{Z}_n)} \right)^{\frac{1}{q_1}} = C' \delta^3.$$

Using Holder's inequality as in the bound for the event \mathcal{A}_2 and \mathcal{A}_3 , we get that:

$$\mathbb{E} \left(\mathbb{1}_{\mathcal{A}_1} \sum_{r=1}^5 \frac{\varphi^{(r)}(0)}{r!} \right) = \mathbb{E} \left(\sum_{r=1}^5 \frac{\varphi^{(r)}(0)}{r!} \right) + O(\delta^3) = \delta^2 \mathbb{E} \left(\psi((p+1)\delta, \bar{Z}_{n-(p+1)}) \right) + O(\delta^3),$$

where

$$\begin{aligned} \psi(s, z) &= (\nabla U + \gamma y) \cdot (\nabla_y/2 - \nabla_x) u + \frac{1}{2} \partial_t^2 u - \frac{1}{2} y \cdot \nabla_x \partial_t u + \frac{1}{2} (\nabla U + \gamma y) \cdot \nabla_y^2 y (\nabla U + \gamma y) \\ &\quad - \frac{1}{2} y \cdot \nabla_{x,y}^2 (\nabla U + \gamma y) + \gamma \beta^{-1} \sum_{i=1}^d \partial_{x_i} \partial_{y_i} u - \frac{2}{3} \gamma \beta^{-1} \partial_t \Delta_y u \\ &\quad - \frac{7}{12} \gamma \beta^{-1} (\nabla U + \gamma y) \cdot \nabla_y \Delta_y u + \frac{1}{3} \gamma \beta^{-1} y \cdot \nabla_x \Delta_y u \\ &\quad + \frac{1}{2} (\gamma \beta^{-1})^2 \sum_{i=1}^d \partial_{y_i}^4 u + \frac{1}{6} (\gamma \beta^{-1})^2 \sum_{i \neq j=1}^d \partial_{y_i}^2 \partial_{y_j}^2 u. \end{aligned}$$

The expression of ψ is found using the fact that u solves (2.36). Finally, we have that:

$$\mathbb{E}_z (f(\bar{Z}_n)) - \mathbb{E}_z (f(Z_t)) = \delta^2 \mathbb{E} \left(\sum_{p=1}^n \psi(p\delta, \bar{Z}_{n-p}) \right) + O(\delta^2).$$

The rest follows as in the proof of Talay and Tubaro [158], which we write for the sake of completeness. As ψ is a function of the derivative of u , Theorem 2.2.1 yields that:

$$|\mathbb{E}_z (f(\bar{Z}_n)) - \mathbb{E}_z (f(Z_t))| \leq C \delta^2 \left(\sum_{p=1}^n e^{-qp\delta} \mathbb{E}_z \left(e^{bH(\bar{Z}_{n-p})} + 1 \right) \right) \leq C \delta^2 \left(\frac{1}{\delta} + 1 \right) \leq C \delta. \quad (2.37)$$

The function $s \rightarrow \mathbb{E}_z (\psi(z, Z_{t-s}))$ is smooth and is bounded, hence the weak convergence (2.37) and classical Riemann summation results yield that:

$$\left| \delta \mathbb{E} \left(\sum_{p=1}^n \psi(p\delta, \bar{Z}_{n-p}) \right) - \int_0^t \mathbb{E}_z (\psi(z, Z_{t-s})) ds \right| = O(\delta),$$

which concludes the proof. \square

2.4.2 Expansion for the invariant measure of the numerical scheme with rejection

To establish an expansion of the invariant measure of the numerical scheme, we first need to prove its existence, and ergodicity of the scheme. For this purpose, we define a metric on $\mathcal{M}^1(\mathbb{R}^{2d})$. Fix some $0 < b < \beta$, and write for $z_1, z_2 \in \mathbb{R}^{2d}$:

$$\mathbf{d}(z_1, z_2) = \mathbb{1}_{z_1 \neq z_2} (1 + V_b(z_1) + V_b(z_2)),$$

where V_b is the Lyapunov function from Lemma 2.4.2. For any two probability measures μ, ν , we call (Z_1, Z_2) a coupling of μ and ν if the law of Z_1 (resp. Z_2) is μ (resp. ν). From the distance \mathbf{d} on \mathbb{R}^{2d} , we define the corresponding Kantorovich distance on $\mathcal{M}^1(\mathbb{R}^{2d})$ by:

$$W_{\mathbf{d}}(\mu, \nu) = \inf \{ \mathbb{E}(\mathbf{d}(Z_1, Z_2)) \mid (Z_1, Z_2) \text{ coupling of } \mu \text{ and } \nu \}.$$

This distance makes $\mathcal{M}^1(\mathbb{R}^{2d})$ complete. Hence, if we show that the map $\mathcal{L}aw(z) \mapsto \mathcal{L}aw(\bar{Z}_k)$, where \bar{Z}_k is the numerical scheme given by (2.4) with initial condition z , for some $k \in \mathbb{N}$, is a contraction, then this would imply the existence of a unique stationary measure, as well as exponentially fast convergence towards it for this Kantorovich distance. It can be shown that convergence for such a distance would imply ergodicity of the numerical scheme, in the sense of the convergence of the average

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=1}^n \mathbb{E}_{(x,y)} (f(\bar{X}_k, \bar{Y}_k)) = \mu(f). \quad (2.38)$$

Write $K_2 = \{H \leq K\}$, where K is the constant from Lemma 2.4.2. Because V_b is a Lyapunov function, we only need to show that there exists $c > 0$, $k \in \mathbb{N}$, such that for all $z \in K_2$, we have the following Doeblin condition:

$$\mathbb{P}_z(\bar{Z}_k \in \cdot) \geq c\lambda(\cdot \cap K_2), \quad (2.39)$$

where λ stands for the Lebesgue measure, see for example [52, Theorem 24]. In other words, we want to show that the numerical scheme creates density.

Lemma 2.4.4. *Under Assumptions 2.2.1 and 2.2.2, there exists $\delta_0, \ell_0 > 0$ such that for all $0 < \delta < \delta_0$, $0 < \ell < \ell_0$, the numerical scheme (2.4) admits a unique stationary measure $\mu_{\beta, \delta} \in \mathcal{M}^1(\mathbb{R}^{2d})$, and for all $(x, y) \in \mathcal{H}_{\delta, \ell}$ and $f : \mathcal{H}_{\delta, \ell} \rightarrow \mathbb{R}$ continuous:*

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=1}^n \mathbb{E}_{(x,y)} (f(\bar{X}_k, \bar{Y}_k)) = \mu_{\beta, \delta}(f).$$

Proof. As explained before, it suffices to show the so-called Doeblin condition (2.39). To achieve such inequality, we first begin by showing, using a controllability argument, that this is locally true, in the sense that: there exists $c > 0$ such that for all $z \in K_2$, $z_0 \in B(z, \delta)$ and $A \subset B(z, \delta)$,

$$\mathbb{P}_{z_0}(\bar{Z}_2 \in A) \geq c\lambda(A).$$

To this end, we want to show that there exists (g_0, g_1) such that if $\sqrt{2\gamma\beta^{-1}\delta}(G_0, G_1) = (g_0, g_1)$ and $\bar{Z}_0 = z_0$, then $\bar{Z}_2 = z_1$. Since Gaussian random variables have a density with respect to the Lebesgue measure, then if $z_1 \mapsto (g_0, g_1)$ is a diffeomorphism, the result will hold. Fix

$z_0, z_1 \in B(z, \delta)$ and write:

$$F(x, y) = (x + \delta(y - \delta \nabla U(x) - \delta \gamma y), y - \delta \nabla U(x) - \delta \gamma y),$$

and $\mathbf{G}(g_0, g_1) = (\mathbf{G}_1(g_0, g_1), \mathbf{G}_2(g_0, g_1))$ where

$$\mathbf{G}_1(g_0, g_1) = \delta(2 - \delta\gamma)g_0 - \delta^2 \nabla U(x_0 + \delta(y_0 - \delta U(x_0) - \delta \gamma y_0 + g_0)) + \delta g_1,$$

and

$$\mathbf{G}_2(g_0, g_1) = (1 - \delta\gamma)g_0 - \delta \nabla U(x_0 + \delta(y_0 - \delta U(x_0) - \delta \gamma y_0 + g_0)) + g_1.$$

Now, the goal is to show that there exists $g_0, g_1 \in \mathbb{R}^d$ such that:

$$H(F(z_0) + (\delta g_0, g_0)) \leq \delta^{-\ell}, \quad (2.40)$$

and

$$\begin{aligned} \mathbf{G}(g_0, g_1) &= z_1 - z_0 \\ &+ (\delta^2(2 - \gamma\delta)\nabla U(x_0) - \delta(2 - 3\delta\gamma + (\delta\gamma)^2)y_0, \delta(1 - \gamma\delta)\nabla U(x_0) + (2\gamma\delta - (\gamma\delta)^2)y_0). \end{aligned} \quad (2.41)$$

We have:

$$\mathbf{G} = \tilde{G}(I_d + \delta\tilde{G}),$$

where \tilde{G} is the invertible matrix:

$$\tilde{G} = \begin{pmatrix} 2\delta I_d & \delta I_d \\ I_d & I_d \end{pmatrix}, \quad \tilde{G}^{-1} = \begin{pmatrix} \delta^{-1} I_d & -I_d \\ -\delta^{-1} I_d & 2I_d \end{pmatrix},$$

and where \tilde{G} and its derivative are bounded on $B(0, \rho)$, for all $\rho > 0$, uniformly with respect to $\delta < \delta_0$ and $z_0 \in K_2$. Write $h = I_d + \delta\tilde{G}$. The goal now is to show that for all $\rho_2 > 0$, there exists $\rho_1 > 0$ such that h is a diffeomorphism from a neighborhood $W \subset B(0, \rho_1)$ of 0 to $B(h(0), \rho_2)$, by following the proof of the local inverse theorem. To this end, for $v, g \in \mathbb{R}^{2d}$, write:

$$\phi_v(g) = g - (d_0 h)^{-1}(h(g) - v).$$

There exists $\delta_0 > 0$ such that, for all $z_0 \in K_2$ and $0 < \delta < \delta_0$, this function is well defined, i.e. $d_0 h$ is invertible. For all $\rho_1 > 0$, there exists $\delta_0 > 0$ such that for all $\delta < \delta_0$, $g \in B(0, \rho_1)$, $\|d_g \phi_v\| \leq 1/2$. Hence for $g, g' \in B_{\mathbb{R}^{2d}}(0, \rho_1)$, we have

$$|\phi_v(g) - \phi_v(g')| \leq \frac{1}{2}|g - g'|.$$

For all $\rho_2 > 0$, $v \in B(h(0), \rho_2)$, and δ small enough we have that

$$|(d_0 h)^{-1}(h(0) - v)| < 2\rho_2.$$

This implies that if $\rho_1 > 4\rho_2$, then for all $g \in B(0, \rho_1)$, we have $\phi_v(g) \in B(0, \rho_1)$:

$$|\phi_v(g)| \leq |\phi_v(g) - \phi_v(0)| + |\phi_v(0)| \leq \frac{1}{2}|g| + 2\rho_2 < \rho_1.$$

Hence we may apply Banach fixed point theorem to get that for all $v \in B(0, \rho_2)$, there exists $g_v \in B(0, \rho_1)$ such that $\phi_v(g_v) = g_v$, or equivalently $h(g_v) = v$. The fact that $v \mapsto g_v$ is smooth

is proved in the same way as in the proof of the inverse function theorem. Thus, for all $\rho > 0$, there exists $\delta_0, r > 0$ such that for all $z_0 \in K_2$, $0 < \delta < \delta_0$, there exists a bounded neighborhood $W \subset B_{\mathbb{R}^{2d}}(0, r)$ of 0, such that G is a diffeomorphism from W to $B_{\mathbb{R}^{2d}}(G(0, 0), \rho\delta)$. We fix

$$\rho > 3 + 2 \sup_{(x,y) \in K_2} |y| + |\nabla U(x)|.$$

Write $I(z_0, z_1)$ for the left hand side of Equation (2.41). For δ small enough, $I \in B(G(0, 0), \rho\delta)$ for all $z_0, z_1 \in B(z, \delta)$, so that Equation (2.41) has a solution $G^{-1}(I(z_0, z_1))$. The fact that $W \subset B(0, r)$ yields condition (2.40) for $\delta < \Delta/r$, where Δ is the distance between K_2 and \mathcal{D}^c . Finally, because (G_0, G_1) has a positive density, for $z_0 \in B(z, \delta)$ and $A \subset B(z, \delta)$ we have:

$$\begin{aligned} \mathbb{P}_{z_0}(\bar{Z}_2 \in A) &\geq \mathbb{P}((G_0, G_1) \in G^{-1} \circ I(\cdot, z_0)(A)) \\ &\geq c \int_{G^{-1} \circ I(\cdot, z_0)(A)} dz' = c \int_A |\det(\nabla G \circ I(z', z_0))|^{-1} dz' \geq c' \lambda(A). \end{aligned}$$

Now we are able to show condition (2.39). Fix δ small enough so that the local Doeblin condition holds true. Since K_2 is compact, there exists z_1, \dots, z_N such that $K_2 = \cup_{i=1}^N B(z_i, \delta)$. For all measurable $A \subset K_2$, we have that

$$\lambda(A) \leq \sum_{i=1}^N \lambda(A \cap B(z_i, \delta)).$$

Hence we may restrict ourselves to $A \subset B(z_j, \delta)$, for some $j \in \llbracket 1, N \rrbracket$. Up to increasing the value of K , we may suppose that K_2 is connected. In this case, there exists $k \in \mathbb{N}$ and $\varepsilon > 0$ such that for all $z \in B(z_i, \delta)$ and $A \subset B(z_j, \delta)$, there exists a finite sequence $z'_0, z'_1, \dots, z'_k \in K_2$ satisfying the following condition: $z'_0 = z$, $z'_k \in B(z_j, \delta)$, and for all $0 \leq p \leq k-1$, there is i_p such that $B(z_p, \varepsilon), B(z_{p+1}, \varepsilon) \subset B(z_{i_p}, \delta)$. Hence we have:

$$\mathbb{P}(Z_{2(k+1)} \in A) \geq \mathbb{P}(Z_{2p} \in B(z'_p, \varepsilon), 1 \leq p \leq k, Z_{2(k+1)} \in A) \geq (cw)^k \lambda(A),$$

where w is the volume of $B_{\mathbb{R}^{2d}}(0, \varepsilon)$, and this concludes the proof. \square

All function $f \in \mathcal{P}(U)$ are continuous on $\mathcal{H}_{\delta, \ell}$, thus we do indeed have the convergence (2.38) for such function. To prove Theorem 2.2.3, we first need weak convergence of the stationary measure of the numerical scheme, for functions that depends on time.

Lemma 2.4.5. *Let $g \in \mathcal{C}^\infty(\mathbb{R}_+ \times \mathbf{X}, \mathbb{R})$ be such that for all $\alpha \in \mathbb{N}^{2d}$, there exists $C_\alpha, q_\alpha > 0$ and $b_\alpha < \beta$ such that:*

$$|\partial^\alpha g(t, z)| \leq C_\alpha e^{-q_\alpha t} e^{b_\alpha H(z)}.$$

Under Assumption 2.2.1, 2.2.2 and 2.2.3, there exists $C > 0$ such that for δ small enough:

$$|\mu_{\beta, \delta}(g(t, \cdot)) - \mu_\beta(g(t, \cdot))| \leq C e^{-qt} \delta.$$

Proof. The proof is very close to the proof Theorem 2.2.2, hence we will omit some details. We fix g satisfying the assumptions of Lemma 2.4.5, $t > 0$, and we write $u(s, z) = \mathbb{E}_z(g(t, Z_s))$, where $Z = (X, Y)$ is the continuous process (2.3). $g(t, \cdot) \in \mathcal{P}(U)$, and we have for any $n \in \mathbb{N}$:

$$\frac{1}{n} \sum_{k=1}^n \mathbb{E}_z(u(0, \bar{Z}_k) - u(k\delta, z)) = \frac{1}{n} \sum_{k=1}^n \sum_{p=0}^{k-1} \mathbb{E}_z(u(p\delta, \bar{Z}_{k-p}) - u((p+1)\delta, \bar{Z}_{k-(p+1)})). \quad (2.42)$$

Lemma 2.4.4 yields that:

$$\frac{1}{n} \sum_{k=1}^n \mathbb{E}_z (u(0, \bar{Z}_k)) = \frac{1}{n} \sum_{k=1}^n \mathbb{E}_z (g(t, \bar{Z}_k)) \xrightarrow{n \rightarrow \infty} \mu_{\beta, \delta}(g(t, \cdot)).$$

The continuous process is also ergodic, as shown by Theorem 2.3.1. Hence we have:

$$\frac{1}{n} \sum_{k=1}^n \mathbb{E}_z (u(k\delta, z)) = \frac{1}{n} \sum_{k=1}^n P_{k\delta} g(t, \cdot)(z) \xrightarrow{n \rightarrow \infty} \mu_{\beta}(g(t, \cdot)).$$

As in the proof of Theorem 2.2.2, a Taylor expansion yields:

$$\left| \sum_{p=0}^{k-1} \mathbb{E}_z (u(p\delta, \bar{Z}_{k-p}) - u((p+1)\delta, \bar{Z}_{k-(p+1)})) \right| \leq C e^{-qt} \delta,$$

and letting n go to infinity in (2.42) concludes the proof. \square

Proof of Theorem 2.2.3. Fix $f \in \mathcal{P}(U)$ and write $u(t, z) = \mathbb{E}_z(f(Z_t))$, where $Z = (X, Y)$ is the continuous process (2.3). We write a Taylor expansion of higher order than in the proof of Lemma 2.4.5 to get:

$$\sum_{p=0}^{k-1} \mathbb{E}_z (u(p\delta, \bar{Z}_{k-p}) - u((p+1)\delta, \bar{Z}_{k-(p+1)})) = \delta^2 \sum_{p=0}^{k-1} \mathbb{E}_z (\psi((p+1)\delta, \bar{Z}_{k-(p+1)})) + O(\delta^2),$$

where the term $O(\delta^2)$ is independent of k . Hence we may write:

$$\begin{aligned} & \frac{1}{n} \sum_{k=1}^n \sum_{p=0}^{k-1} \mathbb{E}_z (u(p\delta, \bar{Z}_{k-p}) - u((p+1)\delta, \bar{Z}_{k-(p+1)})) \\ &= \frac{1}{n} \sum_{k=1}^n \sum_{p=0}^{k-1} \delta^2 \mathbb{E}_z (\psi((p+1)\delta, \bar{Z}_{k-(p+1)})) + O(\delta^2) \\ &= \frac{\delta^2}{n} \sum_{i=1}^n \sum_{j=0}^n \mathbb{E}_z (\psi(i\delta, \bar{Z}_j)) - \frac{\delta^2}{n} \sum_{k=1}^n \sum_{p=k}^n \mathbb{E}_z (\psi((p+1)\delta, \bar{Z}_{k-(p+1)})) + O(\delta^2). \end{aligned}$$

Using Theorem 2.2.1 and Corollary 2.4.1, we bound:

$$\begin{aligned} \left| \frac{1}{n} \sum_{k=1}^n \sum_{p=k}^n \mathbb{E}_z (\psi((p+1)\delta, \bar{Z}_{k-(p+1)})) \right| &\leq \frac{1}{n} \sum_{k=1}^n \sum_{p=k}^n \mathbb{E}_z \left(C e^{-q(p+1)\delta} e^{bH(\bar{Z}_{k-(p+1)})} \right) \\ &\leq \frac{C'}{n} \sum_{k=1}^n \sum_{p=k}^{\infty} e^{-q(p+1)\delta} \\ &\leq \frac{C''}{n} \sum_{k=1}^n e^{-qk\delta} \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

Ergodicity of the numerical scheme yields that

$$\frac{1}{n} \sum_{j=0}^n \mathbb{E}_z (\psi ((i\delta, \bar{Z}_j))) \xrightarrow{n \rightarrow \infty} \mu_{\beta, \delta} (\psi(i\delta, \cdot)),$$

and Theorem 2.2.1 and Corollary 2.4.1 that:

$$\left| \frac{1}{n} \sum_{j=0}^n \mathbb{E}_z (\psi ((i\delta, \bar{Z}_j))) \right| \leq C e^{-qi\delta}.$$

Hence the dominated convergence theorem yields that:

$$\frac{1}{n} \sum_{i=1}^n \sum_{j=0}^n \mathbb{E}_z (\psi ((i\delta, \bar{Z}_j))) \xrightarrow{n \rightarrow \infty} \sum_{i \geq 0} \mu_{\beta, \delta} (\psi(i\delta, \cdot)).$$

Now Lemma 2.4.5 and Riemann sum tells us that:

$$\sum_{i \geq 0} \mu_{\beta, \delta} (\psi(i\delta, \cdot)) = \int_0^{\infty} \mu_{\beta} (\psi(t, \cdot)) dt + O(\delta).$$

Letting n go to infinity in Equation (2.42) (with $g(t, \cdot) = f$) then concludes the proof. \square

Chapter 3

Long-time behavior of the velocity jump Langevin process

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Abstract : We study the long-time convergence in Sobolev spaces of the velocity jump Langevin process, which is a process designed to sample from the Gibbs measure with a reduced number of computation of the gradient of the potential compared to the Langevin process.

3.1 Introduction

3.1.1 Motivation

As in the previous chapter, we are interested in the sampling of the Gibbs measure

$$\mu = \frac{1}{\mathcal{Z}_\mu} \exp(-\beta H(x, v)) dx dv \tag{3.1}$$

where $\mathcal{Z}_\mu = \int_{\mathbb{R}^{2d}} \exp(-\beta H(x, v)) dx dv$ is a normalization constant. A popular process that allows for the sampling of the Gibbs measure is the kinetic Langevin diffusion, defined as the solution of the following SDE:

$$\begin{cases} dX_t &= V_t dt \\ dV_t &= -\nabla U(X_t) dt - \gamma V_t dt - \sqrt{2\beta^{-1}\gamma} dW_t, \end{cases} \tag{3.2}$$

where $(W_t)_{t \geq 0}$ is a standard Brownian motion in \mathbb{R}^d and $\gamma > 0$ is a friction parameter. When simulating this dynamic, the most expensive part is the computation of the forces ∇U . A common approach is to substitute this gradient with a stochastic version, as in the stochastic gradient descent in optimization, see [20, 146, 92], or to treat various parts of the potentials with different time steps (multi-time-step methods), see [162]. We are interested here in an alternative approach that involves replacing (3.2) with a hybrid model combining a classical Langevin diffusion and a piecewise deterministic Markov process. This hybrid model still samples from μ but can be simulated using a numerical splitting scheme that requires fewer gradient computations per time step.

The idea involves decomposing the potential as

$$\nabla U = \sum_{i=0}^K F_i,$$

where F_0 denotes the computationally inexpensive component (typically the short-range forces exhibiting fast variation), while the F_i terms, for $i \geq 1$, represent long-range forces, which are computationally more demanding than F_0 (as each atom interacts with all others through these forces, unlike the short-range ones). Then, define the so-called velocity jump Langevin process $(X_t, V_t)_{t \geq 0}$ as the Langevin diffusion process associated with the force F_0 :

$$\begin{cases} dX_t &= V_t dt \\ dV_t &= -F_0(X_t) dt - \gamma V_t dt - \sqrt{2\beta^{-1}\gamma} dW_t, \end{cases}$$

with additional jumps at rate $\lambda_i(x, v)$, corresponding to a jump kernel $q_i(x, v, dv')$ depending on F_i in such a way that ensures that the equilibrium measure of the process is indeed the Gibbs measure μ . The Langevin velocity jump process can be simulated using a splitting scheme similar to the BAOAB scheme introduced by Leimkuhler, where the parts corresponding to the free transport, the forces, the friction/dissipation, and the jumps are simulated separately, see [21, 107, 105, 106]. More precisely, the generator \mathcal{L} will be decomposed as a sum of Markov generators

$$\mathcal{L} = \mathcal{L}_A + \mathcal{L}_B + \mathcal{L}_O + \mathcal{L}_J,$$

each corresponding to a part of the dynamic, see Section 3.1.2 below. The process can then be discretized based on the Trotter/Strang formula

$$e^{t\mathcal{L}} = e^{\frac{t}{2}\mathcal{L}_B} e^{\frac{t}{2}\mathcal{L}_J} e^{\frac{t}{2}\mathcal{L}_A} e^{t\mathcal{L}_O} e^{\frac{t}{2}\mathcal{L}_A} e^{\frac{t}{2}\mathcal{L}_J} e^{\frac{t}{2}\mathcal{L}_B} + o(t^2).$$

The simulation of the jump part of the process is based on the thinning method, see [113, 116]. Suppose that $\lambda_i \leq \bar{\lambda}_i$ for $1 \leq i \leq K$, and denote $\bar{\lambda} = \sum_i \bar{\lambda}_i$. A direct computation on the generator shows that the jumps can be exactly simulated this way: starting from (x, v) ,

1. Draw \mathcal{E} a standard exponential random variable, and let $T = \mathcal{E}/\bar{\lambda}$ be the next jump time proposal.
2. Draw I in $\llbracket 1, K \rrbracket$ such that $\mathbb{P}(I = i) = \bar{\lambda}_i/\bar{\lambda}$. Propose a jump of type I at time T .
3. Accept the jump with probability $\lambda_I(x, v)/\bar{\lambda}_I$, in which case the velocity is re-sampled at time T according to $q_I(x, v, dv')$, otherwise the velocity at time T is simply v (there is no jump).

Unlike a traditional numerical scheme for the Langevin diffusion (like BAOAB), where the gradient ∇U is computed at every time step, here we only need to evaluate F_i when a jump of type

i is proposed (at step 3 above), which does not occur at every time step for every i . Moreover, the jump rate and jump kernel, first defined in [138], will depend on a parameter, in such a way that when this parameter goes to 0, the velocity jump Langevin process converges to the classical Langevin diffusion (in the sense that the distributions of the processes are close in the space of càdlàg trajectories endowed with the Skorohod topology, see [138, Theorem 3.6]). As a consequence, in addition to the sampling of the Gibbs measure, dynamical properties such as the diffusion constants may be computed using this process.

Motivated by a weak error expansion *à la Talay-Tubaro* of a splitting scheme for the velocity jump Langevin process as in Chapter 2, we prove convergence of its semi-group in Sobolev space of arbitrary order. The derivation of estimates on the semi-group and weak error expansion is left for future work.

3.1.2 Mathematical setting

Fix some smooth $U : \mathbb{R}^d \rightarrow \mathbb{R}$. We will work under the following set of assumptions.

Assumption 3.1.1. • *The Gibbs measure is well defined*

$$\int_{\mathbb{R}^d} e^{-U(x)} dx < \infty.$$

- $U = U_0 + U_1$ where the derivatives of U_1 of all order are bounded.
- $\nabla^2 U_0$ as well as its derivatives of all order are bounded, and there exist $\kappa > 0$ and a compact set $\mathcal{K} \subset \mathbb{R}^d$ such that for all $x \notin \mathcal{K}$

$$-x \cdot \nabla U_0(x) \leq -\kappa|x|^2.$$

- $\Psi \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{R}_+)$ is a smooth non-negative function such that Ψ' and all its derivative are bounded, and

$$\Psi(s) - \Psi(-s) = s. \tag{3.3}$$

For simplicity, in the remainder of this work, we fix $\beta = 1$, and consider a particular decomposition of the forces. Let us denote $(e_i)_{1 \leq i \leq d}$ the canonical basis of \mathbb{R}^d , let $K = d$, and

$$F_0 = \nabla U_0, \quad F_i = \partial_i U_1 e_i, \quad i \in \llbracket 1, d \rrbracket. \tag{3.4}$$

In other words, we write U as $U_0 + U_1$ and decompose ∇U_1 in a similar fashion as in the Zig-Zag process:

$$\nabla U_1(x) = \sum_{i=1}^d \partial_i U_1(x) e_i.$$

Fix a friction parameter $\gamma > 0$ and a constant $\theta > 0$. Write $\mathcal{C}_c^\infty(\mathbb{R}^{2d})$ for the set of smooth function with compact support from \mathbb{R}^{2d} to \mathbb{R} . The Markov process we are going to study is the so-called velocity jump Langevin process, whose Markov generator is given by

$$\mathcal{L} = \mathcal{L}_H + \mathcal{L}_D + \mathcal{L}_J$$

where for any function $h \in \mathcal{C}_c^\infty(\mathbb{R}^{2d})$:

$$\mathcal{L}_H h(x, v) = v \cdot \nabla_x h(x, v) - \nabla U_0(x) \cdot \nabla_v h(x, v) \quad (\text{Hamiltonian part})$$

$$\mathcal{L}_D h(x, v) = -\gamma v \cdot \nabla_v h(x, v) + \gamma \Delta_v h(x, v) \quad (\text{diffusion})$$

$$\mathcal{L}_J h(x, v) = \sum_{i=1}^d \mathcal{L}_J^i h(x, v) \quad (\text{jumps})$$

where

$$\mathcal{L}_J^i h(x, v) = \lambda_i(x, v) \int_{\mathbb{R}^d} (h(x, v') - h(x, v)) q_i(x, v, dv'),$$

$$\begin{aligned} \lambda_i(x, v) \int_{\mathbb{R}^d} h(x, v') q_i(x, v, dv') \\ = \frac{1 + \theta^2}{\theta^2} \mathbb{E} \left[h \left(x, v - \frac{2\theta}{1 + \theta^2} (\theta v_i + G) e_i \right) \Psi \left(\frac{\theta \partial_i U_1(x)}{1 + \theta^2} (\theta v_i + G) \right) \right], \end{aligned}$$

and $G \sim \mathcal{N}(0, 1)$ is a one-dimensional standard Gaussian variable. In the definition above, $q_i(x, v, \cdot)$ is a probability measure for all $(x, v) \in \mathbb{R}^{2d}$, in other words λ_i , for all $i \in \llbracket 1, d \rrbracket$, is obtained by taking $h = 1$ in the formula above. As explained above, this is the generator of a Langevin process with drift given by U_0 , and that jumps at rate λ_i according to the kernel q_i . Let (X_t, V_t) be a Markov process with generator \mathcal{L} , and let $(P_t)_{t \geq 0}$ be the semi-group associated to this process

$$P_t f(x, v) = \mathbb{E}_{(x, v)} [f(X_t, V_t)],$$

defined for $f : \mathbb{R}^{2d} \rightarrow \mathbb{R}$ bounded. Fix $k \in \mathbb{N}$ and define the Sobolev space of order k by

$$H^k(\mu) = \left\{ f : \mathbb{R}^{2d} \rightarrow \mathbb{R} \text{ measurable, } \sum_{i+j \leq k} \int_{\mathbb{R}^{2d}} |\nabla_x^i \nabla_y^j f|^2 d\mu < \infty \right\},$$

where we denoted

$$|\nabla_x^i \nabla_y^j f|^2 = \sum_{|\alpha_1|=i; |\alpha_2|=j} |\partial_x^{\alpha_1} \partial_y^{\alpha_2} f|^2, \quad |\alpha_p| = \sum_{i=1}^d (\alpha_p)_i.$$

Write as well

$$\|f\|_{H^k(\mu)} = \sum_{i+j \leq k} \int_{\mathbb{R}^{2d}} |\nabla_x^i \nabla_y^j f|^2 d\mu$$

the Sobolev norm for $f \in H^k(\mu)$, and

$$\mu(f) = \int_{\mathbb{R}^{2d}} f d\mu.$$

Theorem 3.1.1. *Suppose Assumptions 3.1.1. For all $k \in \mathbb{N}$, there exist $C_k, \rho_k > 0$ such that for all $f \in H^k(\mu)$ and $t \geq 0$*

$$\|P_t f - \mu(f)\|_{H^k(\mu)} \leq C_k e^{-\rho_k t} \|f - \mu(f)\|_{H^k(\mu)}.$$

Let's make a few comments on the assumptions and the theorem. First, we take $\theta > 0$ as a positive constant for simplicity, but it can actually be taken as a function of x (for instance $\theta(x) = \theta_0 |\nabla U_1(x)|$ with $\theta_0 > 0$). As explained in [138], the case $\theta = \infty$ corresponds to the bouncy particle sampler (see [22]), whereas when $\theta \rightarrow 0$, we retrieve the kinetic Langevin process. Secondly, the condition (3.3) on Ψ is here to ensure the invariance of μ . In the Zigzag process, the jump rate is usually taken such that $\Psi(s) = \max(0, s)$, which indeed satisfies the equality (3.3). However, the computations in Sobolev spaces require that the generator has smooth coefficients, which prevent such a Ψ . An admissible example is given by $\Psi(s) = a \log(\exp(s/a) + 1)$ for any $a > 0$. Finally, the choice of the decomposition (3.4) is made in order to avoid singular terms of the form $\nabla U / |\nabla U|$ in the hypocoercivity computations. As explained in Section 3.1.1, this theorem is a first step in proving uniform bounds on the semi-group of the velocity jump process, in order to show weak error expansion of numerical schemes. The main addition with respect to Chapter 2 is the treatment of the jump terms.

3.1.3 Notation

In all the following, $|\cdot|$ denotes the euclidean norm in \mathbb{R}^d as well as the Frobenius norm for matrices, and \cdot the standard dot product on \mathbb{R}^d or the Frobenius scalar product when it's applied on matrices. For any operators A and B , we denote $[A, B] = AB - BA$ their commutator. In some computations, it will be useful to work with $\rho = \frac{1-\theta^2}{1+\theta^2} \in (-1, 1)$ instead of θ . In the remainder of this work, we will denote by C various constants that may change from line to line.

3.2 Proof of Theorem 3.1.1

The proof of Theorem 3.1.1 relies on hypocoercive computations *à la Villani* in Sobolev spaces. The velocity jump Langevin process is hypocoercive, in the sense that the generator of this process is not coercive for the usual Sobolev norm. To prove exponential convergence to equilibrium, for a given $k \in \mathbb{N}$, we are going to introduce a norm equivalent to the classical Sobolev norm, defined for $f \in H^k(\mu)$ by

$$\mathcal{N}_k(f) = \int_{\mathbb{R}^{2d}} f^2 d\mu + \sum_{p=1}^k \int_{\mathbb{R}^{2d}} \left(\sum_{i=0}^{p-1} \omega_{i,p} |\nabla_x^i \nabla_v^{p-i} f|^2 + \omega_{p,p} |(\nabla_x^p - \nabla_x^{p-1} \nabla_v) f|^2 \right) d\mu \quad (3.5)$$

where $(\omega_{i,p})_{p \in \mathbb{N}, 1 \leq i \leq p}$ are positive numbers. In the remainder of this work, we are going to refer to this norm as the modified Sobolev norm. Following [163], we are going to show that we may choose $(\omega_{i,p})_{p \in \mathbb{N}, 1 \leq i \leq p}$ such that for $f \in H^k$, we have

$$\partial_t \mathcal{N}_k(P_t f - \mu(f)) \leq -\rho_k \mathcal{N}_k(P_t f - \mu(f)),$$

for some $\rho_k > 0$. Theorem 3.1.1 is a direct consequence of the following result:

Theorem 3.2.1. *There exist positive $(\omega_{i,p})_{p \in \mathbb{N}, 1 \leq i \leq p}$ and $(\rho_k)_{k \in \mathbb{N}^*}$ such that for all $k \in \mathbb{N}^*$, $f \in H^k(\mu)$ and $t \geq 0$,*

$$\mathcal{N}_k(P_t f - \mu(f)) \leq e^{-\rho_k t} \mathcal{N}(f - \mu(f)),$$

where \mathcal{N}_k was defined in (3.5).

The proof of this theorem relies on an induction argument and Gamma calculus, as presented in Section 1.2.1. Fix $\phi : \mathcal{C}_c^\infty(\mathbb{R}^{2d}) \rightarrow \mathcal{C}_c^\infty(\mathbb{R}^{2d})$. Recall the definition of the generalized *carré du*

champ

$$\Gamma_\phi(h) = \frac{1}{2} (\mathcal{L}(\phi(h)) - D_h\phi(h)\mathcal{L}h), \quad (3.6)$$

where $D_h\phi$ denotes the differential operator of ϕ . When $\phi(h) = h^2$ we retrieve the usual carré du champ, which is simply denoted by Γ . We will show in Section 3.2.1 that μ is indeed an invariant measure of the velocity jump process. This formally implies that:

$$\partial_t \mathcal{N}_k(P_t f - \mu(f)) = - \int_{\mathbb{R}^{2d}} \Gamma(P_t f) d\mu - \sum_{p=1}^k \int_{\mathbb{R}^{2d}} \left(\sum_{i=0}^{p-1} \omega_{i,p} \Gamma_{i,p}(P_t f) + \omega_{p,p} \Gamma_{p,p}(P_t f) \right) d\mu, \quad (3.7)$$

where, for $i < p$,

$$\Gamma_{i,p}(h) = \Gamma_{|\nabla_x^i \nabla_v^{p-i} \cdot|^2}(h) \quad \text{and} \quad \Gamma_{p,p}(h) = \Gamma_{|\nabla_x^p - \nabla_x^{p-1} \nabla_v \cdot|^2}(h).$$

If we could show that for all $h \in \mathcal{C}_c^\infty(\mathbb{R}^{2d})$

$$\int_{\mathbb{R}^{2d}} \Gamma(h) d\mu + \sum_{p=1}^k \int_{\mathbb{R}^{2d}} \left(\sum_{i=0}^{p-1} \omega_{i,p} \Gamma_{i,p}(h) + \omega_{p,p} \Gamma_{p,p}(h) \right) d\mu \geq \rho_k \mathcal{N}_k(h - \mu(h)),$$

for some $\rho_k > 0$, then Theorem 3.2.1 would follow, at least formally, in the sense that we haven't justified the time derivatives. We will actually prove a slightly stronger result (see Proposition 3.2.5 below) for the induction argument. Recall also the proposition that allows for the computations of this generalized *carré du champ*.

Proposition 3.2.1. *If there exists $A = (A_1, \dots, A_p) : \mathcal{C}^\infty \rightarrow (\mathcal{C}^\infty)^p$ a linear operator such that $\phi(h) = |Ah|^2$, then*

$$\Gamma_\phi(h) = \Gamma(Ah) + Ah \cdot [\mathcal{L}, A]h,$$

where $\Gamma(Ah) = \sum_{i=1}^p \Gamma(A_i h)$ and $[\mathcal{L}, A] = ([\mathcal{L}, A_1], \dots, [\mathcal{L}, A_p])$.

For all i, j, i', j' such that $i + j = i' + j'$, the scalar product here has to be understood as

$$\nabla_x^i \nabla_v^j h \cdot \nabla_x^{i'} \nabla_v^{j'} h := \sum_{|\alpha_1|=i} \sum_{|\alpha_2|=j'} \sum_{|\nu|=i'-i} (\partial_x^{\alpha_1} \partial_v^{\alpha_2 + \nu} h) (\partial_x^{\alpha_1 + \nu} \partial_v^{\alpha_2} h).$$

We will also extensively use the fact that

$$[\mathcal{L}, A] = [\mathcal{L}_H, A] + [\mathcal{L}_J, A] + [\mathcal{L}_D, A].$$

In order to justify the discussion above, we will start by proving that the Gibbs measure is indeed invariant for the velocity jump Langevin process in Section 3.2.1. Section 3.2.2 will treat the case $k = 1$ which is the initialization of the induction argument. Section 3.2.3 will conclude with the proof of convergence in H^k space through Theorem 3.2.1.

3.2.1 Invariance of μ

The use of the velocity jump process for the sampling of μ , as well as the use of hypocoercivity method rely on the fact that μ is indeed an invariant measure of this process. Let us prove this property by computing the adjoint of \mathcal{L} in $L^2(\mu)$, denoted as \mathcal{L}^* .

Proposition 3.2.2. Denote \mathcal{L}^* the adjoint of \mathcal{L} in $L^2(\mu)$. For all $h \in C_c^\infty(\mathbb{R}^{2d})$, we have:

$$\mathcal{L}^* h = -v \cdot \nabla_x h + \nabla U_0 \cdot \nabla_v h - \gamma v \cdot \nabla_v h + \gamma \Delta_v h + \frac{1 + \theta^2}{\theta^2} \sum_{i=1}^d \mathbb{E} \left[(h(\cdot, V^i) - h) \Psi \left(\frac{\partial_i U_1}{2} (V_i^i - v_i) \right) \right],$$

with

$$V^i = v - \frac{2\theta}{1 + \theta^2} (\theta v_i + G) e_i,$$

where G is a random variable with standard Gaussian distribution.

Proof. Let $g, h \in C_c^\infty(\mathbb{R}^{2d})$. By integrating by parts, we get

$$\begin{aligned} \int_{\mathbb{R}^{2d}} g \mathcal{L}_H h d\mu &= \mathcal{Z}_\mu^{-1} \int_{\mathbb{R}^{2d}} g (v \cdot \nabla_x h - \nabla U_0 \cdot \nabla_v h) e^{-U(x)} e^{-|v|^2/2} dx dv \\ &= -\mathcal{Z}_\mu^{-1} \int_{\mathbb{R}^{2d}} h v \cdot \nabla_x (g e^{-U(x)}) e^{-|v|^2/2} dx dv \\ &\quad + \mathcal{Z}_\mu^{-1} \int_{\mathbb{R}^{2d}} h \nabla_v \cdot (g e^{-|v|^2/2} \nabla U_0(x)) e^{-U(x)} dx dv \\ &= - \int_{\mathbb{R}^{2d}} h v \cdot \nabla_x g d\mu + \int_{\mathbb{R}^{2d}} g h v \cdot \nabla U(x) d\mu + \int_{\mathbb{R}^{2d}} h \nabla U_0(x) \cdot \nabla_v g d\mu \\ &\quad - \int_{\mathbb{R}^{2d}} g h v \cdot \nabla U_0(x) d\mu \\ &= \int_{\mathbb{R}^{2d}} h (-v \cdot \nabla_x g + \nabla U_0 \cdot \nabla_v g) d\mu + \int_{\mathbb{R}^{2d}} g h v \cdot \nabla U_1 d\mu. \end{aligned}$$

We also have

$$\begin{aligned} \int_{\mathbb{R}^{2d}} g \mathcal{L}_D h d\mu &= \mathcal{Z}_\mu^{-1} \int_{\mathbb{R}^{2d}} g (-\gamma v \cdot \nabla_v h + \gamma \Delta_v h) e^{-U(x)} e^{-|v|^2/2} dx dv \\ &= \gamma \mathcal{Z}_\mu^{-1} \left(\int_{\mathbb{R}^{2d}} g \nabla_v (e^{-|v|^2/2}) \cdot \nabla_v h e^{-U(x)} dx dv + \int_{\mathbb{R}^{2d}} h \Delta_v (g e^{-|v|^2/2}) e^{-U(x)} dx dv \right) \\ &= \gamma \mathcal{Z}_\mu^{-1} \left(\int_{\mathbb{R}^{2d}} \nabla_v (g e^{-|v|^2/2}) \cdot \nabla_v h e^{-U(x)} dx dv - \int_{\mathbb{R}^{2d}} \nabla_v g \cdot \nabla_v h e^{-U(x)} e^{-|v|^2/2} dx dv \right. \\ &\quad \left. + \int_{\mathbb{R}^{2d}} h \Delta_v (g e^{-|v|^2/2}) e^{-U(x)} dx dv \right) \\ &= -\gamma \int_{\mathbb{R}^{2d}} \nabla_v g \cdot \nabla_v h d\mu = \int_{\mathbb{R}^{2d}} h \mathcal{L}_D g d\mu \end{aligned}$$

For the jump part, denote $k_0(x, v, \cdot)$ the law of the random variable V^i . Then k_0 is reversible with respect to the standard Gaussian measure, in the sense that for all $x \in \mathbb{R}^d$,

$$k_0(x, v, dv') e^{-|v|^2/2} dv = k_0(x, v', dv) e^{-|v'|^2/2} dv'. \quad (3.8)$$

Indeed, since $V_j^i = v_j$ for $j \neq i$ and

$$V_i^i = \frac{1 - \theta^2}{1 + \theta^2} v_i + \frac{2\theta}{1 + \theta^2} G = \rho v_i + \sqrt{1 - \rho^2} G,$$

where $\rho = \frac{1-\theta^2}{1+\theta^2}$, the coordinates of V^i are independent and each transition $v_j \mapsto V_j^i$ is reversible for the standard one-dimensional Gaussian. Using this reversibility, and the fact that $\Psi(s) - \Psi(-s) = s$, we get that

$$\begin{aligned}
\int_{\mathbb{R}^{2d}} g \mathcal{L}_J h d\mu &= \frac{1+\theta^2}{\theta^2} \sum_{i=1}^d \int_{\mathbb{R}^{2d}} g \mathbb{E} \left[(h(x, V^i) - h(x, v)) \Psi \left(\frac{\partial_i U_1(x)}{2} (v_i - V_i^i) \right) \right] d\mu \\
&= \frac{1+\theta^2}{\theta^2} \sum_{i=1}^d \int_{\mathbb{R}^{2d}} h \mathbb{E} \left[(g(x, V^i) - g) \Psi \left(-\frac{\partial_i U_1(x)}{2} (v_i - V_i^i) \right) \right] \\
&\quad + \frac{1+\theta^2}{\theta^2} \sum_{i=1}^d \int_{\mathbb{R}^{2d}} g h \mathbb{E} \left[\Psi \left(-\frac{\partial_i U_1(x)}{2} (v_i - V_i^i) \right) - \Psi \left(\frac{\partial_i U_1(x)}{2} (v_i - V_i^i) \right) \right] d\mu \\
&= \frac{1+\theta^2}{\theta^2} \sum_{i=1}^d \int_{\mathbb{R}^{2d}} h \mathbb{E} \left[(g(x, V^i) - g) \Psi \left(-\frac{\partial_i U_1(x)}{2} (v_i - V_i^i) \right) \right] \\
&\quad - \frac{1+\theta^2}{2\theta^2} \sum_{i=1}^d \int_{\mathbb{R}^{2d}} g h \partial_i U_1 \mathbb{E} [(v_i - V_i^i)] d\mu \\
&= \frac{1+\theta^2}{\theta^2} \sum_{i=1}^d \int_{\mathbb{R}^{2d}} h \mathbb{E} \left[(g(x, V^i) - g) \Psi \left(-\frac{\partial_i U_1(x)}{2} (v_i - V_i^i) \right) \right] - \int_{\mathbb{R}^{2d}} g h v \cdot \nabla U_1 d\mu
\end{aligned}$$

Therefore, by summing the three terms, we get the result. \square

Corollary 3.2.1. *Under Assumption 3.1.1, for all $h \in \mathcal{C}_c^\infty(\mathbb{R}^{2d})$*

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} \mathcal{L} h d\mu = 0.$$

Proof. This is a direct consequence of the fact that $\mathcal{L}^* 1 = 0$. \square

Notice in particular that \mathcal{L}_D is symmetric in $L^2(\mu)$, whereas neither \mathcal{L}_H nor \mathcal{L}_J are left invariant by μ , only $\mathcal{L}_H + \mathcal{L}_J$ is.

3.2.2 Exponential decay for the $H^1(\mu)$ -norm

In this section, we prove convergence of the process in $H^1(\mu)$. The modified Sobolev norm here reads

$$\mathcal{N}_1(h) = \int_{\mathbb{R}^{2d}} h^2 d\mu + \int_{\mathbb{R}^{2d}} \omega_{0,1} |\nabla_v h|^2 + \omega_{1,1} |(\nabla_x - \nabla_v) h|^2 d\mu,$$

and Equation (3.7) can be written:

$$\partial_t \mathcal{N}_1(P_t f - \mu(f)) = - \int_{\mathbb{R}^{2d}} \Gamma(P_t f) d\mu - \int_{\mathbb{R}^{2d}} (\omega_{0,1} \Gamma_{0,1}(P_t f) + \omega_{1,1} \Gamma_{1,1}(P_t f)) d\mu.$$

The initialisation of the induction argument to prove Theorem 3.2.1 is

Lemma 3.2.1. *Under Assumption 3.1.1, there exist $\omega_{0,1}, \omega_{1,1}, \rho_1$ such that for all $h \in \mathcal{C}_c^\infty(\mathbb{R}^{2d})$ satisfying $\mu(h) = 0$:*

$$\int_{\mathbb{R}^{2d}} \Gamma(h) d\mu + \int_{\mathbb{R}^{2d}} (\omega_{0,1} \Gamma_{0,1}(h) + \omega_{1,1} \Gamma_{1,1}(h)) d\mu \geq \rho_1 \left(\mathcal{N}_1(h) + \int_{\mathbb{R}^{2d}} |\nabla_x \nabla_v h|^2 + |\nabla_v^2 h|^2 d\mu \right).$$

The terms of order 2 are present to compensate future terms in the induction, but are not required for the convergence in $H^1(\mu)$. This convergence relies on the so-called Poincaré inequality

Proposition 3.2.3. *Under Assumption 3.1.1, the Gibbs measure (3.1) satisfy a Poincaré inequality: there exists $C_P > 0$ such that*

$$\int_{\mathbb{R}^{2d}} (h - \mu(h))^2 d\mu \leq C_P \int_{\mathbb{R}^{2d}} |\nabla h|^2 d\mu. \quad (3.9)$$

for all $h \in \mathcal{C}_c^\infty(\mathbb{R}^{2d})$.

Proof. Proof of such inequality can be found in [6]. □

In order to apply Proposition 3.2.1, we need to express the commutators. For the Hamiltonian part we get:

$$[\mathcal{L}_H, \nabla_x] = \nabla^2 U_0 \nabla_v, \quad [\mathcal{L}_H, \nabla_v] = -\nabla_x.$$

For the diffusion part we get:

$$[\mathcal{L}_D, \nabla_x] = 0, \quad [\mathcal{L}_D, \nabla_v] = \gamma \nabla_v.$$

Regarding the jump part, we have

Lemma 3.2.2. *Under Assumption 3.1.1, there exists $C > 0$ such that for all $h \in \mathcal{C}_c^\infty(\mathbb{R}^{2d})$:*

$$\int_{\mathbb{R}^{2d}} |[\nabla_x, \mathcal{L}_J]h|^2 d\mu + \int_{\mathbb{R}^{2d}} |[\nabla_v, \mathcal{L}_J]h|^2 d\mu \leq C \left(\int_{\mathbb{R}^{2d}} |\nabla_v h|^2 d\mu + \int_{\mathbb{R}^{2d}} |\nabla_v^2 h|^2 d\mu \right).$$

To prove Lemma 3.2.2, we need two intermediate results:

Lemma 3.2.3. *For any function $g \in \mathcal{C}_c^\infty(\mathbb{R}^d)$,*

$$\int_{\mathbb{R}^d} |v|^2 g^2(v) e^{-|v|^2/2} dv \leq 2d \int_{\mathbb{R}^d} g^2(v) e^{-|v|^2/2} dv + 4 \int_{\mathbb{R}^d} |\nabla_v g(v)|^2 e^{-|v|^2/2} dv.$$

Proof. This is a particular case of the Lemma A.24 of [163]. Notice that $ve^{-|v|^2/2} = -\nabla e^{-|v|^2/2}$. Hence, an integration by parts and Young's inequality yield, for any x ,

$$\begin{aligned} \int_{\mathbb{R}^d} |v|^2 g^2(v) e^{-|v|^2/2} dv &= - \int_{\mathbb{R}^d} g^2(v) v \cdot \nabla e^{-|v|^2/2} dv \\ &= \int_{\mathbb{R}^d} \nabla \cdot (g^2(v) v) e^{-|v|^2/2} dv \\ &= d \int_{\mathbb{R}^d} g^2(v) e^{-|v|^2/2} dv + \int_{\mathbb{R}^d} 2g(v) \nabla g(v) \cdot v e^{-|v|^2/2} dv \\ &\leq d \int_{\mathbb{R}^d} g^2(v) e^{-|v|^2/2} dv + \int_{\mathbb{R}^d} 2|\nabla g(v)|^2 e^{-|v|^2/2} dv \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^d} |v|^2 g^2(v) e^{-|v|^2/2} dv, \end{aligned}$$

and thus the result. □

Proposition 3.2.4 (Poincaré for Gaussians). *For any function $g \in \mathcal{C}_c^\infty(\mathbb{R}^d)$,*

$$\int_{\mathbb{R}^d} \left(g(v) - \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} h(w) e^{-|w|^2/2} dw \right)^2 e^{-|v|^2/2} dv \leq \int_{\mathbb{R}^d} |\nabla g(v)|^2 e^{-|v|^2/2} dv. \quad (3.10)$$

Proof. Proof of such inequality can be found in [6]. \square

Proof of Lemma 3.2.2. For all $i \in \llbracket 1, d \rrbracket$, denote

$$g_i(x, v, G) = \left(x, v - \frac{2\theta}{1+\theta^2} (\theta v_i + G) e_i \right), \quad \varphi_i(x, v, G) = \frac{\theta \partial_i U_1(x)}{1+\theta^2} (\theta v_i + G).$$

We then have

$$[\nabla_x, \mathcal{L}_J]h = \sum_{i=1}^d [\nabla_x, \mathcal{L}_J^i]h = \frac{1}{\theta} \sum_{i=1}^d \mathbb{E} [(\theta v_i + G)(h(g_i(G)) - h) \Psi'(\varphi_i(G))] \nabla \partial_i U_1,$$

and

$$[\nabla_v, \mathcal{L}_J]h = \sum_{i=1}^d [\nabla_v, \mathcal{L}_J^i]h = \sum_{i=1}^d \mathbb{E} [\partial_i U_1 (h(g_i(G)) - h) \Psi'(\varphi_i(G)) - 2\partial_{v_i} h(g_i(G)) \Psi(\varphi_i(G))] e_i.$$

Using the fact that Ψ' , ∇U_1 and $\nabla^2 U_1$ are bounded, there exists a constant $C > 0$ such that

$$|[\nabla_x, \mathcal{L}_J]h|^2 \leq C \sum_{i=1}^d \mathbb{E} [(v_i^2 + G^2)(h(g_i(G)) - h)^2],$$

and

$$|[\nabla_v, \mathcal{L}_J]h|^2 \leq C \sum_{i=1}^d \mathbb{E} [(h(g_i(G)) - h)^2 + (\partial_{v_i} h(g_i(G)))^2 (1 + v_i^2 + G^2)].$$

Recall that by denoting $k_0(x, v, \cdot)$ the law of the random variable

$$V^i = v - \frac{2\theta}{1+\theta^2} (\theta v_i + G) e_i$$

where G is a random variable with standard normal distribution, $k_0(x, v, \cdot)$ is reversible with respect to the standard Gaussian measure, see (3.8). By using this reversibility, and the fact that v being fixed, $V_i^i \sim \mathcal{N}(\rho v_i, 1 - \rho^2)$, we have that for any function $h \in \mathcal{C}_c^\infty(\mathbb{R}^{2d})$

$$\begin{aligned} \int_{\mathbb{R}^{2d}} \mathbb{E} \left[(1 + v_i^2 + G^2) (\partial_{v_i} h(g_i(G)))^2 \right] d\mu &= \int_{\mathbb{R}^{2d}} (\partial_{v_i} h)^2 \left(1 + \mathbb{E} \left[(V_i^i)^2 + \frac{(v_i^2 - \rho V_i^i)^2}{1 - \rho^2} \right] \right) d\mu \\ &= \int_{\mathbb{R}^{2d}} (\partial_{v_i} h)^2 (2 + v_i^2) d\mu \\ &\leq 4 \int_{\mathbb{R}^{2d}} ((\partial_{v_i} h)^2 + (\partial_{v_i}^2 h)^2) d\mu, \end{aligned}$$

where we applied Proposition 3.2.3 to with $d = 1$ to $v_i \mapsto \partial_{v_i} h(x, v)$ in the last inequality. By

denoting Π_{v_i} the projection

$$\Pi_{v_i} h(x, v) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} h(x, v_1, \dots, v_{i-1}, w_i, v_{i+1}, \dots, v_d) e^{-w_i^2/2} dw_i,$$

we also have

$$\begin{aligned} \int_{\mathbb{R}^{2d}} \mathbb{E} [(1 + v_i^2 + G^2)(h(g_i(G)) - h)^2] d\mu &\leq 2 \int_{\mathbb{R}^{2d}} \mathbb{E} [(1 + v_i^2 + G^2)((h(g_i(G)) - \Pi_{v_i} h)^2 + (h - \Pi_{v_i} h)^2)] d\mu \\ &\leq 2 \int_{\mathbb{R}^{2d}} \left(3 + v_i^2 + \mathbb{E} \left[(V_i^i)^2 + \frac{(v_i^2 - \rho V_i^i)^2}{1 - \rho^2} \right] \right) (h - \Pi_{v_i} h)^2 d\mu \\ &\leq 2 \int_{\mathbb{R}^{2d}} (4 + 2v_i^2)(h - \Pi_{v_i} h)^2 d\mu \\ &\leq 16 \int_{\mathbb{R}^{2d}} (h - \Pi_{v_i} h)^2 d\mu + 16 \int_{\mathbb{R}^{2d}} (\partial_{v_i} h)^2 d\mu, \end{aligned}$$

where we applied again Proposition 3.2.3 with $d = 1$ to $v_i \mapsto h(x, v) - \Pi_{v_i}(x, v)$ in the last inequality. The Poincaré inequality (3.10) can be written

$$\int_{\mathbb{R}^{2d}} (h - \Pi_{v_i} h)^2 d\mu \leq \int_{\mathbb{R}^{2d}} |\partial_{v_i} h|^2 d\mu,$$

and thus

$$\int_{\mathbb{R}^{2d}} \mathbb{E} [(1 + v_i^2 + G^2)(h(g_i(G)) - h)^2] d\mu \leq 32 \int_{\mathbb{R}^{2d}} (\partial_{v_i} h)^2 d\mu.$$

Therefore, there exists $C > 0$ such that

$$\int_{\mathbb{R}^{2d}} |[\nabla, \mathcal{L}_J]h|^2 d\mu \leq C \sum_{i=1}^d \int_{\mathbb{R}^{2d}} ((\partial_{v_i} h)^2 + |\nabla_v \partial_{v_i} h|^2) d\mu = C \left(\int_{\mathbb{R}^{2d}} |\nabla_v h|^2 d\mu + \int_{\mathbb{R}^{2d}} |\nabla_v^2 h|^2 d\mu \right),$$

which concludes the proof. \square

We now have everything to prove Lemma 3.2.1.

Proof of Lemma 3.2.1. Fix $\omega_{0,1} > \omega_{1,1} > 0$ that we are going to chose later. Let's first treat the derivative of the L^2 norm. We have for all $h \in C_c^\infty(\mathbb{R}^{2d})$, $(x, v) \in \mathbb{R}^{2d}$

$$\Gamma(h)(x, v) = 2\gamma |\nabla_v h(x, v)|^2 + \sum_{i=1}^d \lambda_i(x, v) \int_{\mathbb{R}^d} (h(x, v') - h(x, v))^2 q_i(x, v, dv'). \quad (3.11)$$

This already implies that

$$\Gamma(h) \geq 2\gamma |\nabla_v h|^2.$$

To get a lower bound on $\Gamma_{0,1}(h)$ and $\Gamma_{1,1}(h)$, we use Proposition 3.2.1. Equation (3.11) yields:

$$\Gamma(\nabla_v h) \geq 2\gamma |\nabla_v^2 h|^2, \quad \Gamma((\nabla_x - \nabla_v)h) \geq 2\gamma |(\nabla_x \nabla_v - \nabla_v^2)h|^2,$$

so that using $\omega_{0,1} > \omega_{1,1}$ and Young inequality:

$$\omega_{0,1} \Gamma(\nabla_v h) + \omega_{1,1} \Gamma((\nabla_x - \nabla_v)h) \geq 2\gamma(\omega_{0,1} - \omega_{1,1}) |\nabla_v^2 h|^2 + \omega_{1,1} (\gamma |\nabla_v^2 h|^2 + 2\gamma/3 |\nabla_x \nabla_v h|^2).$$

Let us now look at the commutators. Fix $\varepsilon > 0$ and write using Young inequality and Lemma 3.2.2:

$$\begin{aligned} \int_{\mathbb{R}^{2d}} \nabla_v h \cdot [\mathcal{L}, \nabla_v] h d\mu &= \int_{\mathbb{R}^{2d}} \nabla_v h \cdot (-\nabla_x h + \gamma \nabla_v + [\mathcal{L}_J, \nabla_v] h) d\mu \\ &\geq - \int_{\mathbb{R}^{2d}} \left(\frac{1}{\varepsilon} + 1 \right) |\nabla_v h|^2 + \frac{\varepsilon}{2} |\nabla_x - \nabla_v h|^2 + \frac{\varepsilon}{2} C (|\nabla_v h|^2 d\mu + |\nabla_v^2 h|^2) d\mu, \end{aligned}$$

for some $C > 0$. Using again Young inequality and Lemma 3.2.2, we get that there exists $C > 0$ such that:

$$\begin{aligned} \int_{\mathbb{R}^{2d}} (\nabla_x - \nabla_v) h \cdot [\mathcal{L}, \nabla_x - \nabla_v] h d\mu &= \int_{\mathbb{R}^{2d}} (\nabla_x - \nabla_v) h \cdot (\nabla^2 U_0 \nabla_v h + \nabla_x h - \gamma \nabla_v h + [\mathcal{L}_J, \nabla_x - \nabla_v] h) d\mu \\ &\geq \int_{\mathbb{R}^{2d}} \frac{1}{2} |\nabla_x - \nabla_v h|^2 - C (|\nabla_v h|^2 + |\nabla_v^2 h|^2) d\mu. \end{aligned}$$

Now all is left to do is to choose ε , $\omega_{0,1}$ and $\omega_{1,1}$. We choose them such that

$$\frac{\omega_{1,1}}{\omega_{0,1}} \leq \frac{2\gamma - C\varepsilon}{2\gamma + C}, \quad \varepsilon < \min \left(\frac{\omega_{1,1}}{2\omega_{0,1}}, \frac{2\gamma}{C} \right), \quad C\omega_{1,1} + \omega_{0,1} \left(\frac{1}{\varepsilon} + 1 + \frac{C\varepsilon}{2} \right) \leq \gamma$$

so that

$$\begin{aligned} \int_{\mathbb{R}^{2d}} \Gamma(h) d\mu + \int_{\mathbb{R}^{2d}} (\omega_{0,1} \Gamma_{0,1}(h) + \omega_{1,1} \Gamma_{1,1}(h)) d\mu \\ \geq \int_{\mathbb{R}^{2d}} \gamma |\nabla_v h|^2 + \frac{\omega_{1,1}}{4} |\nabla_x - \nabla_v h|^2 + \omega_{1,1} \gamma \left(|\nabla_v^2 h|^2 + \frac{2}{3} |\nabla_x \nabla_v h|^2 \right) d\mu \\ \geq \tilde{\rho}_1 \int_{\mathbb{R}^{2d}} \omega_{0,1} |\nabla_v h|^2 + \omega_{1,1} (|\nabla_x - \nabla_v h|^2 + |\nabla_x \nabla_v h|^2 + |\nabla_v^2 h|^2) d\mu, \end{aligned}$$

for some $\tilde{\rho}_1 > 0$. Since we consider h such that $\mu(h) = 0$, the Poincaré inequality (3.9) yields that there exists $\rho_1 > 0$ such that

$$\tilde{\rho}_1 \int_{\mathbb{R}^{2d}} \omega_{0,1} |\nabla_v h|^2 + \omega_{1,1} (|\nabla_x - \nabla_v h|^2 + |\nabla_x \nabla_v h|^2 + |\nabla_v^2 h|^2) d\mu \geq \rho_1 \left(\mathcal{N}_1(h) + \int_{\mathbb{R}^{2d}} |\nabla_x \nabla_v h|^2 + |\nabla_v^2 h|^2 d\mu \right),$$

which concludes the proof. \square

3.2.3 Exponential decay for the H^k -norm

Recall that we defined the modified Sobolev norm as

$$\mathcal{N}_k(h) := \int_{\mathbb{R}^{2d}} h^2 d\mu + \sum_{p=1}^k \int_{\mathbb{R}^{2d}} \left(\sum_{i=0}^{p-1} \omega_{i,p} |\nabla_x^i \nabla_v^{p-i} h|^2 + \omega_{p,p} |(\nabla_x^p - \nabla_x^{p-1} \nabla_v) h|^2 \right) d\mu$$

In order to control its derivative (3.7), we prove by induction the following lemma.

Proposition 3.2.5. *Under Assumption 3.1.1, there exist $(\omega_{i,p})_{1 \leq i \leq p}$ such that for all $k \in \mathbb{N}$,*

there exists ρ_k such that for all $h \in \mathcal{C}_c^\infty(\mathbb{R}^{2d}, \mathbb{R})$ such that $\mu(h) = 0$:

$$\int_{\mathbb{R}^{2d}} \Gamma(h) d\mu + \sum_{p=1}^k \int_{\mathbb{R}^{2d}} \left(\sum_{i=0}^{p-1} \omega_{i,p} \Gamma_{i,p}(h) + \omega_{p,p} \Gamma_{p,p}(h) \right) d\mu \geq \rho_k \left(\mathcal{N}_k(h) + \int_{\mathbb{R}^{2d}} \sum_{i=0}^k |\nabla_x^i \nabla_v^{k+1-i} h|^2 d\mu \right). \quad (3.12)$$

To prove this Lemma, we will need formulas for partial derivatives of products, provided by the Leibniz formula

Proposition 3.2.6. For all $g, h \in \mathcal{C}_c^\infty$ and $\alpha_1, \alpha_2 \in \mathbb{N}^d$,

$$\partial_x^{\alpha_1} \partial_v^{\alpha_2} (gh) = \sum_{\nu_1 \leq \alpha_1, \nu_2 \leq \alpha_2} \binom{\alpha_1}{\nu_1} \binom{\alpha_2}{\nu_2} (\partial_x^{\nu_1} \partial_v^{\nu_2} g) (\partial_x^{\alpha_1 - \nu_1} \partial_v^{\alpha_2 - \nu_2} h)$$

where for $\alpha = (\alpha_1, \dots, \alpha_d)$ and $\nu = (\nu_1, \dots, \nu_d)$,

$$\binom{\alpha}{\nu} = \prod_{i=1}^d \binom{\alpha_i}{\nu_i},$$

and

$$\nu \leq \alpha \iff \forall i \in \llbracket 1, d \rrbracket, \nu_i \leq \alpha_i.$$

Let us look at the commutators. As in the H^1 case, we will look separately the parts associated to the Hamiltonian dynamic \mathcal{L}_H , the diffusion \mathcal{L}_D and the jump process \mathcal{L}_J .

Lemma 3.2.4 (Hamiltonian commutators). Let $i \in \llbracket 0, k \rrbracket$. There exists $C > 0$ such that the following holds. If $i < k$, we have

$$\nabla_x^i \nabla_v^{k+1-i} h \cdot [\mathcal{L}_H, \nabla_x^i \nabla_v^{k+1-i}] h \geq -|\nabla_x^i \nabla_v^{k+1-i} h|^2 - C \left(|\nabla_x^{i+1} \nabla_v^{k-i} h|^2 + \sum_{j=0}^{i-1} |\nabla_x^j \nabla_v^{k+2-i} h|^2 \right).$$

In the case $i = k$, for all $\eta > 0$, we have

$$\nabla_x^k \nabla_v h \cdot [\mathcal{L}_H, \nabla_x^k \nabla_v] h \geq -\frac{\eta}{8} |(\nabla_x^{k+1} - \nabla_x^k \nabla_v) h|^2 - C \left(1 + \frac{1}{\eta} \right) |\nabla_x^k \nabla_v h|^2 - C \sum_{j=0}^{k-1} |\nabla_x^j \nabla_v^2 h|^2.$$

Finally, we have

$$(\nabla_x^{k+1} - \nabla_x^k \nabla_v) h \cdot [\mathcal{L}_H, \nabla_x^{k+1} - \nabla_x^k \nabla_v] h \geq \frac{1}{2} |(\nabla_x^{k+1} - \nabla_x^k \nabla_v) h|^2 - C \left(\sum_{j=0}^k |\nabla_x^j \nabla_v h|^2 + \sum_{j=0}^{k-1} |\nabla_x^j \nabla_v^2 h|^2 \right).$$

Proof. For all $\alpha_1, \alpha_2 \in \mathbb{N}^d$ with $|\alpha_1| = i$ and $|\alpha_2| = k + 1 - i$, where $\alpha_2 = (\alpha_{2,1}, \dots, \alpha_{2,d})$, write

$$\alpha_2^j = (\alpha_{2,1}, \dots, \alpha_{2,j-1}, \alpha_{2,j} - 1, \alpha_{2,j+1}, \dots, \alpha_{2,d}),$$

and we have

$$\begin{aligned}
\partial_x^{\alpha_1} \partial_v^{\alpha_2} \mathcal{L}_H h &= \sum_{j=1}^d \partial_x^{\alpha_1} \partial_v^{\alpha_2} (v_j \partial_{x_j} h - \partial_j U_0 \partial_{v_j} h) \\
&= \sum_{j=1}^d \partial_v^{\alpha_2} (v_j \partial_x^{\alpha_1} \partial_{x_j} h) - \partial_x^{\alpha_1} (\partial_j U_0 \partial_v^{\alpha_2} \partial_{v_j} h) \\
&= \sum_{j=1}^d \left(\sum_{\nu_2 \leq \alpha_2} \binom{\alpha_2}{\nu_2} \partial_v^{\nu_2} (v_j) \partial_v^{\alpha_2 - \nu_2} \partial_x^{\alpha_1} \partial_{x_j} h - \sum_{\nu_1 \leq \alpha_1} \binom{\alpha_1}{\nu_1} \partial_x^{\nu_1} \partial_j U_0 \partial_x^{\alpha_1 - \nu_1} \partial_v^{\alpha_2} \partial_{v_j} h \right) \\
&= \sum_{j=1}^d \left(\alpha_{2,j} \partial_v^{\alpha_2} \partial_x^{\alpha_1} \partial_{x_j} h + v_j \partial_v^{\alpha_2} \partial_x^{\alpha_1} \partial_{x_j} h - \sum_{\nu_1 \leq \alpha_1} \binom{\alpha_1}{\nu_1} \partial_x^{\nu_1} \partial_j U_0 \partial_x^{\alpha_1 - \nu_1} \partial_v^{\alpha_2} \partial_{v_j} h \right).
\end{aligned}$$

Therefore,

$$[\mathcal{L}_H, \partial_x^{\alpha_1} \partial_v^{\alpha_2}] h = \sum_{j=1}^d \left(\sum_{\nu_1 \leq \alpha_1; \nu_1 \neq 0} \binom{\alpha_1}{\nu_1} \partial_x^{\nu_1} \partial_j U_0 \partial_x^{\alpha_1 - \nu_1} \partial_v^{\alpha_2} \partial_{v_j} h - \alpha_{2,j} \partial_v^{\alpha_2} \partial_x^{\alpha_1} \partial_{x_j} h \right).$$

Using the bound on the derivatives of U_0 , this yields that there exists a $C > 0$ such that

$$\nabla_x^i \nabla_v^{k+1-i} h \cdot [\mathcal{L}_H \nabla_x^i \nabla_v^{k+1-i}] h \geq -|\nabla_x^i \nabla_v^{k+1-i} h|^2 - C \left(|\nabla_x^{i+1} \nabla_v^{k-i} h|^2 + \sum_{j=0}^{i-1} |\nabla_x^j \nabla_v^{k+2-i} h|^2 \right).$$

If $i = k$, then for any $\eta > 0$, using the Young inequality

$$\begin{aligned}
\sum_{\substack{|\alpha_1|=k; |\alpha_2|=1 \\ j \in \llbracket 1, d \rrbracket}} (\partial_x^{\alpha_1} \partial_v^{\alpha_2} h) (\alpha_{2,j} \partial_v^{\alpha_2} \partial_x^{\alpha_1} \partial_{x_j} h) &= \sum_{|\alpha_1|=k; j \in \llbracket 1, d \rrbracket} (\partial_x^{\alpha_1} \partial_{v_j} h) (\partial_x^{\alpha_1} \partial_{x_j} h) \\
&= \sum_{|\alpha_1|=k; j \in \llbracket 1, d \rrbracket} (\partial_x^{\alpha_1} \partial_{v_j} h) (\partial_x^{\alpha_1} \partial_{x_j} - \partial_x^{\alpha_1} \partial_{v_j} + \partial_x^{\alpha_1} \partial_{v_j}) h \\
&\leq \left(1 + \frac{2}{\eta} \right) |\nabla_x^k \nabla_v h|^2 + \frac{\eta}{8} |(\nabla_x^{k+1} - \nabla_x^k \nabla_v) h|^2.
\end{aligned}$$

which again implies that

$$\nabla_x^k \nabla_v h \cdot [\mathcal{L}_H, \nabla_x^k \nabla_v] h \geq -C \left(1 + \frac{1}{\eta} \right) |\nabla_x^k \nabla_v h|^2 - \frac{\eta}{8} |(\nabla_x^{k+1} - \nabla_x^k \nabla_v) h|^2 - C \sum_{j=0}^{k-1} |\nabla_x^j \nabla_v^2 h|^2.$$

Similarly, for β a multi-index such that $|\beta| = k$ and $i \in \llbracket 1, d \rrbracket$,

$$\begin{aligned}
[\mathcal{L}_H, \partial_x^\beta \partial_{x_i} - \partial_x^\beta \partial_{v_i}] h &= \partial_x^\beta \partial_{x_i} h + \sum_{j=1}^d \sum_{\nu \leq \beta} \binom{\beta}{\nu} \partial^\nu \partial_{i,j} U_0 \partial_x^{\beta-\nu} \partial_{v_j} h \\
&\quad + \sum_{j=1}^d \sum_{\nu \leq \beta; \nu \neq 0} \binom{\beta}{\nu} \partial^\nu \partial_j U_0 \partial_x^{\beta-\nu} \partial_{x_i} \partial_{v_j} h - \sum_{j=1}^d \sum_{\nu \leq \beta; \nu \neq 0} \binom{\beta}{\nu} (\partial^\nu \partial_j U_0) (\partial_x^{\beta-\nu} \partial_{v_i} \partial_{v_j} h),
\end{aligned}$$

and thus, by applying Young inequality,

$$(\nabla_x^{k+1} - \nabla_x^k \nabla_v)h \cdot [\mathcal{L}_H, \nabla_x^{k+1} - \nabla_x^k \nabla_v]h \geq \frac{1}{2} |(\nabla_x^{k+1} - \nabla_x^k \nabla_v)h|^2 - C \left(\sum_{j=0}^k |\nabla_x^j \nabla_v h|^2 + \sum_{j=0}^{k-1} |\nabla_x^j \nabla_v^2 h|^2 \right),$$

which concludes the proof. \square

Regarding the diffusion part, we have

Lemma 3.2.5. For $i \in \llbracket 0, k \rrbracket$,

$$\nabla_x^i \nabla_v^{k+1-i} h \cdot [\mathcal{L}_D, \nabla_x^i \nabla_v^{k+1-i}]h = \gamma(k+1-i) |\nabla_x^i \nabla_v^{k+1-i} h|^2,$$

and there exists $C > 0$ such that

$$(\nabla_x^{k+1} - \nabla_x^k \nabla_v)h \cdot [\mathcal{L}_D, \nabla_x^{k+1} - \nabla_x^k \nabla_v]h \geq -\frac{1}{8} |(\nabla_x^{k+1} - \nabla_x^k \nabla_v)h|^2 - C |\nabla_x^k \nabla_v h|^2.$$

Proof. We have, for all $\alpha_1, \alpha_2 \in \mathbb{N}^d$,

$$\begin{aligned} \partial_x^{\alpha_1} \partial_v^{\alpha_2} \mathcal{L}_D h(x, v) &= -\gamma \sum_{j=1}^d \partial_v^{\alpha_2} (v_j \partial_x^{\alpha_1} \partial_{v_j} h) + \gamma \sum_{j=1}^d \partial_x^{\alpha_1} \partial_v^{\alpha_2} (\partial_{v_j^2} h) \\ &= -\gamma \sum_{j=1}^d v_j \partial_v^{\alpha_2} \partial_x^{\alpha_1} \partial_{v_j} h - \gamma \sum_{j=1}^d \alpha_{2,j} \partial_v^{\alpha_2} \partial_x^{\alpha_1} \partial_{v_j} h + \gamma \sum_{j=1}^d \partial_x^{\alpha_1} \partial_v^{\alpha_2} (\partial_{v_j^2} h). \end{aligned}$$

Therefore, if $|\alpha_1| = i$ and $|\alpha_2| = k+1-i$, we have

$$[\mathcal{L}_D, \partial_x^{\alpha_1} \partial_v^{\alpha_2}]h(x, v) = \gamma \sum_{j=1}^d \alpha_{2,j} \partial_v^{\alpha_2} \partial_x^{\alpha_1} h = \gamma(k+1-i) \partial_x^{\alpha_1} \partial_v^{\alpha_2} h$$

and

$$\nabla_x^i \nabla_v^{k+1-i} h \cdot [\mathcal{L}_D, \nabla_x^i \nabla_v^{k+1-i}]h = \gamma(k+1-i) |\nabla_x^i \nabla_v^{k+1-i} h|^2.$$

Similarly, for all $\beta \in \mathbb{N}^d$ and $i \in \llbracket 1, d \rrbracket$,

$$\begin{aligned} (\partial_x^\beta \partial_{x_i} - \partial_x^\beta \partial_{v_i}) \mathcal{L}_D h(x, v) &= -\gamma \sum_{j=1}^d v_i \partial_x^\beta \partial_{x_i} \partial_{v_j} h + \gamma \sum_{j=1}^d \partial_{v_i} (v_j \partial_x^\beta \partial_{v_j} h) + \gamma \sum_{j=1}^d \partial_x^\beta \partial_{x_i} \partial_{v_j^2} h - \gamma \sum_{j=1}^d \partial_x^\beta \partial_{v_i} \partial_{v_j^2} h \\ &= -\gamma \sum_{j=1}^d v_j \partial_x^\beta \partial_{x_i} \partial_{v_j} h + \gamma \sum_{j=1}^d v_j \partial_{v_i} \partial_x^\beta \partial_{v_j} h + \gamma \partial_x^\beta \partial_{v_i} h \\ &\quad + \gamma \sum_{j=1}^d \partial_x^\beta \partial_{x_i} \partial_{v_j^2} h - \gamma \sum_{j=1}^d \partial_x^\beta \partial_{v_i} \partial_{v_j^2} h \end{aligned}$$

Therefore,

$$[\mathcal{L}_D, \partial_x^\beta \partial_{x_i} - \partial_x^\beta \partial_{v_i}]h(x, v) = \gamma \partial_x^\beta \partial_{v_i} h$$

and finally applying Young inequality

$$\begin{aligned}
(\nabla_x^{k+1} - \xi \nabla_x^k \nabla_v)h \cdot [\mathcal{L}_D, \nabla_x^{k+1} - \nabla_x^k \nabla_v]h &= \gamma \sum_{|\beta|=k; j \in \llbracket 1, d \rrbracket} (\partial_x^\beta \partial_{x_j} - \partial_x^\beta \partial_{v_j})h \partial_x^\beta \partial_{v_j} h \\
&\geq \frac{1}{4} |(\nabla_x^{k+1} - \nabla_x^k \nabla_v)h|^2 - C |\nabla_x^k \nabla_v h|^2,
\end{aligned}$$

for some $C > 0$. □

Finally, let us look at the jump part.

Lemma 3.2.6. *For all $k \in \mathbb{N}$, there exists $C > 0$ such that for $i \in \llbracket 0, k \rrbracket$ and $\varepsilon > 0$,*

$$\begin{aligned}
\int_{\mathbb{R}^{2d}} \nabla_x^i \nabla_v^{k+1-i} h \cdot [\mathcal{L}_J, \nabla_x^i \nabla_v^{k+1-i}]h d\mu &\geq -\frac{1}{\varepsilon} \int_{\mathbb{R}^{2d}} |\nabla_x^i \nabla_v^{k+1-i} h|^2 d\mu \\
&\quad - C \varepsilon \int_{\mathbb{R}^{2d}} \left(\sum_{\substack{j \leq i \\ l \leq k+1-j}} |\nabla_x^j \nabla_v^l h|^2 + |\nabla_x^i \nabla_v^{k+2-i} h|^2 \right) d\mu.
\end{aligned}$$

and

$$\begin{aligned}
\int_{\mathbb{R}^{2d}} (\nabla_x^{k+1} - \nabla_x^k \nabla_v h) \cdot [\mathcal{L}_J, \nabla_x^{k+1} - \nabla_x^k \nabla_v]h d\mu &\geq -\frac{1}{8} \int_{\mathbb{R}^{2d}} |\nabla_x^{k+1} - \nabla_x^k \nabla_v h|^2 d\mu \\
&\quad - C \left(\int_{\mathbb{R}^{2d}} \sum_{\substack{i \leq k \\ j \leq k+1-i}} |\nabla_x^i \nabla_v^j h|^2 d\mu + \int_{\mathbb{R}^{2d}} |\nabla_x^k \nabla_v^2 h|^2 d\mu \right).
\end{aligned}$$

To prove this Lemma, we need a generalization of Proposition 3.2.3:

Lemma 3.2.7. *Let $n \in \mathbb{N}^*$. There exists $C > 0$ such that for any $h \in \mathcal{C}_c^\infty(\mathbb{R})$,*

$$\int_{\mathbb{R}} v^{2n} h^2(v) e^{-v^2/2} dv \leq C \sum_{k=0}^n \int_{\mathbb{R}} (h^{(k)}(v))^2 e^{-v^2/2} dv.$$

Proof. We prove the inequality by induction on n . The case $n = 1$ corresponds to Lemma 3.2.3. Suppose that the inequality holds for some $n \in \mathbb{N}$. Then

$$\begin{aligned}
\int_{\mathbb{R}} v^{2n+2} h^2(v) e^{-v^2/2} dv &= \int_{\mathbb{R}} v^{2n} (vh(v))^2 e^{-v^2/2} dv \\
&\leq C \sum_{k=0}^n \int_{\mathbb{R}} ((vh(v))^{(k)})^2 e^{-v^2/2} dv \\
&= C \sum_{k=0}^n \int_{\mathbb{R}} (kh^{(k-1)} + vh^{(k)})^2 e^{-v^2/2} dv \\
&\leq C \sum_{k=0}^n 2 \int_{\mathbb{R}} (k^2 (h^{(k-1)})^2 + v^2 (h^{(k)})^2) e^{-v^2/2} dv \\
&\leq 2Cn^2 \sum_{k=0}^{n-1} \int_{\mathbb{R}} (h^{(k)}(v))^2 e^{-v^2/2} dv + 4C \sum_{k=0}^n \int_{\mathbb{R}} (h^{(k)}(v))^2 e^{-v^2/2} dv
\end{aligned}$$

$$\begin{aligned}
& + 8C \sum_{k=1}^{n+1} \int_{\mathbb{R}} (h^{(k)})^2 e^{-v^2/2} dv \\
& \leq \tilde{C} \sum_{k=0}^{n+1} \int_{\mathbb{R}} (h^{(k)})^2 e^{-v^2/2} dv,
\end{aligned}$$

and hence it holds for $n + 1$. □

Proof of Lemma 3.2.6. Recall that we denote

$$g_i(x, v, G) = \left(x, v - \frac{2\theta}{1 + \theta^2} (\theta v_i + G) e_i\right), \quad \varphi_i(x, v, G) = \frac{\theta \partial_i U_1(x)}{1 + \theta^2} (\theta v_i + G).$$

The functions $(g_i)_i$ are smooth and we have for all $i \in \llbracket 1, d \rrbracket$

$$\partial_{v_j} g_i = \left(0, e_j - \frac{2\theta^2}{1 + \theta^2} e_i \text{frm}[o]_{-j=i}\right), \quad \partial_{x_j} g_i = (e_j, 0), \quad \partial_x^\nu \partial_x^\alpha g_i = 0 \quad \forall |\nu| + |\alpha| \geq 2.$$

As a consequence, for any $\nu_1, \nu_2 \in \mathbb{N}^d$, we have

$$\partial_x^{\nu_1} \partial_v^{\nu_2} (h(g_i)) = \left(1 - \frac{2\theta}{1 + \theta^2}\right)^{\nu_{2,i}} (\partial_x^{\nu_1} \partial_v^{\nu_2} h)(g_i).$$

The functions $(\varphi_i)_i$ are smooth and we have for all $i \in \llbracket 1, d \rrbracket$

$$\partial_x^\nu \varphi_i = \frac{\theta}{1 + \theta^2} (\theta v_i + G) \partial^\nu \partial_i U_1, \quad \partial_x^\nu \partial_{v_i} \varphi_i = \frac{\theta^2}{1 + \theta^2} (\partial^\nu \partial_i U_1).$$

This yields that the only non-vanishing derivatives of $\Psi(\varphi_i)$ are of the type $\partial_x^\alpha \partial_{v_i}^k \Psi(\varphi_i)$. For $k \in \mathbb{N}$ and $\alpha \in \mathbb{N}^d$, we have:

$$\partial_{v_i}^k \Psi(\varphi_i) = \Psi^{(k)}(\varphi_i) \left(\frac{\theta^2}{1 + \theta^2}\right)^k (\partial_i U_1)^k,$$

and

$$\partial_x^\alpha \partial_{v_i}^k \Psi(\varphi_i) = \left(\frac{\theta^2}{1 + \theta^2}\right)^k \sum_{\nu \leq \alpha} \binom{\alpha}{\nu} \partial_x^\nu \Psi^{(k)}(\varphi_i) \partial_x^{\alpha-\nu} (\partial_i U_1)^k.$$

Therefore, using that $\Psi(s) \leq c + |s|$ for some $c > 0$, and that Ψ' and U_1 and their derivatives of all order are bounded, we get that for all $k \in \mathbb{N}$ and $\alpha \in \mathbb{N}^d$ there exists $C > 0$ such that:

$$|\partial_x^\alpha \partial_{v_i}^k \Psi(\varphi_i)| \leq C \left(1 + |\theta v_i + G|^{|\alpha|}\right) \leq C' \left(1 + |v_i|^{|\alpha|} + |G|^{|\alpha|}\right).$$

Thus, for $\alpha = (\alpha_1, \alpha_2) \in \mathbb{N}^{2d}$, we have

$$\begin{aligned} [\partial^\alpha, \mathcal{L}_J^i]h &= \frac{1+\theta^2}{\theta^2} (\mathbb{E}[\partial^\alpha [(h(g_i) - h)\Psi(\varphi_i)]] - \mathbb{E}[(\partial^\alpha h(g_i) - \partial^\alpha h)\Psi(\varphi_i)]) \\ &= \frac{1+\theta^2}{\theta^2} \left(\sum_{\nu < \alpha} \binom{\alpha}{\nu} \mathbb{E}[(\partial^\nu h(g_i) - \partial^\nu h)\partial^{\alpha-\nu}(\Psi(\varphi_i))] + \mathbb{E}[(\partial^\alpha h(g_i) - \partial^\alpha h)\Psi(\varphi_i)] \right) \\ &= \frac{1+\theta^2}{\theta^2} \sum_{\nu < \alpha} \binom{\alpha}{\nu} \mathbb{E} \left[\left(\left(1 - \frac{2\theta}{1+\theta^2} \right)^{\nu, i+d} \partial^\nu h(g_i) - \partial^\nu h \right) \partial^{\alpha-\nu}(\Psi(\varphi_i)) \right] \\ &\quad + \frac{1+\theta^2}{\theta^2} \mathbb{E} \left[\left(\left(1 - \frac{2\theta}{1+\theta^2} \right)^{\alpha, i+d} - 1 \right) \partial^\alpha h(g_i)\Psi(\varphi_i) \right]. \end{aligned}$$

As a consequence, there exists a $C > 0$ such that

$$\begin{aligned} |[\partial^\alpha, \mathcal{L}_J^i]h|^2 &\leq C \mathbb{E}[(h(g_i) - h)^2(1 + |v_i|^{2|\alpha|} + G^{2|\alpha|})] \\ &\quad + C \left(\sum_{0 < \nu < \alpha} \mathbb{E} [(\partial^\nu h(g_i))^2(1 + |v_i|^{2|\alpha-\nu|} + G^{2|\alpha-\nu|})] + (\partial^\nu h)^2(1 + |v_i|^{2|\alpha-\nu|}) \right) \\ &\quad + C \mathbb{E}[(\partial^\alpha h(g_i))^2(1 + v_i^2 + G^2)]. \end{aligned}$$

As in the H^1 case, the integrals with respect to μ of the previous expectations can be bounded using the Poincaré inequality for the Gaussian measure, the reversibility of the law of V^i with respect to the Gaussian measure, as well as Lemma 3.2.7. Recall that thanks to the reversibility (3.8),

$$\int_{\mathbb{R}^{2d}} \mathbb{E}[(\partial^\nu h(g_i))^2] d\mu = \int_{\mathbb{R}^{2d}} (\partial^\nu h)^2 d\mu$$

Recall that $V_i^i = \rho v_i + \sqrt{1 - \rho^2} G$ where G is a random variable with standard normal distribution. Hence, for any $n \in \mathbb{N}^*$,

$$\mathbb{E}[(V_i^i)^{2n}] = \sum_{k=0}^{2n} \binom{2n}{k} (1 - \rho^2)^{k/2} \mathbb{E}[G^k] \rho^{2n-k} v_i^{2n-k} \leq C (1 + v_i^{2n}).$$

Similarly we have:

$$\mathbb{E}[(v_i - \rho V_i^i)^{2n}] = \sum_{k=0}^{2n} \binom{2n}{k} (-1)^k \rho^k \mathbb{E}[(V_i^i)^k] v_i^{2n-k} \leq C (1 + v_i^{2n}).$$

Therefore, for all $\nu \in \mathbb{N}^{2d}$ and $n \in \mathbb{N}^*$:

$$\int_{\mathbb{R}^{2d}} |v_i|^{2n} \mathbb{E}[|\partial^\nu h(g_i)|^2] d\mu = \int_{\mathbb{R}^{2d}} \mathbb{E}[V_i^{2n}] |\partial^\nu h|^2 d\mu \leq C \int_{\mathbb{R}^{2d}} (1 + v_i^{2n}) |\partial^\nu h|^2 d\mu,$$

and using Lemma 3.2.7, we get:

$$\int_{\mathbb{R}^{2d}} |v_i|^{2n} \mathbb{E}[|\partial^\nu h(g_i)|^2] d\mu \leq C \sum_{k=0}^n \int_{\mathbb{R}^{2d}} |\partial_{v_i}^k \partial^\nu h|^2 d\mu.$$

Similarly we have

$$\begin{aligned} \int_{\mathbb{R}^{2d}} \mathbb{E}[G^{2n} |\partial^\nu h(g_i)|^2] d\mu &= \frac{1}{(1-\rho^2)^n} \int_{\mathbb{R}^{2d}} |\partial^\nu h|^2 \mathbb{E}[(v_i - \rho V_i^i)^{2n}] d\mu \\ &\leq C \int_{\mathbb{R}^{2d}} (1 + v_i^{2n}) |\partial^\nu h|^2 d\mu \leq C' \sum_{k=0}^n \int_{\mathbb{R}^{2d}} |\partial_{v_i}^k \partial^\nu h|^2 d\mu. \end{aligned}$$

Now bound

$$\begin{aligned} \int_{\mathbb{R}^{2d}} v_i^{2|\alpha|} \mathbb{E}[(h(g_i) - h)^2] d\mu &\leq 2 \left(\int_{\mathbb{R}^{2d}} v_i^{2|\alpha|} \mathbb{E}[(h(g_i) - \Pi_{v_i} h)^2] d\mu + \int_{\mathbb{R}^{2d}} v_i^{2|\alpha|} (h - \Pi_{v_i} h)^2 d\mu \right) \\ &= 2 \left(\int_{\mathbb{R}^{2d}} \mathbb{E}[(V_i^i)^{2|\alpha|}] (h - \Pi_{v_i} h)^2 d\mu + \int_{\mathbb{R}^{2d}} v_i^{2|\alpha|} (h - \Pi_{v_i} h)^2 d\mu \right) \\ &\leq C \int_{\mathbb{R}^{2d}} (1 + v_i^{2|\alpha|}) (h - \Pi_{v_i} h)^2 d\mu. \end{aligned}$$

The Poincaré inequality (3.10) and Proposition 3.2.7 then yields

$$\int_{\mathbb{R}^{2d}} v_i^{2|\alpha|} \mathbb{E}[(h(g_i) - h)^2] d\mu \leq C \sum_{k=0}^{|\alpha|} \int_{\mathbb{R}^{2d}} (\partial_{v_i}^k h)^2 d\mu,$$

for some $C > 0$. Similarly we have

$$\begin{aligned} \int_{\mathbb{R}^{2d}} \mathbb{E}[G^{2|\alpha|} (h(g_i) - h)^2] d\mu &\leq 2 \left(\int_{\mathbb{R}^{2d}} \mathbb{E}[G^{2|\alpha|} (h(g_i) - \Pi_{v_i} h)^2] d\mu + \int_{\mathbb{R}^{2d}} \mathbb{E}[G^{2|\alpha|}] (h - \Pi_{v_i} h)^2 d\mu \right) \\ &\leq C \left(\int_{\mathbb{R}^{2d}} \mathbb{E}[(v_i - \rho V_i^i)^{2|\alpha|}] (h - \Pi_{v_i} h)^2 d\mu + \int_{\mathbb{R}^{2d}} (h - \Pi_{v_i} h)^2 d\mu \right) \\ &\leq C \sum_{k=0}^{|\alpha|} \int_{\mathbb{R}^{2d}} (\partial_{v_i}^k h)^2 d\mu, \end{aligned}$$

for some constant $C > 0$. Putting everything together, we get that for all $\alpha \in \mathbb{N}^{2d}$, there is $C > 0$ such that

$$\int_{\mathbb{R}^{2d}} |[\partial^\alpha, \mathcal{L}_J^i] h|^2 d\mu \leq C \left(\int_{\mathbb{R}^{2d}} (\partial_{v_i} \partial^\alpha h)^2 d\mu + \sum_{\nu \leq \alpha} \sum_{k=0}^{|\alpha-\nu|} \int_{\mathbb{R}^{2d}} (\partial_{v_i}^k \partial^\nu h)^2 d\mu \right).$$

For any $i \in \llbracket 0, k \rrbracket$ and $\varepsilon > 0$, Young inequality yields

$$\begin{aligned} \int_{\mathbb{R}^{2d}} \nabla_x^i \nabla_v^{k+1-i} h \cdot [\mathcal{L}_J, \nabla_x^i \nabla_v^{k+1-i}] h d\mu &\geq -\frac{1}{\varepsilon} \int_{\mathbb{R}^{2d}} |\nabla_x^i \nabla_v^{k+1-i} h|^2 d\mu \\ &\quad - C\varepsilon \int_{\mathbb{R}^{2d}} \left(\sum_{\substack{j \leq i \\ l \leq k+1-j}} |\nabla_x^j \nabla_v^l h|^2 + |\nabla_x^i \nabla_v^{k+2-i} h|^2 \right) d\mu. \end{aligned}$$

To treat the term with derivative $\nabla_x^{k+1} - \nabla_x^k \nabla_v$, write for $\alpha \in \mathbb{N}^d$

$$[\partial_x^\alpha, \mathcal{L}_J^i]h = \frac{1 + \theta^2}{\theta^2} \sum_{\nu < \alpha} \binom{\alpha}{\nu} \mathbb{E} [(\partial_x^\nu h(g_i) - \partial_x^\nu h) \partial_x^{\alpha-\nu} (\Psi(\varphi_i))] ,$$

so that no derivatives of order $k+2$ appear, nor derivatives of the form ∇_x^{k+1} , and we have

$$\int_{\mathbb{R}^{2d}} |[\partial_x^\alpha, \mathcal{L}_J^i]h|^2 d\mu \leq C \int_{\mathbb{R}^{2d}} \sum_{\nu < \alpha} \sum_{k=0}^{|\alpha-\nu|} (\partial_{v_i}^k \partial_x^\nu h)^2 d\mu.$$

Hence, the only derivatives of order $k+2$ that appear in $[\mathcal{L}_J, \nabla_x^{k+1} - \nabla_x^k \nabla_v]h$ come from the term $[\mathcal{L}_J, \nabla_x^k \nabla_v]h$ that we treated above. Using Young inequality, we get

$$\begin{aligned} & \int_{\mathbb{R}^{2d}} (\nabla_x^{k+1} - \nabla_x^k \nabla_v h) \cdot [\mathcal{L}_J, \nabla_x^{k+1} - \nabla_x^k \nabla_v]h d\mu \\ & \geq -\frac{1}{8} \int_{\mathbb{R}^{2d}} |\nabla_x^{k+1} - \nabla_x^k \nabla_v h|^2 d\mu - C \left(\int_{\mathbb{R}^{2d}} \sum_{\substack{i \leq k \\ j \leq k+1-i}} |\nabla_x^i \nabla_v^j h|^2 d\mu - \int_{\mathbb{R}^{2d}} |\nabla_x^k \nabla_v^2 h|^2 d\mu \right), \end{aligned}$$

which concludes the proof. \square

Combining all the commutator terms, we get that for $i \in \llbracket 0, k-1 \rrbracket$ there exists $C > 0$ such that for all $\varepsilon > 0$ small enough

$$\begin{aligned} & \int_{\mathbb{R}^{2d}} \nabla_x^i \nabla_v^{k+1-i} h \cdot [\mathcal{L}, \nabla_x^i \nabla_v^{k+1-i}]h d\mu \\ & \geq -\frac{C}{\varepsilon} \int_{\mathbb{R}^{2d}} |\nabla_x^i \nabla_v^{k+1-i} h|^2 d\mu - C \int_{\mathbb{R}^{2d}} |\nabla_x^{i+1} \nabla_v^{-i} h|^2 d\mu - C \sum_{j=0}^{i-1} \int_{\mathbb{R}^{2d}} |\nabla_x^j \nabla_v^{k+2-i} h|^2 d\mu \\ & \quad - C\varepsilon \int_{\mathbb{R}^{2d}} \left(\sum_{\substack{j \leq i \\ l \leq k+1-j}} |\nabla_x^j \nabla_v^l h|^2 + |\nabla_x^i \nabla_v^{k+2-i} h|^2 \right) d\mu, \end{aligned}$$

as well as

$$\begin{aligned} & \int_{\mathbb{R}^{2d}} \nabla_x^k \nabla_v h \cdot [\mathcal{L}, \nabla_x^k \nabla_v]h d\mu \geq \\ & -C \left(\frac{1}{\varepsilon} + \frac{1}{\eta} \right) \int_{\mathbb{R}^{2d}} |\nabla_x^k \nabla_v h|^2 d\mu - \frac{\eta}{8} \int_{\mathbb{R}^{2d}} |(\nabla_x^{k+1} - \nabla_x^k \nabla_v)h|^2 d\mu - C \sum_{j=0}^{k-1} \int_{\mathbb{R}^{2d}} |\nabla_x^j \nabla_v^2 h|^2 d\mu \\ & \quad - C\varepsilon \int_{\mathbb{R}^{2d}} \left(\sum_{\substack{j \leq k \\ l \leq k+1-j}} |\nabla_x^j \nabla_v^l h|^2 + |\nabla_x^k \nabla_v^2 h|^2 \right) d\mu, \end{aligned}$$

and finally

$$\begin{aligned} & \int_{\mathbb{R}^{2d}} (\nabla_x^{k+1} - \nabla_x^k \nabla_v h) \cdot [\mathcal{L}, \nabla_x^{k+1} - \nabla_x^k \nabla_v] h d\mu \\ & \geq \frac{1}{4} \int_{\mathbb{R}^{2d}} |\nabla_x^{k+1} - \nabla_x^k \nabla_v h|^2 d\mu - C \int_{\mathbb{R}^{2d}} \sum_{\substack{i \leq k \\ j \leq k+1-i}} |\nabla_x^i \nabla_v^j h|^2 d\mu - C \left(\sum_{j=0}^k |\nabla_x^j \nabla_v h|^2 + \sum_{j=0}^k |\nabla_x^j \nabla_v^2 h|^2 \right). \end{aligned}$$

Thanks to those expressions, we are now able to prove Proposition 3.2.5.

Proof of Proposition 3.2.5. The fact that inequality (3.12) holds for $k = 1$ is proven in Lemma 3.2.1. Let $k \in \mathbb{N}$, and suppose that inequality (3.12) holds for such k and some $\rho_k > 0$ and $\omega_{i,p} > 0$, $0 \leq i \leq p \leq k$. Fix some $\omega_{i,k+1} > 0$, $0 \leq i \leq k+1$, $\varepsilon > 0$ small enough so that the previous formulas for the commutators hold, and choose $\eta = \omega_{k+1,k+1}/\omega_{k,k+1}$. By assumption we have

$$\begin{aligned} & \int_{\mathbb{R}^{2d}} \Gamma(h) d\mu + \sum_{p=1}^{k+1} \int_{\mathbb{R}^{2d}} \left(\sum_{i=0}^{p-1} \omega_{i,p} \Gamma_{i,p}(h) + \omega_{p,p} \Gamma_{p,p}(h) \right) d\mu \\ & \geq \rho_k \left(\mathcal{N}_k(h) + \int_{\mathbb{R}^{2d}} \sum_{i=0}^k |\nabla_x^i \nabla_v^{k+1-i} h|^2 d\mu \right) + \int_{\mathbb{R}^{2d}} \left(\sum_{i=0}^k \omega_{i,k+1} \Gamma_{i,k+1}(h) + \omega_{k+1,k+1} \Gamma_{k+1,k+1}(h) \right) d\mu. \end{aligned}$$

By using Proposition 3.2.1, the bounds on the commutators and the fact that

$$\begin{aligned} \Gamma(\nabla_x^i \nabla_v^j h) & \geq 2\gamma |\nabla_x^i \nabla_v^{j+1} h|^2, \\ \Gamma((\nabla_x^{k+1} - \nabla_x^k \nabla_v)h) & \geq 2\gamma |(\nabla_x^{k+1} \nabla_v - \nabla_x^k \nabla_v^2)h|^2 \geq \gamma |\nabla_x^{k+1} \nabla_v h|^2 - 2\gamma |\nabla_x^k \nabla_v^2 h|^2, \end{aligned}$$

the term of order $k+2$ are bounded below by

$$2\gamma \sum_{i=0}^k \omega_{i,k+1} |\nabla_x^i \nabla_v^{k+2-i} h|^2 + \gamma \omega_{k+1,k+1} |\nabla_x^{k+1} \nabla_v h|^2 - (C_1 + 2\gamma) \omega_{k+1,k+1} |\nabla_x^k \nabla_v^2 h|^2 - C_1 \varepsilon \sum_{i=0}^k \omega_{i,k+1} |\nabla_x^i \nabla_v^{k+2-i} h|^2.$$

for some constant $C_1 > 0$. We may bound from below the terms of order $k+1$ for ε small enough by

$$\rho_k \sum_{i=0}^k |\nabla_x^i \nabla_v^{k+1-i} h|^2 - \sup_{0 \leq i \leq k+1} \omega_{i,k+1} \frac{2C_2}{\varepsilon} \sum_{i=0}^k |\nabla_x^i \nabla_v^{k+1-i} h|^2 - C_2 \frac{\omega_{k,k+1}^2}{\omega_{k+1,k+1}} |\nabla_x^k \nabla_v h|^2 + \frac{\omega_{k+1,k+1}}{8} |(\nabla_x^{k+1} - \nabla_x^k \nabla_v)h|^2,$$

for some constant $C_2 > 0$. Finally, the term of order at most k may be bounded from below by

$$\left(\rho_k \inf_{i+j \leq k} \omega_{i,i+j} - 3C_3 \sup_{0 \leq i \leq k+1} \omega_{i,k+1} \right) \sum_{i+j \leq k} |\nabla_x^i \nabla_v^j h|^2,$$

for some constant $C_3 > 0$. Set $C_4 = \max(C_1, C_2, C_3)$ (which is independent from ε and the weights $\omega_{i,j}$). Now, choose ε and $\omega_{i,k+1}$ for $i \in \llbracket 1, k+1 \rrbracket$ such that

$$\frac{\omega_{k+1,k+1}}{\omega_{k,k+1}} \leq \frac{\gamma - C_4 \varepsilon}{2\gamma + C_4}, \quad \varepsilon < \gamma/C_4, \quad \omega_{i,k+1} < \varepsilon \rho_k / 4C_4, \quad 1 \leq i \leq k-1, \quad \omega_{k,k+1} \left(\frac{2}{\varepsilon} + \frac{\omega_{k,k+1}}{\omega_{k+1,k+1}} \right) < \rho_k / (2C_4)$$

and

$$6C_4 \sup_{0 \leq i \leq k+1} \omega_{i,k+1} < \rho_k \inf_{i+j \leq k} \omega_{i,i+j}.$$

We get

$$\begin{aligned} & \int_{\mathbb{R}^{2d}} \Gamma(h) d\mu + \sum_{p=1}^{k+1} \int_{\mathbb{R}^{2d}} \left(\sum_{i=0}^{p-1} \omega_{i,p} \Gamma_{i,p}(h) + \omega_{p,p} \Gamma_{p,p}(h) \right) d\mu \\ & \geq \tilde{\rho}_{k+1} \left(\sum_{p=1}^{k+1} \int_{\mathbb{R}^{2d}} \left(\sum_{i=0}^{p-1} \omega_{i,p} |\nabla_x^i \nabla_v^{p-i} f|^2 + \omega_{p,p} |(\nabla_x^p - \nabla_x^{p-1} \nabla_v) f|^2 \right) + \sum_{i=0}^k |\nabla_x^i \nabla_v^{k+2-i} h|^2 d\mu \right), \end{aligned}$$

for any

$$\tilde{\rho}_{k+1} < \min \left(\frac{\rho_k}{2}, \frac{\omega_{k+1,k+1}}{8}, \gamma \inf_{i+j \leq k+1} \omega_{i,i+j} \right).$$

As in the $H^1(\mu)$ case, an application of the Poincaré inequality (3.9) yields inequality (3.12), which concludes the induction. \square

Proof of Theorem 3.2.1. Our goal is to apply Lumer-Phillips theorem to the operator $\mathcal{L} + \rho_k/2I$, where I denotes the identity operator of H^k . This theorem can be stated as follows: an operator A on a Hilbert space generates a contraction semi-group if and only if it is maximally dissipative, see [169, Chapter IX, p.250]. Fix $k \in \mathbb{N}$. The scalar product

$$\begin{aligned} & \langle f, g \rangle_k^2 \\ & = \int_{\mathbb{R}^{2d}} f g d\mu + \int_{\mathbb{R}^{2d}} \sum_{p=1}^k \left(\sum_{i=0}^{p-1} \omega_{i,p} \nabla_x^i \nabla_v^{p-i} f \cdot \nabla_x^i \nabla_v^{p-i} g + \omega_{p,p} (\nabla_x^p - \nabla_x^{p-1} \nabla_v) f \cdot (\nabla_x^p - \nabla_x^{p-1} \nabla_v) g \right) d\mu \end{aligned}$$

generates a norm equivalent to the usual norm of H^k . Proposition 3.2.5 and a density argument yield that the operator $\mathcal{L} + \rho_k/2I$, is dissipative:

$$\forall h \in D(\mathcal{L}), \langle (\mathcal{L} + \rho_k/2I)h, h \rangle_k \leq 0,$$

where $D(\mathcal{L})$ denote the domain of \mathcal{L} in H^k defined by:

$$f \in D(\mathcal{L}), g = \mathcal{L}f \Leftrightarrow f \in H^k, \lim_{t \rightarrow 0} \left\| \frac{P_t f - f}{t} - g \right\|_{H^k} = 0.$$

We are left to show that $\mathcal{L} + \rho I$, for some $\rho < \rho_k/2$, is surjective. Fix such a $\rho < \rho_k/2$. Thanks to Proposition 3.2.5, we have that

$$\Lambda : (f, g) \mapsto \langle -(\mathcal{L} + \rho I)f, g \rangle_k$$

is coercive and continuous from $(H^k)^2$ to \mathbb{R} for $k \geq 1$. Hence, we may apply Lax-Milgram theorem to get that for all $g \in H^k$, there exists $f \in H^k$ such that for all $h \in H^k$, we have:

$$\langle -(\mathcal{L} + \rho I)f, h \rangle_{H^k} = \langle -g, h \rangle_{H^k},$$

which implies that f is a solution to the equation

$$(\mathcal{L} + \rho I)f = g,$$

and $\mathcal{L} + \rho_k/2I$ is maximally dissipative. Lumer-Phillips Theorem then yields that the semi-group

generated by $\mathcal{L} + \rho_k/2$ is a contraction on H^k : for all $f \in H^k$

$$\mathcal{N}_k \left(e^{\rho_k t/2} (P_t f - \mu(f)) \right) \leq \mathcal{N}_k (f - \mu(f)),$$

which concludes the proof. □

Part II

Optimisation

Chapter 4

Convergence of the kinetic annealing for general potentials

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Abstract : The convergence of the kinetic Langevin simulated annealing is proven under mild assumptions on the potential U for slow logarithmic cooling schedules, which widely extends the scope of the previous results of [137]. Moreover, non-convergence for fast logarithmic and non-logarithmic cooling schedules is established. The results are based on an adaptation to non-elliptic non-reversible kinetic settings of a localization/local convergence strategy developed by Fournier and Tardif in [64] in the overdamped elliptic case, and on precise quantitative high order Sobolev hypocoercive estimates.

4.1 Introduction and main results

Given a potential $U : \mathbb{R}^d \mapsto \mathbb{R}$, the goal of a simulated annealing procedure is to minimize U by designing a stochastic process $(X_t)_{t \geq 0}$ whose law at time t is close to the probability density

proportional to $e^{-\beta_t U(x)} dx$, where $\beta : \mathbb{R}_+ \mapsto \mathbb{R}_+$ is called the cooling schedule. As β goes to infinity, this probability law concentrates around the global minimizers of U .

The most classical case is based on the overdamped Langevin process:

$$dX_t = -\beta_t \nabla U(X_t) dt + \sqrt{2} dB_t,$$

where $(B_t)_{t \geq 0}$ is a standard Brownian motion on \mathbb{R}^d . For a fixed β , the density $e^{-\beta U(x)} dx$ is a stationary measure for this process. The idea is thus that, if β increases sufficiently slowly, the law of X_t gets and remains close to its instantaneous equilibrium. As a consequence, the convergence of the simulated annealing algorithm, in the sense of convergence in probability of $U(X_t)$ toward $\min U$ as $t \rightarrow +\infty$, is related to the longtime convergence to equilibrium of the process at a fixed but high β . On the contrary, when β goes to infinity too fast, the algorithm is expected to fail with positive probability, i.e. the law of X_t is not expected to be close to $e^{-\beta_t U}$ and $U(X_t)$ to converge to $\min U$.

On the other hand, the simulated annealing based on the kinetic Langevin process:

$$\begin{cases} dX_t = Y_t dt \\ dY_t = -\nabla U(X_t) dt - \beta_t Y_t dt + \sqrt{2} dB_t. \end{cases}$$

was studied in [137]. The present work is concerned with the kinetic Langevin simulated annealing. The contributions with respect to [137] are the following. First, following the method of [64], the conditions on U are considerably weakened. Notice that, in the kinetic case, it means we can consider potentials that grow slower than those considered in [137], but also potentials that grow much faster (arbitrarily fast in fact), while the results of [137] require $U(x)/(|x|^2 + 1)$ and $\nabla^2 U$ to be bounded. Second, we prove the failure of the algorithm with fast cooling schedule, which was yet to be established in an hypocoercive case. Indeed, the failure of the overdamped Langevin simulated annealing is proven in [83] thanks to hypercontractivity results that are not available for the kinetic process, and the hypocoercive convergence results used in [137] to prove convergence are too weak to conclude about the failure of the algorithm in the fast cooling case (see the discussion at the beginning of Section 4.2.4). By proving the non-convergence of the algorithm under the same condition as in the overdamped case, we make rigorous the heuristic discussion in [137] according to which the kinetic process does not change the optimal condition on the cooling schedule. Third, as noted in [31], a technical truncation argument in [137], required for the rigorous computation of the modified entropy dissipation, is incorrect, and we have solved this issue (see Section 4.4 and more precisely Remark 4.4.1).

More precisely, we study the Markov process $(Z_t)_{t \geq 0} = (X_t, Y_t)_{t \geq 0}$ on \mathbb{R}^{2d} that solves

$$\begin{cases} dX_t = Y_t dt \\ dY_t = -\nabla U(X_t) dt - \gamma_t Y_t dt + \sqrt{2\gamma_t \beta_t^{-1}} dB_t, \end{cases} \quad (4.1)$$

where $\gamma : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is a friction parameter. We retrieve the settings of [137] with $\gamma_t = \beta_t$. We remark that the extension to Generalized Langevin processes as in [31] would not raise any particular difficulty, but we don't consider it for the sake of clarity. We will work under the following set of assumptions :

Assumption 4.1.1.

- $U : \mathbb{R}^d \mapsto \mathbb{R}$ is a C^∞ potential such that $\min U = 0$, $\lim_{|x| \rightarrow \infty} U(x) = \infty$, and there exists

$\alpha_0 > 0$ such that :

$$\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)} dx < \infty.$$

- The cooling schedule $\beta : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is given by

$$\beta_t = \frac{\ln(e^{c\beta_0} + t)}{c}, \quad (4.2)$$

for some parameters $c > 0$ and $\beta_0 > 0$.

- The friction $\gamma : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ is a C^1 function and there exists $\kappa > 0$ such that for all $t \geq 0$, $\gamma_t \geq \kappa$ and $\gamma'_t \leq \frac{1}{\kappa(1+t)}$. In particular there exists L such that $\gamma_t \leq L\beta_t$.
- The critical height c^* of U is finite, where $c^* = \sup_{x_1, x_2} c(x_1, x_2)$ and

$$c(x_1, x_2) = \inf \left\{ \max_{0 \leq t \leq 1} U(\xi(t)) - U(x_1) - U(x_2) \right\}$$

where the infimum runs over $\{\xi \in \mathcal{C}([0, 1], \mathbb{R}^d), \xi(0) = x_1, \xi(1) = x_2\}$.

The condition $\min U = 0$ is imposed for simplicity, it can always be enforced by changing U to $U - \min U$. The specific form of β is also made for simplicity, since it is known that, in order to study the convergence in probability for large time for simulated annealing algorithm, only logarithmic schedules are relevant. In particular, notice that, under Assumption 4.1.1, the time-shifted process $(Z_{t_0+t})_{t \geq 0}$ for any $t_0 \geq 0$ satisfies Assumption 4.1.1 with the same U, c, κ, L and with β_0 replaced by β_{t_0} .

The critical height c^* represents the largest energy barrier the process has to cross in order to go from any local minimum to any global one. In the classical overdamped case, disregarding the question of the behavior of U at infinity, it is well known that, at least in the case where the global minimizer of U is unique, the algorithm converges if $c > c^*$ (slow cooling) and has a positive probability to fail (i.e. to never visit a global minimum) if $c < c^*$ (fast cooling). We retrieve this dichotomy in the kinetic case.

In the slow cooling case, we extend the results of [137]:

Theorem 4.1.1. *Under Assumption 4.1.1, assume furthermore that $c > c^*$. Then any solution $(Z_t)_{t \geq 0}$ of (4.1) satisfies*

$$\forall \delta > 0, \quad \mathbb{P}(H(Z_t) \geq \delta) \rightarrow 0.$$

Since $H(x, v) = U(x) + |v|^2/2$, this implies the convergence in probability of X_t to the set of global minimizers of U .

On the other hand, if $c < c^*$, then the process might remain stuck in a region that contains no global minimum of U . In fact, a slightly stronger condition is required. Indeed, it is possible that $c^* > 0$ with all minima of U being global, in which case $H(Z_t)$ may go to zero with fast cooling schedule, while the law of Z_t is not close to its local equilibrium. To be more precise, we need some additional definitions. For $x, y \in \mathbb{R}^d$, let

$$\tilde{c}(x, y) = \inf \left\{ \max_{0 \leq t \leq 1} U(\xi(t)) - U(x) \right\} \quad (4.3)$$

where the infimum runs over $\{\xi \in \mathcal{C}([0, 1], \mathbb{R}^d), \xi(0) = x, \xi(1) = y\}$. We define the depth of $x \in \mathbb{R}^d$ by

$$D(x) = \inf \{ \tilde{c}(x, y), y \in \mathbb{R}^d, U(y) < U(x) \}, \quad (4.4)$$

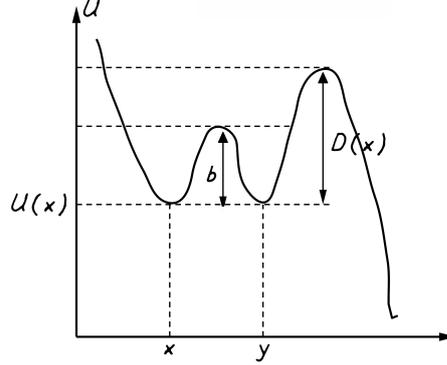


Figure 4.1: Case with two local non-global minima x and y at the same energy level. If $c < b$, then Assumption 4.1.2 holds by choosing either $\tilde{x} = x$ or $\tilde{x} = y$ and any $a \in (c, b)$. If $c \in (b, D(x))$, again Assumption 4.1.2 holds with $\tilde{x} \in \{x, y\}$ and any $a \in (b, D(x))$. However, if $c = b$, Assumption 4.1.2 does not hold with $\tilde{x} \in \{x, y\}$.

with $\inf \emptyset = \infty$. It is clear that $D(x) = 0$ if x is not a local minimum of U . For $x \in \mathbb{R}^d$ with $D(x) > 0$ and $a \in (0, D(x))$, we define the cup of bottom x and height a (this is the vocabulary of [80]) as

$$C(x, a) = \{y \in \mathbb{R}^d, \tilde{c}(x, y) < a\}. \quad (4.5)$$

We want to discard pathological cases where there are two non-global local minima x_1, x_2 with $U(x_1) = U(x_2)$, $D(x_1) = D(x_2) > c$ and $c(x_1, x_2) = c$, see Figure 4.1 (these cases do not prevent the result to hold, but the proof doesn't work directly, see Remark 4.1.1 below. Notice that the problem is not that there are two local minima with the same energy level and depth, which is a pretty common situation as soon as there are some symmetries in the system; the problem is that the elevation $c(x_1, x_2)$ between them is *exactly* the parameter c chosen by the user in the cooling schedule which, now, is a very unlikely situation). Hence, we work under the following condition.

Assumption 4.1.2. *Assumption 4.1.1 holds and there exist $\tilde{x} \in \mathbb{R}^d$ with $D(\tilde{x}) > c$ and $a \in (c, D(\tilde{x}))$ such that for all $y \in C(\tilde{x}, a)$, $\tilde{c}(y, \tilde{x}) < c$.*

Theorem 4.1.2. *Under Assumption 4.1.2, for all initial condition such that $\mathbb{P}(X_0 \in C(\tilde{x}, c)) > 0$ and all $\delta > 0$, the solution of (4.1) is such that*

$$\mathbb{P}(X_t \in C(\tilde{x}, c + \delta) \forall t \geq 0) > 0.$$

If U has a finite number of minima and a unique global minimum, it is easily seen that there exists a non-global minimum x such that $D(x) = c^*$. More generally, since for all $a < D(x)$ the minimum value of U over the cup $C(\tilde{x}, a)$ is $U(\tilde{x})$, if there exists a non-global minimum x of U with depth $D(x) > c$, the previous results implies that, with positive probability, $\inf_{t \geq 0} U(X_t) \geq U(\tilde{x}) > \min U$. Moreover, even if the probability to start in $C(\tilde{x}, c)$ is initially zero, due to the controllability of the process, it is positive for all positive times (see e.g. [137, proposition 5]). As a conclusion, we immediately get the following:

Corollary 4.1.1. *Under Assumption 4.1.2, for all initial condition and all $t_0 > 0$,*

$$\mathbb{P}(U(X_t) \geq U(\tilde{x}) \forall t \geq t_0) > 0.$$

Notice that, in practice, one can keep track of $X_{s(t)}$ where

$$s(t) = \inf\{w \in [0, t], U(X_w) = \min_{w' \in [0, t]} U(X_{w'})\},$$

so that $X_{s(t)}$ may converge to a minimizer of U even if X_t does not. However, our results show that this doesn't solve the issue of non-convergence for fast cooling schedules.

Remark 4.1.1. *In Figure 4.1, in the case $c = b$ (so that Assumption 4.1.2 do not hold) we cannot deduce from our results that the process stays stuck with positive probability in the cusp $C(x, b)$ because, for any $\delta > 0$, $C(x, b + \delta)$ contains y (contrary to $C(x, b)$). In fact it is clear that the process can stay stuck with positive probability in $C(x, b + \delta)$ for any $\delta > 0$ (so that the conclusion of Corollary 4.1.1 also holds), but we cannot deduce it from our proof which requires that the critical depth within the cusp (i.e. for a suitable modification of the potential which only consider the local situation of this cusp, see Section 4.2.4 and Figure 4.2) is strictly smaller than c (in order to apply a variation of Theorem 4.1.1), while it is exactly $b = c$ in this example. We refer to [130] where a fine analysis is conducted on a related question on finite graphs.*

Finally we address the case of faster than logarithmic cooling schedules. For simplicity we restrict this study to the case of a constant friction parameter γ (although as discussed at the end of the proof it can be extended to the non-constant case with suitable conditions on γ depending on β). In the following we do not assume that $t \mapsto \beta_t$ is increasing, and possibly $\beta_t = +\infty$ for some t .

Theorem 4.1.3. *Assume that $\gamma_t = \gamma$ is constant, that $t \in \mathbb{R}_+ \mapsto \beta_t \in (0, +\infty]$ is piecewise continuous with $\ln(t) = o(\beta_t)$ as $t \rightarrow +\infty$, that $U \in C^\infty(\mathbb{R}^d)$ and that $x_* \in \mathbb{R}^d$ is a non-degenerate local minimum of U , i.e. $\nabla U(x_*) = 0$ and $\nabla^2 U(x_*) > 0$. Then there exist $C, r > 0$ such that, denoting*

$$\varepsilon_t = C \left(e^{-rt} + \sup_{s \geq t/2} \ln(s) \beta_s^{-1} \right),$$

the following holds. For all $\delta > 0$ and all initial condition $z_0 = (x_0, y_0) \in \mathbb{R}^{2d}$ with $|x_0 - x_| \leq \delta/2$, the solution $Z = (X, Y)$ of (4.1) is such that*

$$\mathbb{P}_{z_0} (|X_t - x_*| \leq \min(\delta, \sqrt{\varepsilon_t}) \forall t \geq 0) > 0.$$

The rest of the paper is dedicated to the proofs of Theorems 4.1.1, 4.1.2 and 4.1.3. It is organised as follows. The main step of the proofs in the logarithmic case are exposed in Section 4.2, while technical intermediary results are postponed to Sections 4.3, 4.4 and 4.5. More precisely, Section 4.3.1 is dedicated to the proof of a uniform in time energy bound, which is the main ingredient in the proof that the process goes back infinitely many times to a compact set. A result of small-time conditional regularization is proven in Section 4.3.2, which is used to replace deterministic initial conditions by smooth distributions (with some quantitative bounds). Section 4.4 presents hypocoercivity estimates similar to those of [137], which are used to prove the convergence of the algorithm in the slow cooling case. In the fast logarithmic cooling case, similar estimates have to be established in higher order Sobolev norms, which is the topic of Section 4.5. Section 4.6 is dedicated to the faster than logarithmic case, with the proof of Theorem 4.1.3.

4.2 Main steps of the proofs

The sketch of the proofs is the following.

The first point is to get uniform in time moment estimates. This would classically be done using Lyapunov arguments, but this would typically require some assumption on ∇U , which we want to avoid. We adapt an argument from [64]. From these estimates, we get that $\liminf_{t \rightarrow +\infty} H(Z_t)$ is almost surely finite, i.e. there exists a (random) compact set $\{H \leq A\}$ which will be visited infinitely often by the process.

The second step is to prove that, for any $A > 0$, there exists $A' > A$ such that, provided the process is in $\{H \leq A\}$ at some time t_0 , there is a probability at least, say, $1/4$, that the process remains in $\{H \leq A'\}$ for all times $t \geq t_0$. This is reminiscent of the study in [83] of fast cooling schedules, where it is proven that there is a positive probability that, starting in a potential well of depth larger than c , the process never climbs high enough to exit the well (as in Theorem 4.1.2). We will follow a similar proof, except that we have to check the dependency of the estimates with respect to t_0 or, equivalently by taking $t_0 = 0$, to β_0 . That way, we will conclude that, each time the process goes below A , it has a probability $1/4$ to never go above A' again so that, if it goes below A infinitely often, eventually it will stay below A' .

Combining the two previous steps, we get that the process is almost surely bounded. It is thus sufficient to prove the convergence of the process when the position space is a compact torus, which is then similar to [137], but without the issue of the behavior of U at infinity.

The strategy for the non-convergence in the fast cooling case is similar to [83], the technical difficulties coming from the degeneracy of the process. Indeed the estimates used in [137] in the kinetic case to prove convergence are too weak to get that the process has a positive probability to stay forever below some energy level. On the other hand the estimates of [83] are based on hypercontractivity of elliptic diffusions on compact manifold. We are not aware of similar results for hypoelliptic diffusions, and thus we overcome this difficulty by working with higher Sobolev norms.

The faster than logarithmic case is similar and somehow simpler: in that case the process has a positive probability to converge to $(x_*, 0)$, it is thus sufficient to linearize ∇U at this point and to study the corresponding Gaussian process.

4.2.1 Return to a compact set

Diffusions defined by (4.1) are time-inhomogeneous Markov processes with generator :

$$L_t = y \cdot \nabla_x - (\gamma_t y + \nabla_x U) \cdot \nabla_y + \gamma_t \beta_t^{-1} \Delta_y. \quad (4.6)$$

First, let us check that the process is well-defined.

Proposition 4.2.1. *Under Assumption 4.1.1, let $z_0 \in \mathbb{R}^{2d}$. There exists a unique process $Z = (X, Y)$ that solves (4.1) with $Z_0 = z_0$. It is non-explosive (i.e. defined for all $t \geq 0$) and, for all $t \geq 0$, $\mathbb{E}(H(Z_t)) \leq H(z_0) + dLt$.*

Proof. Since the coefficients of the diffusion (4.1) are all smooth, there is existence and uniqueness until a time ξ of explosion. For all $x, y \in \mathbb{R}^d$ and $t \geq 0$,

$$L_t H(x, y) = \gamma_t \beta_t^{-1} d - \gamma_t |y|^2 \leq Ld.$$

Considering for $N \in \mathbb{N}$ the stopping time $\tau_N = \inf \{t \geq 0; H(Z_t) \geq N\}$, we get

$$\mathbb{E}(H(Z_{\tau_N \wedge t})) \leq H(z_0) + dLt$$

which implies

$$\mathbb{P}(\tau_N < t) = \mathbb{P}(H(Z_{\tau_N \wedge t}) \geq N) \leq \frac{H(z_0) + dLt}{N} \xrightarrow{N \rightarrow \infty} 0,$$

hence $\xi < +\infty$ almost surely, which concludes. \square

The first main point is to strengthen the energy bound of Proposition 4.2.1 to a uniform in time estimate. For f a probability law or density on \mathbb{R}^{2d} , we write \mathbb{E}_f and \mathbb{P}_f expectations and probabilities with respect to the process Z solving (4.1) with initial condition Z_0 distributed according to f . If $f = \delta_z$ for some $z \in \mathbb{R}^{2d}$, we write \mathbb{E}_z and \mathbb{P}_z instead.

Lemma 4.2.1. *Under Assumption 4.1.1, there exists $b > \alpha_0$ that depends only on U such that the following holds. Provided $\beta_0 \geq b$ then, for any \mathcal{C}^∞ probability density f_0 with compact support,*

$$\sup_{t \geq 0} \mathbb{E}_{f_0} (H(Z_t)) \leq \frac{\kappa^{\beta_0}(f_0) + \ln(\mathcal{Z}_{\alpha_0})}{\beta_0 - \alpha_0},$$

where

$$\kappa^{\beta_0}(f_0) = \int_{\mathbb{R}^{2d}} f_0 \ln(1 + f_0 e^{\beta_0 H}), \quad \mathcal{Z}_{\alpha_0} = \int_{\mathbb{R}^{2d}} e^{-\alpha_0 H}.$$

The proof is postponed to Section 4.3.1. The next result enables the use of Lemma 4.2.1 when the initial condition is not smooth.

Lemma 4.2.2. *Under Assumption 4.1.1 with $c > c^*$, fix $A > 1$ and $\varepsilon > 0$. Then there exist $t^*, b_A, C_A^1, C > 0$ that do not depend on β_0 such that, for all $\beta_0 \geq b_A$ and $z_0 \in \mathbb{R}^{2d}$ with $H(z_0) \leq A$, the following holds. Writing $\mathcal{B} = \{\sup_{t \leq t^*} H(Z_t) \leq A + 1\}$,*

$$\mathbb{P}_{z_0}(\mathcal{B}) \geq 1 - \varepsilon.$$

Moreover, the law at time t^* of the process (4.1) with initial condition $Z_0 = z_0$ conditioned on the event \mathcal{B} has a density $f_{t^*}^c$ that satisfies

$$f_{t^*}^c \leq C e^{C_A^1 \beta_0} \mathbb{1}_{\{H \leq A+1\}}.$$

This is proven in Section 4.3.2. The two previous lemmas yield the following.

Proposition 4.2.2. *Under Assumption 4.1.1, $\liminf_{t \rightarrow \infty} H(Z_t) < \infty$ almost surely.*

Proof. For t large enough, $\beta_t \geq b$ where $b > \alpha_0$ is the constant from Lemma 4.2.1. Notice that, for $t_0 \geq 0$, $(Z_{t_0+t})_{t \geq 0}$ solves (4.1) except that β_0 is replaced by β_{t_0} and γ is also time-shifted. Hence, by the Markov property, without loss of generality, we can assume that $\beta_0 \geq b$. Moreover, by conditioning with respect to the initial condition, it is sufficient to consider the case of a deterministic initial condition $z_0 \in \mathbb{R}^{2d}$.

Fix $\varepsilon > 0$ and $A = H(z_0)$. From Lemma 4.2.2, there exist $t^*, C' > 0$ such that $\mathbb{P}_{z_0}(\mathcal{B}) \geq 1 - \varepsilon$ where $\mathcal{B} = \{\sup_{t \leq t^*} H(Z_t) \leq A + 1\}$, and such that the law of the process at time t^* and conditioned on \mathcal{B} has a density $\tilde{f}_{t^*} \leq C' \mathbb{1}_{\{H \leq A+1\}}$. Let $C > 0$ and f_0 be a \mathcal{C}^∞ probability density on \mathbb{R}^{2d} with compact support such that $C f_0 \geq C' \mathbb{1}_{\{H \leq A+1\}}$. Then, denoting by $(\mathcal{F}_t)_{t \geq 0}$ the filtration associated with $(Z_t)_{t \geq 0}$, by the strong Markov property and Lemma 4.2.1, for all $t \geq 0$,

$$\mathbb{E}_{z_0}(H(Z_{t^*+t})|\mathcal{B}) = \mathbb{E}_{z_0}(\mathbb{E}(H(Z_{t^*+t})|\mathcal{F}_{t^*})|\mathcal{B}) \leq C \mathbb{E}_{f_0}(H(Z_t)) \leq C \frac{\kappa^{\beta_0}(f_0) + \ln(\mathcal{Z}_{\alpha_0})}{\beta_0 - \alpha_0}.$$

As a consequence, by Fatou's Lemma,

$$\mathbb{E}_{z_0} \left(\liminf_{t \rightarrow \infty} H(Z_t) | \mathcal{B} \right) \leq \sup_{t \geq 0} \mathbb{E}_{z_0}(H(Z_t)|\mathcal{B}) < \infty.$$

Finally

$$\mathbb{P}_{z_0} \left(\liminf_{t \rightarrow \infty} H(Z_t) = \infty \right) \leq \mathbb{P}_{z_0}(\mathcal{B}^c) + \mathbb{P}_{z_0} \left(\liminf_{t \rightarrow \infty} H(Z_t) = \infty | \mathcal{B} \right) \leq \varepsilon,$$

which concludes since ε is arbitrary. \square

4.2.2 Position in a compact set

As in [64], with Proposition 4.2.2 at hand, we can now focus on the behavior of the process when the position is in a compact set, ignoring the behavior of U at infinity. To this end, we fix some parameter $K > 0$, let $L_K > 0$ be such that $\{U \leq K\} \subset [-(L_K - 1), (L_K - 1)]^d$ and consider the torus $M_K = (\mathbb{R}/2L_K\mathbb{Z})^d$ (i.e. we consider periodic boundary conditions, which will be technically simpler than e.g. reflecting boundary conditions). We now define a process (X_t^K, Y_t^K) on $M_K \times \mathbb{R}^d$ and a potential $U^K : M_K \mapsto \mathbb{R}$ to replace the initial one.

More precisely, write $\theta_K : \mathbb{R}^d \mapsto M_K$ the canonical projection and $\tilde{M}_K =]-L_K, L_K]^d$, so that $M_K = \theta_K(\tilde{M}_K)$. For a non-negative function $V : \mathbb{R}^d \rightarrow \mathbb{R}$, we define the critical height $c^*(V)$ with the same definition as c^* except that U is replaced by V .

Let $\tilde{U}^K \in C^\infty(\mathbb{R}^d)$ be equal to U on some open set O_K containing $\{U \leq K\}$, non-negative, $2L_K$ -periodic, and such that $c_K^* = c^*(\tilde{U}^K) \leq c^*$. Such a function exists from [64, Notation 9]. We write U^K the corresponding function on M_K , given by $U^K(\theta_K(x)) = \tilde{U}^K(x)$, and $H_K(x, y) = U^K(x) + |y|^2/2$.

Finally, given the same Brownian motion as in (4.1), we consider $Z^K = (X^K, Y^K)$ the process on $M_K \times \mathbb{R}^d$ that solves

$$\begin{cases} dX_t^K = Y_t^K dt \\ dY_t^K = -\nabla_x U^K(X_t) dt - \gamma_t Y_t^K dt + \sqrt{2\gamma_t \beta_t^{-1}} dB_t, \end{cases} \quad (4.7)$$

with $(X_0^K, Y_0^K) = (\theta_K(X_0), Y_0)$. Write $\tau_K = \inf \{t \geq 0, X_t \notin O_K\}$. Then, by design,

$$(U^K(X_t^K), Y_t^K)_{t \leq \tau_K} = (U(X_t), Y_t)_{t \leq \tau_K}. \quad (4.8)$$

For $\beta > 0$, write μ_β^K the probability measure on $M_K \times \mathbb{R}^d$ with density proportional to $e^{-\beta H_K}$.

Lemma 4.2.3. *Fix $\delta, \alpha > 0$. There exists $C > 0$ such that for all $\beta > 0$,*

$$\mu_\beta^K(H_K > \delta) \leq C e^{-\beta(\delta - \alpha)}.$$

Proof. For completeness, we recall the short proof of [137, section 3.1]. First,

$$\int_{M_K \times \mathbb{R}^d} e^{-\beta H_K(z)} dz \geq \int_{\{H_K \leq \alpha\}} e^{-\beta H_K(z)} dz \geq e^{-\beta \alpha} / C,$$

for some constant $C > 0$ because $\{H^K \leq \alpha\}$ is compact. Likewise, $\{\delta \leq H^K \leq \delta + |y|\}$ is compact and

$$\begin{aligned} \int_{\{H^K \geq \delta\}} e^{-\beta H_K(z)} dz &\leq \int_{\{\delta \leq H_K \leq \delta + |y|\}} e^{-\beta H_K(z)} dz + \int_{\{H_K \geq \delta + |y|\}} e^{-\beta H_K(z)} dz \\ &\leq e^{-\beta \delta} \left(C + C \int_{\mathbb{R}^d} e^{-|y|} dy \right) \end{aligned}$$

for some $C > 0$. The ratio of those two inequalities concludes the proof. \square

The goal of this section is to prove a similar result but with the law of Z_t^K instead of $\mu_{\beta_t}^K$, with an explicit dependency of the constants in term of β_0 .

Denote by f_t^K the law of Z_t^K . Since ∇U^K and its derivatives are all bounded, if f_0 is smooth, so is f_t^K for all $t \geq 0$ (see Section 4.4 for details). Consider the relative density $h_t^K = f_t^K / \mu_{\beta_t}^K$. We start with a uniform in time quantitative bound of the norm of h_t^K in $L^2(\mu_{\beta_t}^K)$, for nice initial conditions.

Proposition 4.2.3. *Under Assumption 4.1.1 with $c > c^*$, let $K \geq 1$. There exists $b_K > 0$, which depends on U and K , such that, if $\beta_0 \geq b_K$ and $f_0 \in \mathcal{C}^\infty(M_K \times \mathbb{R}^d)$ with compact support, then for all $t \geq 0$,*

$$\begin{aligned} \int_{M_K \times \mathbb{R}^d} (h_t^K)^2 d\mu_{\beta_t}^K \\ \leq 1 + \int_{M_K \times \mathbb{R}^d} \left(|(\nabla_x + \nabla_y)h_0^K|^2 + 4\sqrt{\gamma_0^{-1}\beta_0}(\|\nabla_x^2 U^K\|_\infty + 1 + \gamma_0)^2 (h_0^K)^2 \right) d\mu_0^K. \end{aligned}$$

The proof of this proposition is postponed to Section 4.4.

Lemma 4.2.4. *Under Assumption 4.1.1 with $c > c^*$, fix $A > 1$, $\varepsilon = 1/4$ and consider $\mathcal{B}, C_A^1, b_A, t^*$ as in Lemma 4.2.2. Set $D_A = 2C_A^1 + A + 4 + 4c$ and $K_A = D_A + 1$. There exist $C_A > 0$ and $b'_A \geq b_A$ that do not depend on β_0 such that, for all $\beta_0 \geq b'_A$ and $z_0 \in \mathbb{R}^{2d}$ with $H(z_0) \leq A$, we have that, \mathbb{P}_{z_0} -a.s., $\sup_{t \in [0, t^*]} H_{K_A}(Z_t^{K_A}) \mathbb{1}_{\mathcal{B}} < D_A$, and for all $t \geq 0$*

$$\mathbb{P}_{z_0} \left(H_{K_A} \left(Z_{t+t^*}^{K_A} \right) \geq D_A \mid \mathcal{B} \right) \leq \frac{C_A}{(e^{c\beta_0} + t)^2}.$$

Proof. The first point is clear since, by definition of \mathcal{B} , $\sup_{[0, t^*]} H_{K_A}(Z_t^{K_A}) \mathbb{1}_{\mathcal{B}} < A + 1 \leq D_A$.

In the rest of the proof we denote by C different constants.

Let us introduce a function which will serve as a new initial condition. Let v_d and w_d be respectively the volumes of $\{H \leq A + 1\}$ and $\{H \leq A + 2\}$ in $M_K \times \mathbb{R}^d$, and $f_0 \in \mathcal{C}^\infty$ be such that $(2v_d)^{-1} \mathbb{1}_{\{H \leq A+1\}} \leq f_0 \leq 2(w_d)^{-1} \mathbb{1}_{\{H \leq A+2\}}$. Notice that f_0 does not depend on β_0 , and that ∇f_0 is bounded since f_0 is smooth on a compact set. As in the proof of Lemma 4.2.2, from Lemma 4.2.2 and the strong Markov property,

$$\mathbb{P}_{z_0} \left(H_{K_A} \left(Z_{t+t^*}^{K_A} \right) \geq D_A \mid \mathcal{B} \right) \leq 2v_d C e^{C_A \beta_0} \mathbb{P}_{f_0} \left(H_{K_A} \left(Z_t^{K_A, \beta_{t^*}} \right) \geq D_A \right),$$

where $Z^{K_A, \beta_{t^*}}$ is a process similar to Z^{K_A} except that β_0 has been replaced by β_{t^*} and $(\gamma_t)_{t \geq 0}$ by $(\gamma_{t+t^*})_{t \geq 0}$. Denote by h_t^* the relative density of the law of $Z_t^{K_A, \beta_{t^*}}$ with respect to $\mu_{\beta_{t+t^*}}^{K_A}$. By the Cauchy-Schwartz inequality,

$$\begin{aligned} \mathbb{P}_{f_0} \left(H_{K_A} \left(Z_t^{K_A, \beta_{t^*}} \right) \geq D_A \right) &= \int_{\{H_{K_A} \geq D_A\}} h_t^* d\mu_{\beta_{t+t^*}}^{K_A} \\ &\leq \sqrt{\int_{\mathbb{R}^d \times \mathbb{R}^d} (h_t^*)^2 d\mu_{\beta_{t+t^*}}^{K_A}} \sqrt{\mu_{\beta_{t+t^*}}^{K_A} (H_{K_A} \geq D_A)}. \end{aligned} \quad (4.9)$$

For the second term, applying Lemma 4.2.3 with $\alpha = 1$,

$$\mu_{\beta_{t+t^*}}^{K_A} (H_{K_A} \geq D_A) \leq C e^{-\beta_{t+t^*} (D_A - 1)}.$$

For the first term, Proposition 4.2.3 applies if $\beta_0 \geq b_{K_A}$, which yields

$$\begin{aligned} & \int_{M_K \times \mathbb{R}^d} (h_t^*)^2 d\mu_{\beta_{t+t^*}}^{K_A} \\ & \leq 1 + \int_{M_K \times \mathbb{R}^d} \left(|(\nabla_x + \nabla_y)h_0^*|^2 + 4\sqrt{\gamma_{t^*}^{-1}\beta_{t^*}} (\|\nabla_x^2 U^K\|_\infty + 1 + \gamma_{t^*})^2 (h_0^*)^2 \right) d\mu_{\beta_{t^*}}^{K_A} \\ & \leq C\beta_{t^*}^{\frac{5}{2}} \int_{\{H_{K_A} \leq A+2\}} \frac{1}{\mu_{\beta_{t^*}}^{K_A}(z)} dz \end{aligned}$$

for some $C > 0$ that does not depend on β_0 , where we used Assumption 4.1.1, that $\beta_{t^*} \geq \beta_0$, $h_0^K = f_0^K/\mu_{\beta_0}^K$, and a uniform bound on f_0 and ∇f_0 . For any $\beta \geq 1$, using that $e^{-\beta U^{K_A}(x)} \leq 1$,

$$\int_{M_{K_A}} e^{-\beta U^{K_A}(x)} dx \leq (2L_{K_A})^d \quad \text{and} \quad \mathcal{Z}_\beta \int_{M_{K_A} \times \mathbb{R}^d} e^{-\beta H_{K_A}(z)} dz \leq (2\sqrt{2\pi}L_{K_A})^d,$$

for all $\beta > 0$. Hence,

$$\int_{M_{K_A} \times \mathbb{R}^d} (h_t^*)^2 d\mu_{\beta_{t+t^*}}^{K_A} \leq C\beta_{t^*}^{\frac{5}{2}} \mathcal{Z}_{\beta_{t^*}} \int_{\{H_{K_A} \leq A+2\}} e^{\beta_{t^*} H_{K_A}(z)} dz \leq C' e^{\beta_{t^*}(A+3)}$$

Everything put together gives, if $\beta_0 \geq \max(1, b_{K_A}, b_A)$, using the monotonicity of $t \mapsto \beta_t$, we conclude with

$$\mathbb{P}\left(H_{K_A}\left(Z_{t+t^*}^{K_A}\right) \geq D_A \mid \mathcal{B}\right) \leq C e^{-\frac{1}{2}\beta_{t^*+t}(D_A-1-2C_A^1-A-3)} \leq C e^{-2c\beta_t} = \frac{C}{(e^{c\beta_0} + t)^2}.$$

□

In fact, a similar proof already yields the convergence of the kinetic annealing on the compact torus:

Proposition 4.2.4. *Under Assumption 4.1.1 with $c > c^*$, for all $K > 1$ and $\delta > 0$,*

$$\mathbb{P}(H_K(Z_t^K) > \delta) \xrightarrow[t \rightarrow +\infty]{} 0.$$

Proof. As in the proof of Proposition 4.2.2, by the Markov property, without loss of generality we assume that $\beta_0 \geq b_K$ and that the initial condition is a Dirac mass at some $z_0 \in M_K \times \mathbb{R}^d$. Fix $\varepsilon > 0$, let $A = H(z_0)$ and, from Lemma 4.2.2 (applied to the process Z^K rather than Z , the proof is the same) let $t_0, C > 0$ be such that the event $\mathcal{B} = \{\forall t \in [0, t_0], H(Z^K) \leq A+1\}$ has a probability larger than $1 - \varepsilon$ and the law of $Z_{t_0}^K$ conditioned on \mathcal{B} has a density $\tilde{f}_{t_0}^K \leq C' \mathbb{1}_{\{H_K \leq A+1\}}$. Let $C > 0$ and f_0 be a smooth probability density on $M_K \times \mathbb{R}^d$ with compact support such that $C' \mathbb{1}_{\{H_K \leq A+1\}} \leq C f_0$. We then have:

$$\mathbb{P}(H_K(Z_{t+t_0}^K) > \delta \mid \mathcal{B}) = \mathbb{E}(\mathbb{P}(H_K(Z_{t+t_0}^K) > \delta \mid \mathcal{F}_{t_0}) \mid \mathcal{B}) \leq C \mathbb{P}_{f_0}(H_K(\tilde{Z}_t) > \delta),$$

where \tilde{Z} is a process similar to Z^{K_A} except that β_0 has been replaced by β_{t_0} and γ has been time-shifted. Denoting by \tilde{f}_t the law of \tilde{Z}_t (with initial condition f_0), Proposition 4.2.3 means that $t \mapsto \|\tilde{f}_t/\mu_{\beta_{t+t_0}}^K\|_{L^2(\mu_{\beta_{t+t_0}}^K)}$ is bounded. As in the previous proof, applying the Cauchy-Schwartz

inequality and Lemma 4.2.3 with $\alpha = \delta/2$ then yields :

$$\mathbb{P}_{f_0}^2 \left(H_K(\tilde{Z}_t) > \delta \right) \leq C \mu_{\beta_{t+t_0}}^K (H_K > \delta) \leq C e^{-\frac{\beta_t \delta}{2}} \rightarrow 0.$$

As a consequence,

$$\limsup_{t \rightarrow \infty} \mathbb{P}(H_K(Z_t^K) > \delta) \leq \mathbb{P}(\mathcal{B}^c) + \limsup_{t \rightarrow \infty} \mathbb{P}(H_K(Z_t^K) > \delta \mid \mathcal{B}) \leq \varepsilon,$$

which concludes since ε is arbitrary. \square

4.2.3 Localization and convergence

Building upon the results of the previous section, we can now prove the following.

Proposition 4.2.5. *Under Assumption 4.1.1 with $c > c^*$, fix some $A > 1$. There exist $b_A > 1$, $K_A > A$ which depends on A , U , c , and κ but not β_0 such that, for all $\beta_0 \geq b_A$ and all initial condition $z_0 \in \{H \leq A\}$,*

$$\mathbb{P}_{z_0} \left(\sup_{t \geq 0} H(Z_t) \leq K_A \right) \geq \frac{1}{4}.$$

Proof. It is enough to show the same result for the process Z^{K_A} since, from (4.8),

$$\begin{aligned} & \left\{ \sup_{t \geq 0} H(Z_t) \leq K_A \right\} \\ &= \left\{ \sup_{t \geq 0} H(Z_t) \leq K_A, (U^K(X_t^{K_A}), Y_t^{K_A})_{t \leq \tau_{K_A}} = (U(X_t), Y_t)_{t \leq \tau_{K_A}}, \tau_{K_A} = \infty \right\} \\ &= \left\{ \sup_{t \geq 0} H_{K_A}(Z_t^{K_A}) \leq K_A, (U^K(X_t^{K_A}), Y_t^{K_A})_{t \leq \tau_{K_A}} = (U(X_t), Y_t)_{t \leq \tau_{K_A}}, \tau_{K_A} = \infty \right\} \\ &= \left\{ \sup_{t \geq 0} H_{K_A}(Z_t^{K_A}) \leq K_A \right\}. \end{aligned}$$

We use the definitions and notations of Lemma 4.2.4. Let $\Psi_A \in \mathcal{C}^\infty(\mathbb{R}_+, [0, 1])$ equal to 0 outside of $[D_A, K_A]$ and such that $\Psi_A\left(\frac{D_A + K_A}{2}\right) = 1$, and let $\Phi_A = \Psi_A \circ H^{K_A}$. Then, there exists $C > 0$, independent of β , such that, for all $t \geq 0$, $|L_t \Phi_A| \leq C(1 + \gamma_t) \mathbb{1}_{\{H^{K_A} \geq D_A\}}$.

Recall the definition $\mathcal{B} = \{\sup_{t \leq t^*} H(Z_t) \leq A + 1\}$. From Ito's formula,

$$\Phi_A \left(Z_{t+t^*}^{K_A} \right) \mathbb{1}_{\mathcal{B}} = (M_t + R_t) \mathbb{1}_{\mathcal{B}}$$

where M_t is a local martingale and $R_t = \int_{t^*}^t L_s \Phi_A(Z_s^{K_A}) ds$. We then get that for $\beta_0 \geq b'_A$,

$$\begin{aligned} \mathbb{E} \left(\sup_{t \geq 0} |R_t| \mathbb{1}_{\mathcal{B}} \right) &\leq C \int_0^\infty (1 + \gamma_s) \mathbb{E} \left(\mathbb{1}_{\{H^{K_A}(Z_{s+t^*}^{K_A}) \geq D_A\}} \mid \mathcal{B} \right) ds \\ &\leq C \int_0^\infty (1 + L\beta_s) \mathbb{P} \left(H \left(Z_{s+t^*}^{K_A} \right) \geq D_A \mid \mathcal{B} \right) ds \\ &\leq C \int_0^\infty \frac{1 + L \ln(e^{c\beta_0} + t)}{c(e^{c\beta_0} + t)^2} ds. \end{aligned}$$

We take β_0 large enough to get that, by Markov's inequality, $\mathbb{P}(\mathcal{E}|\mathcal{B}) \geq 3/4$, where $\mathcal{E} = \{\sup_{t \geq 0} |R_t| \leq 1/10\}$. Now,

$$\mathcal{E} \cap \mathcal{B} \cap \left\{ \sup_{t \geq 0} H_{K_A}(Z_t^{K_A}) \geq K_A \right\} \subset \mathcal{E} \cap \mathcal{B} \cap \left\{ \sup_{t \geq 0} M_t \geq \frac{9}{10} \right\},$$

so that

$$\mathbb{P} \left(\sup_{t \geq 0} H_{K_A}(Z_t^{K_A}) \geq K_A \mid \mathcal{B} \right) \leq \mathbb{P}(\mathcal{E}^c \mid \mathcal{B}) + \mathbb{P} \left(\mathcal{E}, M_t \text{ up-crosses } \left[\frac{1}{10}, \frac{9}{10} \right] \mid \mathcal{B} \right).$$

Consider the stopping time

$$\sigma = \inf \left\{ t \geq 0, M_t \notin \left[-\frac{1}{10}, \frac{11}{10} \right] \right\}.$$

Then $M_{t \wedge \sigma}$ is a bounded local martingale, hence a martingale. Moreover, since Φ_A takes values in $[0, 1]$, $M_t = M_{t \wedge \sigma}$ for all $t \geq 0$ on $\mathcal{E} \cap \mathcal{B}$. By Doob's up-crossing inequality, for any $T > 0$, the probability that M_t up-crosses $[1/10, 9/10]$ before time T is bounded by $\mathbb{E}(M_{T \wedge \sigma} - \frac{1}{10}) / (8/10) \leq \frac{1}{4}$. As a consequence,

$$\mathbb{P} \left(\mathcal{E}, M_t \text{ up-crosses } \left[\frac{1}{10}, \frac{9}{10} \right] \mid \mathcal{B} \right) \leq \frac{1}{4}.$$

As a conclusion,

$$\begin{aligned} \mathbb{P} \left(\sup_{t \geq 0} H_{K_A}(Z_t^{K_A}) \geq K_A \right) \\ \leq \mathbb{P}(\mathcal{B}^c) + \mathbb{P}(\mathcal{E}^c|\mathcal{B}) + \mathbb{P} \left(\mathcal{E}, M_t \text{ up-crosses } \left[\frac{1}{10}, \frac{9}{10} \right] \mid \mathcal{B} \right) \leq \frac{3}{4}. \end{aligned}$$

□

As announced, combining this result with Proposition 4.2.2 yields the following.

Proposition 4.2.6. *Under Assumption 4.1.1 with $c > c^*$, almost surely, $\sup_{t \geq 0} H(Z_t) < +\infty$.*

Proof. For $A > 0$, let

$$\Omega_A = \left\{ \liminf_{t \rightarrow \infty} H(Z_t) < A \right\}.$$

It is sufficient to show that, for all $A > 0$, $(Z_t)_{t \geq 0}$ is bounded on Ω_A since, from Proposition 4.2.2, $\mathbb{P}(\cup_{A \geq 0} \Omega_A) = 1$. Hence, we fix $A > 0$.

Let b_A, K_A be as in Proposition 4.2.5 and $S_0 = t_A$ where t_A satisfies $\beta_{t_A} \geq b_A$. By induction, for $k \in \mathbb{N}$, define $T_k = \inf \{t \geq S_k; H(Z_t) \leq A\}$ and $S_{k+1} = \inf \{t \geq T_k; H(Z_t) \geq K_A\}$. From Proposition 4.2.5 and the Markov property,

$$\begin{aligned} \mathbb{P}(S_{k+1} < \infty | S_k < \infty) &= \mathbb{P}(S_{k+1} < \infty, T_k < \infty | S_k < \infty) \\ &= \mathbb{E}(\mathbb{1}_{T_k < \infty} \mathbb{P}(S_{k+1} < \infty | \mathcal{F}_{T_k}) | S_k < \infty) \leq \frac{3}{4}, \end{aligned}$$

where we used that $\beta_{T_k} \geq \beta_{t_A} \geq b_A$ for all $k \in \mathbb{N}$. This implies that a.s. there exists $J \in \mathbb{N}$ such that $S_J = \infty$. On Ω_A , T_J is finite and $\sup_{t \geq T_J} H(Z_t) \leq K_A$, which concludes. □

We can now finally prove Theorem 4.1.1.

Proof of Theorem 4.1.1. Let $\varepsilon > 0$ and, thanks to Proposition 4.2.6, let $K > 1$ be such that $\mathbb{P}(\sup_{t \geq 0} H(Z_t) \geq K) \leq \varepsilon$. Using Proposition 4.2.4, for $t \geq 0$,

$$\begin{aligned} \mathbb{P}(H(Z_t) > \delta) &\leq \varepsilon + \mathbb{P}\left(\sup_{t \geq 0} H(Z_t) \leq K; H(Z_t) > \delta\right) \\ &= \varepsilon + \mathbb{P}\left(\sup_{t \geq 0} H_K(Z_t^K) \leq K; H_K(Z_t^K) > \delta\right) \\ &\leq \varepsilon + \mathbb{P}(H_K(Z_t^K) > \delta) \xrightarrow{t \rightarrow +\infty} \varepsilon. \end{aligned}$$

As a consequence, $\limsup_{t \rightarrow \infty} \mathbb{P}(H(Z_t) > \delta) \leq \varepsilon$ for all $\varepsilon > 0$, which concludes. \square

4.2.4 Full process on a compact space

One of the main point of the proof of Theorem 4.1.2 is essentially to get something of the form

$$\forall \delta > 0, \quad \mathbb{P}_{z_0}\left(\sup_{t \geq 0} H(Z_t) < c + \delta\right) > 0$$

for suitable initial conditions z_0 . First, let us highlight some of the difficulties in order to motivate the rest of this section. Refining the proof of Proposition 4.2.5, we would obtain a similar result but with c replaced by $4c$. The factor 4 is due to two things. First, in Lemma 4.2.4, we prove a bound of order $1/t^2$ while the proof of Proposition 4.2.5 in fact only requires an integrable bound, i.e. $1/t^{1+\delta}$ for any $\delta > 0$ is enough. The second factor 2 is lost when the Cauchy-Schwartz inequality is used in (4.9). To solve this, the Cauchy-Schwartz inequality has to be replaced by the Hölder inequality, which means the L^2 estimate of Proposition 4.2.3 is not sufficient and we need L^p estimates for all $p > 2$, or even better, L^∞ estimates (besides, in [137], the convergence is stated in relative entropy, which is weaker than L^p for any $p > 1$, which is why we said in the introduction that these results were not sufficient to conclude in the fast cooling case). In fact in the elliptic case the proof of [83] relies on L^∞ bounds. In order to get such bounds in an hypocoercive case, we will work with H^k -Sobolev norms for $k \geq 1$, as in the work [170] of Zhang, and then use Sobolev embeddings. This should be done with a correct control of the dependency in time of the constants, and to do so it is convenient to work with a process (both position and velocity) in a compact manifold. This is done by replacing the Hamiltonian $H(x, y) = U(x) + |y|^2/2$ by $H_K(x, y) = U^K(x) + W(y)$ where W is some periodic potential with $W(y) = |y|^2/2$ below some threshold. This raises an issue in the dissipation of the hypocoercive modified entropy. Indeed, in the modified H^1 -norm of Villani (and similarly in the modified H^k -norm of Zhang), the key point is that the missing coercivity in x is recovered through a term

$$\nabla_x h \cdot [\nabla_y, y \nabla_x] h = |\nabla_x h|^2$$

where $[A, B] = AB - BA$ stands for the commutator of A and B . When H is replaced by H_K , this term becomes

$$\nabla_x h \cdot [\nabla_y, \nabla W(y) \nabla_x] h = \nabla_x h \cdot \nabla^2 W \nabla_x h$$

which is negative at maxima of W . For this reason, and since anyway we are not really interested in the process above some energy threshold, we will add some Brownian noise in the position variable where $W(y) \neq |y|^2/2$.

As a conclusion, for these reasons, in this section, we consider a process $Z^K = (X^K, Y^K)$ on

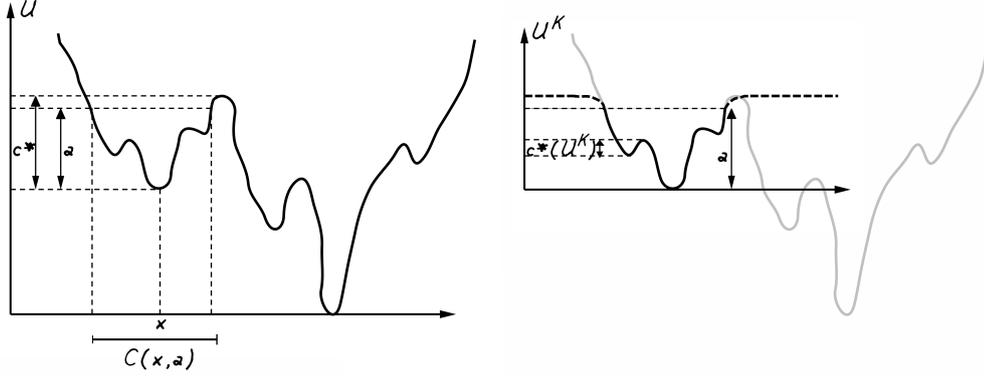


Figure 4.2: Construction of U^K from U , with \tilde{x} chosen so that $c^*(U) = D(\tilde{x})$.

a periodic torus M_K^2 solution of

$$\begin{cases} dX_t^K = \nabla W(Y_t^K)dt - \sigma(Y_t^K)\nabla U^K(X_t^K)dt + \sqrt{2\sigma(Y_t^K)\beta_t^{-1}}d\tilde{B}_t \\ dY_t^K = -\nabla U^K(X_t^K)dt - \gamma_t\nabla W(Y_t^K)dt + \sqrt{2\gamma_t\beta_t^{-1}}dB_t \end{cases} \quad (4.10)$$

where B is as in (4.1), \tilde{B} is another independent d -dimensional Brownian motion, and σ, W and U^K are $2L_K$ -periodic non-negative functions on \mathbb{R}^d (with $M_K = (\mathbb{R}/2L_K\mathbb{Z})^d$). The term $\sigma\nabla U^K$ has been added so that, for fixed γ, β , this new process admits the explicit stationary measure

$$\mu_\beta^K \propto e^{-\beta H_K(x,y)} dx dy$$

that satisfies a Poincaré inequality (see Section 4.5). Here and in all this section, when there is no ambiguity we identify $2L_K$ -periodic functions on \mathbb{R}^d and functions on M_K . Let us now give the precise definition of L_K, σ, W and U^K .

In all this section we consider fixed $U \in C^\infty(\mathbb{R}^d)$, $\beta, \gamma, \tilde{x} \in \mathbb{R}^d$ and $a > 0$ satisfying Assumption 4.1.2. Setting $K = a + 1$, similarly to Section 4.2.2 we fix some $L_K > \sqrt{2K} + 2$ large enough so that $C(\tilde{x}, a) \subset [-L_K + 1, L_K - 1]^d$. We consider a non-negative $U^K \in C^\infty(M_K)$ with $c^*(U^K) < c$ and such that, seen as a periodic function on \mathbb{R}^d , $U^K(x) = U(x) - U(\tilde{x})$ for all $x \in C(\tilde{x}, a)$. Such a function exists: indeed, since \tilde{c} is continuous, $C(\tilde{x}, a)$ is a compact set, and then, under Assumption 4.1.2, $\sup\{\tilde{c}(y, \tilde{x}), y \in C(\tilde{x}, a)\} < c$. We can thus choose $\delta \in (0, a - c)$ small enough so that $\sup\{\tilde{c}(y, \tilde{x}) : y \in C(\tilde{x}, a)\} + 2\delta < c$ and, using that the boundary of $C(\tilde{x}, a)$ is in $\{U = U(\tilde{x}) + a\}$, we let U^K be any C^∞ potential on $[-L_K, L_K]^d$ with $U^K(x) = U(x) - U(\tilde{x})$ on $C(\tilde{x}, a)$, $U^K(x) \in [a - \delta, a + \delta]$ for $x \in [-L_K, L_K]^d \setminus C(\tilde{x}, a)$ with $U^K(x) = a$ for all $x \in [-L_K, L_K]^d \setminus [-L_K + 1/2, L_K + 1/2]^d$ so that we can extend it to a $2L_K$ -periodic C^∞ potential on \mathbb{R}^d . The fact that $c^*(U^K) < c$ is straightforward since a path from any $y \in [-L_K, L_K]^d$ to \tilde{x} can be obtained by a straight line from y to some $y_* \in C(\tilde{x}, a)$ with $\tilde{c}(y, y_*) \leq 2\delta$ and then a path to \tilde{x} , where Assumption 4.1.2 is used. See Figure 4.2 for an illustration of the construction of U^K .

Concerning the new potential W for the velocity, first, write $n = \sqrt{2K} + 1$ and $m = \sqrt{2K} + 2$. Then, fix some $2L_K$ -periodic $W_1 \in C^\infty(\mathbb{R}, \mathbb{R})$ such that for all $s \in [-m, m]$, $W_1(s) = s^2/2$, W_1 is symmetric on $[-L_K, L_K]$, and increasing on $[0, L_K]$. For $y \in [-L_K, L_K]^d$, we set $W(y) = \sum_{i=1}^d W_1(y_i)$.

Similarly, fix some $2L_K$ -periodic non-negative $\sigma^0 \in C^\infty(\mathbb{R}^d, \mathbb{R}_+)$ with $\sigma^0(y) = 0$ for $y \in [-n, n]^d$, $\sigma^0(y) = \sigma_*^0$ for $y \in [-L_K, L_K]^d \setminus [-m, m]^d$ for some constant $\sigma_*^0 > 0$, and $|\nabla \sigma^0|^2 \leq C\sigma^0$ for some $C > 0$. Set $\sigma = r\sigma^0$ where $r > 0$ is chosen small enough that $\|\nabla \sigma\|_\infty \|\nabla U^K\|_\infty \leq \frac{1}{2}$ and $|\nabla \sigma|^2 \leq \sigma$.

The useful properties of W and σ can be summarized as follows :

Lemma 4.2.5. • *Seeing W as a periodic function from \mathbb{R}^d to \mathbb{R} , there exists $m \in (\sqrt{2K}, L_K)$ such that $W(y) = |y|^2/2$ for all $y \in [-m, m]^d$.*

- *On M_K , W has a unique local minimum, which is global.*
- *There exist $n \in (\sqrt{2K}, m)$ and $\sigma_* > 0$ such that, seeing σ as a periodic function from \mathbb{R}^d to \mathbb{R}_+ , $\sigma(y) = \sigma_*$ for all $y \in [-L_K, L_K]^d \setminus [-m, m]^d$ and $\sigma(y) = 0$ for all $y \in [-n, n]^d$.*
- *σ satisfies $\|\nabla \sigma\|_\infty \|\nabla U^K\|_\infty \leq 1/2$ and $|\nabla \sigma(y)|^2 \leq \sigma(y)$ for all $y \in M_K$.*

We write $H_K(x, y) = U^K(x) + W(y)$,

$$\mathcal{M} = \{y \in M_K; \nabla^2 W(y) = I_d\}$$

and notice that, by construction, for $y \in M_K \setminus \mathcal{M}$, $\sigma(y) = \sigma_*$. Moreover, if $|y|^2/2 \leq K$ then $W(y) = |y|^2/2$ and $\sigma(y) = 0$.

By construction of U^K , W and σ , if we consider Z and Z^K the solutions respectively of (4.1) and (4.10) with the same initial condition in $C(\tilde{x}, c)$ and the same Brownian motion B , then $H(Z_t) = H_K(Z_t^K)$ for all $t \leq \tau := \inf\{s \geq 0, H(Z_s) \geq a\}$. In particular, for $\delta > 0$ small enough so that $c + \delta < \inf\{U^K(x), x \in [-L_K, L_K]^d \setminus C(\tilde{x}, a)\}$,

$$\{H_K(Z_t^K) < c + \delta \forall t \geq 0\} \subset \{X_t \in C(\tilde{x}, c + \delta) \forall t \geq 0\}, \quad (4.11)$$

which means we are lead to prove that the left hand side has a positive probability.

Denote by f_t^K the law of the solution of (4.10), write $\mu_\beta^K = \mathcal{Z}_\beta^{K-1} e^{-\beta H_K(z)} dz$ where \mathcal{Z}_β^K makes μ_β^K a probability measure, and let $h_t^K = f_t^K / \mu_{\beta_t}^K$. Similarly to Section 4.2.3, the key point is the following estimate, proven in Section 4.5.

Proposition 4.2.7. *Let $f_0^K \in C^\infty(M_K \times M_K)$. Under Assumption 4.1.2, $t \mapsto \|h_t^K\|_\infty$ is bounded.*

Lemma 4.2.6. *Under Assumption 4.1.2, for all probability density $f_0^K \in C^\infty(M_K \times M_K)$ and $\delta > 0$, there exists $C > 0$ such that for all $t \geq 0$,*

$$\mathbb{P}_{f_0^K}(H_K(Z_t^K) \geq c + \delta) \leq \frac{C}{(1+t)^{1+\frac{\delta}{2c}}}.$$

Proof. Applying Proposition 4.2.7, for $t \geq 0$

$$\begin{aligned} \mathbb{P}(H_K(Z_t^K) \geq c + \delta) &= \int_{\{H_K \geq c + \delta\}} h_t^K d\mu_{\beta_t}^K \\ &\leq \sup_{s \geq 0} \|h_s^K\|_\infty \mu_{\beta_t}^K(H_K \geq c + \delta) \leq \frac{C}{(1+t)^{1+\frac{\delta}{2c}}} \end{aligned}$$

for some $C > 0$, where we used Lemma 4.2.3 with $\alpha = \delta/2$. □

Lemma 4.2.7. *Under Assumption 4.1.2, for all probability density $f_0^K \in \mathcal{C}^\infty(M_K \times M_K)$ and $\delta > 0$, there exists $t_b > 1$ such that*

$$\mathbb{P}_{f_0^K} \left(\sup_{t \geq t_b} H_K(Z_t^K) < c + \delta \right) > 0.$$

Proof. It is enough to show the result for δ satisfying $c + \delta < a$. Let \mathcal{B} the event $\{H(Z_{t_b}) < c\}$. Let $\psi_K : \mathbb{R} \mapsto [0, 1]$ be a \mathcal{C}^∞ function equal to zero outside of $[c + \frac{\delta}{2}, c + \delta + 1]$ such that $\psi_K < 1$ on $[c + \frac{\delta}{2}, c + \delta[$ and $\psi_K(c + \delta) = 1$ and write $\Psi_K = \psi_K \circ H_K$. We have :

$$\left\{ \sup_{t \geq t_b} H(Z_t^K) < c + \delta \right\} = \left\{ \sup_{t \geq t_b} \Psi_K(Z_t^K) < 1 \right\}.$$

There exists some constant $C > 0$ such that $|L\Psi_K| \leq C(1 + \beta_t)\mathbb{1}_{\{H_K \geq c + \frac{\delta}{2}\}}$, and from Ito's formula we can write :

$$\Phi(Z_{t+t_b}^K) \mathbb{1}_{\mathcal{B}} = (M_t + R_t) \mathbb{1}_{\mathcal{B}}$$

where $R_t = \int_{t_b}^t L\Psi_K(Z_s^K) ds$, and if $t_b \geq t_0$:

$$\begin{aligned} \mathbb{E} \left(\sup_{t \geq t_b} |R_t| \mathbb{1}_{\mathcal{B}} \right) &\leq C \int_{t_b}^{\infty} (1 + \beta_s) \mathbb{E} \left(\mathbb{1}_{H_K(Z_t^K) \geq c + \frac{\delta}{2}} \mid \mathcal{B} \right) ds \\ &\leq C \int_{t_b}^{\infty} (1 + \beta_s) \mathbb{P} \left(H_K(Z_s^K) \geq c + \frac{\delta}{2} \mid \mathcal{B} \right) ds \\ &\leq C \int_{t_b}^{\infty} \frac{1 + \ln(1+t)}{(1+t)^{1+\frac{\delta}{8c}}} ds \end{aligned}$$

where the constant C depends only on U^K and its derivative, but not on t_b . Since $(1 + \ln(1+t))/(1+t)^{1+\frac{\delta}{8c}}$ is integrable, we can take t_b great enough so that the event $E = \{\sup_{t \geq t_b} |R_t| \leq \frac{1}{10}\}$ has probability at least $\frac{3}{4}$. On $E \cap \mathcal{B}$, M_t takes value in $[-\frac{1}{10}, \frac{11}{10}]$ because $0 \leq \psi_A \leq 1$. Using Doob's up-crossing inequality as in the proof of Lemma 4.2.5, we get that the probability of Ψ_K going to 1 knowing \mathcal{B} is less then $\frac{1}{2}$. We conclude by :

$$\mathbb{P} \left(\sup_{t \geq 0} H_{K_A}(Z_t^{K_A}) < c + \delta \right) \geq \mathbb{P}(\mathcal{B}) \times \mathbb{P} \left(\sup_{t \geq 0} H_{K_A}(Z_t^{K_A}) < c + \delta \mid \mathcal{B} \right) > 0.$$

□

4.2.5 Non-convergence with fast cooling schedules

We are now ready to prove Theorem 4.1.2. In this section, Assumption 4.1.2 is enforced and we use the definitions and notations of Section 4.2.4.

We start with a result on the position of the process for small times, as well as a Doeblin-like condition, which will be proven in Section 4.3.2 :

Lemma 4.2.8. *For all $t, \delta > 0$, write :*

$$\mathcal{B}_t = \{X_s \in C(\tilde{x}, c + \delta) \forall s \in [0, t]\}.$$

Then, for all $z_0 = (x_0, y_0)$ with $x_0 \in C(\tilde{x}, c)$, $\mathbb{P}_{z_0}(\mathcal{B}_t) > 0$, and more precisely for all compact set \mathcal{K} included in the interior of $C(\tilde{x}, c + \delta) \times \mathbb{R}^d$, there exists $\varepsilon > 0$ such that

$$\mathbb{P}_{z_0}(\mathcal{B}_t, Z_t \in \cdot) \geq \varepsilon \ell(\cdot \cap \mathcal{K}),$$

where ℓ stands for the Lebesgue measure.

Proof of Theorem 4.1.2. By conditioning on the initial condition, it is sufficient to prove the result with a fixed initial condition $z_0 = (x_0, y_0)$ with $x_0 \in C(\tilde{x}, c)$. Moreover it is sufficient to prove the result for $\delta > 0$ small enough. We consider a fixed $\delta > 0$ such that $c + \delta < \inf\{U^K(x), x \in [-L_K, L_K]^d \setminus C(\tilde{x}, a)\} \leq a$, which means (4.11) holds and $\{U^K \leq c + \delta\} = C(\tilde{x}, c + \delta)$ (seeing $\{U^K \leq c + \delta\}$ as a subset of $[-L_K, L_K]^d$).

Let $f_0^K \in \mathcal{C}^\infty(M_K \times M_K)$ a probability density and $t_b > 0$ as in Lemma 4.2.7 applied with $\delta/2$ instead of δ such that:

$$\mathbb{P}_{f_0^K} \left(\sup_{t \geq t_b} H_K(Z_t^K) \leq c + \delta/2 \right) > 0.$$

In other words, denoting by \tilde{f} the law at time t_b of the process solution to equation (4.10) with initial condition f_0^K and conditioned to $\{H^K(Z_{t_b}) \leq c + \delta/2\}$, and $(Z^{K, t_b})_{t \geq 0}$ the solution to equation (4.10) with initial condition \tilde{f} at time t_b ,

$$\mathbb{P}_{\tilde{f}} \left(\sup_{t \geq 0} H_K(Z_t^{K, t_b}) \leq c + \delta/2 \right) > 0.$$

Let \mathcal{B}_{t_b} be as in Lemma 4.2.8. From Lemma 4.2.8 and the fact \tilde{f} has a bounded density on its support $\{H^K \leq c + \delta/2\}$ (which we see as a subset of $[-L_K, L_K]^{2d}$), there exists $\varepsilon > 0$ such that

$$\mathbb{P}_{z_0}(\mathcal{B}_{t_b}, Z_{t_b} \in \cdot) \geq \varepsilon \tilde{f}.$$

Finally, thanks to (4.11), we conclude that

$$\begin{aligned} \mathbb{P}_{z_0}(X_t \in C(\tilde{x}, c + \delta) \forall t \geq 0) &\geq \mathbb{P}_{z_0}(\mathcal{B}_{t_b}, X_t \in C(\tilde{x}, c + \delta) \forall t \geq t_b) \\ &\geq \varepsilon \mathbb{P}_{\tilde{f}} \left(\sup_{t \geq 0} H(Z_t^{K, t_b}) < c + \delta \right) > 0. \end{aligned}$$

□

4.3 Auxiliary results

4.3.1 Uniform energy bounds

This section is dedicated to the proof of Lemma 4.2.1. First, we consider a family of approximation functions $\eta_m \in \mathcal{C}_c^\infty$ for $m \geq 1$ in order to justify some PDE computations below. Let

$$\Phi(s) = \begin{cases} e^{\frac{1}{s^2-1}} / \int e^{\frac{1}{u^2-1}} du & \text{for } s \in (-1, 1) \\ 0 & \text{for } s \in \mathbb{R} \setminus (-1, 1) \end{cases}$$

and, for $m \geq 1$, $\Phi_m(s) = \Phi(s/m)/m$, $\nu_m = \mathbb{1}_{(-\infty, m^2]} * \Phi_m$ where $*$ denotes the convolution, and finally, for $z \in \mathbb{R}^{2d}$,

$$\eta_m(z) = \nu_m(\ln(H(z) + 1)).$$

Proposition 4.3.1. *Assume $U \rightarrow +\infty$ at infinity and ∇U is bounded.*

- For all $m \geq 1$, $\eta_m \in C^\infty(\mathbb{R}^d)$, has a compact support, and satisfies $0 \leq \eta_m \leq 1$.
- For all $z \in \mathbb{R}^{2d}$, $\eta_m(z) \rightarrow 1$ as $m \rightarrow \infty$.
- There exists $C > 0$ such that $L_t \eta_m \leq C\beta_t/m$ and $|\nabla \eta_m| \leq C\beta_t/m$ for all $m \geq 1$.

Proof. This is [31, Lemma 4]. □

Proof of Lemma 4.2.1. We first show the result when ∇U and its derivative are bounded, the general case being then obtained by approximating U .

Hence, suppose for now that ∇U and its derivative are bounded. In this case, it can be shown that the law of the process at time t admits a bounded density f_t such that $(t, z) \mapsto f_t(z) \in C^\infty(\mathbb{R}_+ \times \mathbb{R}^{2d})$, see the proof of Lemma 4.4.2. Define $g_t(z) = f_t(z)e^{\beta_t H(z)}$ and $u(t) = \mathbb{E}(H(Z_t))$. Since f and U are smooth, so is g . Consider

$$N(t) = \int_{\mathbb{R}^{2d}} g_t(z) \ln(1 + g_t(z)) e^{-\beta_t H(z)} dz.$$

From the inequality $\ln(1 + x) \leq \ln(x) + 1/x$ for all $x > 0$,

$$N(t) \leq \int_{\mathbb{R}^{2d}} f_t(z) \ln(f_t(z)) dx dy + \beta_t \mathbb{E}(H(Z_t)) + \int_{\mathbb{R}^{2d}} e^{-\beta_t H(z)} dz.$$

Since f_t is bounded on $[0, T] \times \mathbb{R}^{2d}$, and is in $L^1(dz)$ for all $t \geq 0$, $t \mapsto \int_{\mathbb{R}^{2d}} f_t \ln(f_t)$ is locally bounded and so is $N(t)$. In order to differentiate N , we introduce for $m \geq 1$ the approximation

$$N_m(t) = \int_{\mathbb{R}^{2d}} \eta_m(z) g_t(z) \ln(1 + g_t(z)) e^{-\beta_t H(z)} dz.$$

Integrating by parts, we see that the dual of the generator L_t in $L^2(e^{-\beta_t H})$ is

$$L_t^* = -y \cdot \nabla_x + (-\gamma_t y + \nabla_x U) \cdot \nabla_y + \gamma_t \beta_t^{-1} \Delta_y \quad (4.12)$$

Since f_t solves $\partial_t f_t = L_t^*(f_t e^{\beta_t H}) e^{-\beta_t H}$, g_t solves $\partial_t g_t = \beta_t' H g_t + L_t^* g_t$. Using that η_m is compactly supported for all $m \geq 1$, we can differentiate

$$\begin{aligned} N_m'(t) &= \int_{\mathbb{R}^{2d}} \eta_m \left(-\beta_t' H g_t \ln(1 + g_t) e^{-\beta_t H} + \partial_t g_t \ln(1 + g_t) e^{-\beta_t H} + \frac{g_t}{1 + g_t} \partial_t g_t e^{-\beta_t H} \right) \\ &= \int_{\mathbb{R}^{2d}} \eta_m L_t^* g_t \left(\ln(1 + g_t) + \frac{g_t}{1 + g_t} \right) e^{-\beta_t H} + \int_{\mathbb{R}^{2d}} \eta_m \frac{g_t^2}{1 + g_t} \beta_t' H e^{-\beta_t H}. \end{aligned}$$

Now, using that $g_t \geq 0$,

$$\int_{\mathbb{R}^{2d}} \eta_m \frac{g_t^2}{1 + g_t} \beta_t' H e^{-\beta_t H} \leq \beta_t' \int_{\mathbb{R}^{2d}} f_t H = \beta_t' u(t).$$

Consider the carré du champ operator Γ_t associated to L_t^* given by

$$\Gamma_t(g_1, g_2) := \frac{1}{2} (L_t^*(g_1 g_2) - g_2 L_t^*(g_1) - g_1 L_t^*(g_2)) = \gamma_t \beta_t^{-1} \nabla_y g_1 \cdot \nabla_y g_2 \quad (4.13)$$

for smooth g_1, g_2 , and $\Gamma_t(g) := \Gamma_t(g, g)$. Using that $e^{-\beta_t H}$ is invariant for L_t^* so that

$$\int L_t^* g e^{-\beta_t H} = 0$$

for all smooth g and the diffusion property

$$L_t^*(\phi(g)) = \phi'(g) L_t^*(g) + \phi''(g) \Gamma_t(g)$$

for any smooth ϕ , we get

$$\begin{aligned} & \int_{\mathbb{R}^{2d}} \eta_m L_t^* g_t \left(\ln(1 + g_t) + \frac{g_t}{1 + g_t} \right) e^{-\beta_t H} \\ &= \int_{\mathbb{R}^{2d}} \eta_m L_t^* g_t \left(\ln(1 + g_t) + \frac{g_t}{1 + g_t} \right) e^{-\beta_t H} - \int_{\mathbb{R}^{2d}} L_t^*(\eta_m g_t \ln(1 + g_t)) e^{-\beta_t H} \\ &= - \int_{\mathbb{R}^d \times \mathbb{R}^d} \eta_m \Gamma_t(g_t) \left(\frac{1}{1 + g_t} + \frac{1}{(1 + g_t)^2} \right) e^{-\beta_t H} - \int_{\mathbb{R}^{2d}} L_t^*(\eta_m) g_t \ln(1 + g_t) e^{-\beta_t H} \\ &\quad - 2 \int_{\mathbb{R}^{2d}} \Gamma_t(\eta_m, g_t \ln(1 + g_t)) e^{-\beta_t H}. \end{aligned}$$

The first term is negative (since $\eta_m \Gamma_t(g_t) \geq 0$) and the others are bounded as follows:

$$\begin{aligned} & - \int_{\mathbb{R}^d \times \mathbb{R}^d} L_t^*(\eta_m) g_t \ln(1 + g_t) e^{-\beta_t H} - 2 \int_{\mathbb{R}^d \times \mathbb{R}^d} \Gamma(\eta_m, g_t \ln(1 + g_t)) e^{-\beta_t H} \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^d} \eta_m L_t^*(g_t \ln(1 + g_t)) e^{-\beta_t H} \\ &= \int_{\mathbb{R}^d \times \mathbb{R}^d} L_t(\eta_m) g_t \ln(1 + g_t) e^{-\beta_t H} dx dy \\ &\leq \frac{C \beta_t}{m} N(t) \end{aligned}$$

thanks to Proposition 4.3.1. We conclude that for all $m \geq 1$, $0 \leq s \leq t$:

$$N_m(t) - N_m(s) \leq \int_s^t \beta'_r u(r) + \frac{C \beta_r}{m} N(r) dr.$$

By the monotone convergence theorem, $N_m(t) \rightarrow N(t)$ as $m \rightarrow \infty$, hence :

$$N(t) - N(s) \leq \int_s^t \beta'_r u(r) dr.$$

On the other hand, from the variational formula for the entropy:

$$\int_{\mathbb{R}^{2d}} f_t \ln f_t = \max \left\{ \int_{\mathbb{R}^{2d}} f_t \ln g; g : \mathbb{R}^{2d} \mapsto \mathbb{R}_+, \int_{\mathbb{R}^{2d}} g = 1 \right\},$$

we get with $g_0 = e^{-\alpha_0 H} / \mathcal{Z}_{\alpha_0}$, where $\mathcal{Z}_{\alpha_0} = \int e^{-\alpha_0 H}$,

$$N(t) \geq \beta_t u(t) + \int_{\mathbb{R}^{2d}} f_t \ln f_t \geq \beta_t u(t) + \int_{\mathbb{R}^{2d}} f_t \ln g_0 = (\beta_t - \alpha_0)u(t) - \ln(\mathcal{Z}_{\alpha_0}).$$

As a consequence, writing $\phi(t) = N(t) + \ln(\mathcal{Z}_{\alpha_0})$ for $t \geq 0$,

$$\phi(t) \leq \phi(0) + \int_0^t \frac{\beta'_s}{\beta_s - \alpha_0} \phi(s) ds.$$

Then Gronwall's lemma gives $\phi(t) \leq \phi(0) \frac{\beta_t - \alpha_0}{\beta_0 - \alpha_0}$ and using again that $u(t) \leq \phi(t) / (\beta_t - \alpha_0)$ concludes the proof in the case where ∇U and all its derivatives are bounded.

Let us now consider the general case, without any assumption on ∇U . For n large enough, we fix some $U_n \in \mathcal{C}^\infty(\mathbb{R}^d)$ equal to U on $B(0, n)$, to $|x|$ outside of $B(0, n+1)$ and such that for all $x \in \mathbb{R}^d$, $U_n(x) \geq \min(U(x), |x|) - 1$. Let $(Z_t^n)_{t \geq 0} = (X_t^n, Y_t^n)_{t \geq 0}$ be the diffusion defined by Equation (4.1) where U is replaced by U_n and starting from the same initial distribution f_0 . By design, Z_t and Z_t^n are equal up to the time $\tau_n = \inf\{t \geq 0; |X_t| \geq n\}$. As Z does not explode in finite time, $\lim_n \tau_n = \infty$ and, for all $t \geq 0$, $\lim_n H_n(Z_t^n) = H(Z_t)$ almost surely, where $H_n(x, y) = U_n(x) + |y|^2/2$. By Fatou's lemma, for all $t \geq 0$,

$$\mathbb{E}(H(Z_t)) = \mathbb{E}\left(\liminf_{n \rightarrow \infty} H_n(Z_t^n)\right) \leq \liminf_{n \rightarrow \infty} \mathbb{E}(H_n(Z_t^n)) \leq \liminf_{n \rightarrow \infty} \frac{\kappa^{\beta_0, n}(f_0) + \ln(\mathcal{Z}_{\alpha_0}^n)}{\beta_0 - \alpha_0}$$

where $\kappa^{\beta_0, n}(f_0)$ is define as $\kappa^{\beta_0, n}(f_0)$ but with U replaced by U_n . Now, since f_0 is compactly supported, $\kappa^{\beta_0, n}(f_0)$ is independent of n for n large enough. Finally, using that $e^{-\beta_0 U_n(x)} \leq e^{\alpha_0}(e^{-\alpha_0 U(x)} + e^{-\alpha_0 |x|})$, we can apply the Dominated Convergence Theorem to get that $\mathcal{Z}_{\alpha_0}^n \rightarrow \mathcal{Z}_{\alpha_0}$ as $n \rightarrow \infty$, which concludes. □

4.3.2 Small time regularisation

Proof of Lemma 4.2.2. It is enough to show the first point for ∇U bounded. Indeed, for all \tilde{U} equal to U on $\{U \leq A+1\}$, and $(\tilde{Z})_{t \geq 0}$ the corresponding process, we have the equality

$$\left\{ \sup_{t \leq t^*} H(Z_t) \leq A+1 \right\} = \left\{ \sup_{t \leq t^*} \tilde{H}(\tilde{Z}_t) \leq A+1 \right\}.$$

We only need a bound on $\sup_{t \leq t^*} |Y_t - y_0|$ because :

$$\sup_{t \leq t^*} |U(X_t) - U(x_0)| \leq \|\nabla U\|_\infty t^* \sup_{t \leq t^*} |Y_t|.$$

From

$$Y_t = e^{-\int_0^t \gamma_s ds} \left(y_0 + \int_0^t \nabla U(X_s) e^{\int_0^s \gamma_u du} ds + \int_0^t \sqrt{2\gamma_s \beta_s^{-1}} e^{\int_0^s \gamma_u du} dB_s \right),$$

we get

$$\sup_{s \leq t} |Y_s| \leq |y_0| + \|\nabla U\|_\infty t + \sup_{s \leq t} |W_s|,$$

where $W_t = e^{-\int_0^t \gamma_s ds} \int_0^t \sqrt{2\gamma_s \beta_s^{-1}} e^{\int_0^s \gamma_u du} dB_s$. Since $(W_t)_{0 \leq t \leq 1}$ is a L^2 -martingale, Doob's inequality implies

$$\mathbb{E} \left(\sup_{0 \leq s \leq t} |W_s|^2 \right) \leq 4\mathbb{E}(W_t^2) = 4e^{-2\int_0^t \gamma_s ds} \int_0^t 2\gamma_s \beta_s^{-1} e^{2\int_0^s \gamma_u du} ds \leq 8Lt.$$

Now we can take t_1^* such that $t_1^* \|\nabla U\|_\infty + \sup_{t \leq t_1^*} W_t \leq \frac{1}{8\sqrt{A}}$ with probability larger than $1 - \varepsilon$. Thus, with probability at least $1 - \varepsilon$, we have :

$$\sup_{t \leq t_1^*} |Y_t|^2 \leq |y_0|^2 + \frac{1}{4} + \frac{1}{32A}.$$

Since $A > 1$, this is less than $|y_0|^2 + \frac{1}{2}$ and we write $t_2^* = t_1^* \wedge (2\|\nabla U\|_\infty \sqrt{1 + |y_0|^2})^{-1}$.

For the second point, fix some $t^* \leq t_2^*$ and let, for $t \leq t^*$, (\bar{X}_t, \bar{Y}_t) be the solution of the system

$$\begin{cases} d\bar{X}_t = \bar{Y}_t dt \\ d\bar{Y}_t = \sqrt{2\gamma_t \beta_t^{-1}} dB_t \\ (\bar{X}_0, \bar{Y}_0) = (x_0, y_0), \end{cases}$$

let

$$N_t = - \int_0^t \frac{\sqrt{\beta_s}}{\sqrt{2\gamma_s}} (\nabla U(\bar{X}_s) + \gamma_s \bar{Y}_s) dB_s$$

and $\mathbb{Q} = e^{N_{t^*} - \frac{1}{2}\langle N \rangle_{t^*}} \mathbb{P}$. Ito's formula gives for $t \leq t^*$:

$$\begin{aligned} & \frac{\beta_t}{2\gamma_t} \bar{Y}_t \cdot (\nabla U(\bar{X}_t) + \gamma_t \bar{Y}_t) - \frac{\beta_0}{2\gamma_0} y_0 \cdot (\nabla U(x_0) + \gamma_0 y_0) \\ &= -N_t + \int_0^t \left(\frac{\beta_s}{2\gamma_s} \Delta U(\bar{X}_s) |\bar{Y}_s|^2 + \frac{\beta'_s}{2\gamma_s} \bar{Y}_s \cdot (\nabla U(\bar{X}_s) + \gamma_s \bar{Y}_s) - \frac{\beta_s \gamma'_s}{2\gamma_s^2} \bar{Y}_s \cdot \nabla U(\bar{X}_s) + \frac{\beta_s}{4} \right) ds. \end{aligned} \quad (4.14)$$

Using $\beta' \leq c$ and $\beta_t \leq \beta_0 + \frac{t^*}{c}$, we then get $\mathbb{1}_{\mathcal{B}} N_t \leq C(\beta_0 + 1)$ where C is independent from β_0 and γ and depends only on $\sup_{\{U \leq A+1\}} |\nabla U|$, $\sup_{\{U \leq A+1\}} |\Delta U|$, κ and c .

Girsanov's theorem yields that, under the change of probability $\mathbb{P} \rightarrow \mathbb{Q}$, $(\bar{X}_t, \bar{Y}_t)_{t \leq t^*}$ is a solution to the original Equation (4.1) and, for all $\phi \geq 0$, $t \leq t^*$,

$$\mathbb{E}(\phi(X_t, Y_t) \mathbb{1}_{\mathcal{B}}) = \mathbb{E}(e^{N_{t^*} - \frac{1}{2}\langle N \rangle_{t^*}} \phi(\bar{X}_t, \bar{Y}_t) \mathbb{1}_{\mathcal{B}}) \leq C e^{C_A(\beta_0 + 1)} \mathbb{E}(\phi(\bar{X}_t, \bar{Y}_t) \mathbb{1}_{\mathcal{B}}).$$

It only remains to show that (\bar{X}_t, \bar{Y}_t) has a density bounded by some $e^{C\beta_0}$. As a Gaussian process, the density of (\bar{X}_t, \bar{Y}_t) is bounded by $(2\pi)^{-d/2} / \det(Q_d)$ where Q_d is the covariance matrix of the process at time t^* . By independence, $\det(Q_d) = (\det(Q_1))^d$, and a straightforward computation yields

$$\det(Q_1) = 8 \int_0^{t^*} \gamma_s \beta_s^{-1} ds \int_0^{t^*} (t^* - s) \int_0^s \gamma_u \beta_u^{-1} du ds - 4 \left(\int_0^{t^*} \int_0^s \gamma_u \beta_u^{-1} du ds \right)^2.$$

Now, let $\varpi, \lambda > 1$ be such that $\varpi \lambda^2 < 4/3$ and take t^* small enough (depending only on c and

κ) so that uniformly in $\beta_0 \geq 1$

$$\beta_0 \leq \beta_{t^*} \leq \varpi \beta_0 \quad \text{and} \quad \lambda^{-1} \gamma_0 \leq \gamma_{t^*} \leq \lambda \gamma_0.$$

This choice ensures

$$\det(Q_1) \geq \kappa \beta_0^{-1} t^{*4} \left(\frac{4}{3\varpi\lambda} - \lambda^2 \right)$$

and thus the result. \square

Proof of Lemma 4.2.8. The first part follows from the controllability of the process, see [137, proposition 5]. The second part follows from the fact the distribution of the process killed when it leaves $C(\tilde{x}, c+\delta) \times \mathbb{R}^d$ solves a parabolic hypoelliptic Dirichlet problem, hence has a continuous positive density. In fact, in the time-homogeneous case, this is exactly [109, Theorem 2.20]. In our time-inhomogeneous case, we can proceed as follows. First, for some $A' > \max(|y_0|, A)$ large enough, consider \mathcal{D} the interior of $C(\tilde{x}, c+\delta) \times [-A', A']$ and $\tau = \inf\{s \geq 0, Z_t \notin \mathcal{D}\}$. Then, for all $t > 0$,

$$\mathbb{P}_{z_0}(\mathcal{B}_t, Z_t \in \cdot) \geq \mathbb{P}_{z_0}(\tau > t, Z_t \in \cdot) := p_t^{\mathcal{D}}(z_0, \cdot).$$

It is well-known that $p_t^{\mathcal{D}}$ solves a parabolic equation with generator L_t on \mathcal{D} . Since L_t is hypoelliptic, $p_t^{\mathcal{D}}(z_0, \cdot)$ has a continuous density. Finally, the coefficients of L_t being smooth and bounded on \mathcal{D} , $p_t^{\mathcal{D}}(z_0, \cdot)$ being not identically zero and the process being controllable, we can use the strong maximum principle of [155, Theorem 6.1] to deduce that $p_t^{\mathcal{D}}(z_0, \cdot)$ cannot take the value 0 in \mathcal{D} . As a continuous positive function, $p_t^{\mathcal{D}}(z_0, \cdot)$ is thus lower bounded by a positive constant over any compact subset of \mathcal{D} , which concludes. \square

4.4 L^2 -hypoercivity

In this section we use the definitions and notations of Section 4.2.2

The hypoercivity issue arises in the proof of Proposition 4.2.3 when computing the evolution of the L^2 -norm of h_t^K . In the standard elliptic case, as in [83], one would simply differentiate this quantity and concludes with a Poincaré inequality of the form :

$$\int \left(h - \int h d\mu \right)^2 d\mu \leq C \int \Gamma(h) d\mu$$

where Γ is the carré du champ associated to the process. However, in the kinetic case, as we saw in (4.13), $\Gamma_t(f) = \gamma_t \beta_t^{-1} |\nabla_y f|^2$, which means such an inequality cannot hold since, for non-constant functions of x , the left hand side is positive while the right hand side vanishes. For this reason, we work with a modified norm as in [163].

More precisely, at a formal level, the proof of Proposition 4.2.3 is the following: writing $\phi_t(h) = |(\nabla_x + \nabla_y)h|^2 + \sigma_t h^2$ with $\sigma_t = \frac{1}{2} + 2\sqrt{\gamma_t^{-1} \beta_t (1 + \|\nabla U^K\|_\infty + \gamma_t)^2}$, we introduce

$$\tilde{N}(t) = \int_{M_K \times \mathbb{R}^d} \phi_t(h_t^K - 1) d\mu_{\beta_t}^K, \quad \tilde{I}(t) = \int_{M_K \times \mathbb{R}^d} |\nabla h_t^K|^2 d\mu_{\beta_t}^K.$$

Differentiating \tilde{N} , one can (formally) check that

$$\tilde{N}'(t) \leq -\frac{1}{2} \tilde{I}(t) + C \beta_t'(1 + \beta_t) \tilde{N}(t)$$

for some constant $C > 0$, the definition of \tilde{N} being motivated by the $-\tilde{I}$ term in this inequality. Using a Poincaré inequality for $\mu_{\beta_t}^K$ (with the full gradient rather than Γ_t) with a constant $\lambda(\beta_t)$ that scales as $1/t^{c^*/c} \gg \beta_t' \beta_t$, we get that $\tilde{N}'(t) \leq 0$ for t large enough (or equivalently for all $t \geq 0$ if β_0 is large enough), hence \tilde{N} is bounded. We conclude the proof of Proposition 4.2.3 by bounding

$$\|h_t\|_{L^2(\mu_{\beta_t})} \leq 1 + \|h_t - 1\|_{L^2(\mu_{\beta_t})} \leq 1 + 2\tilde{N}(t).$$

In the remainder of this section, this formal proof is made rigorous and we give the details of the computations.

Remark 4.4.1. *The proof of [137] is based on a similar argument but, as mentioned in the introduction, and as noticed by the authors of [31], it contains an error. The problem occurs when it comes to justify rigorously the derivation of \tilde{N} . In [137], a compactly-supported truncation function is added within the integral. This leads to additional terms in $\partial_t \tilde{N}$. One of these terms is said to be non-positive in [137, Lemma 16], which is false (there is a sign error). In [31], the authors add a small elliptic term to the dynamics, use elliptic regularity results to justify the computation and then let the small ellipticity parameter vanish afterwards. In this section, we make a correct version of the argument of [137], combining some bounds on the density of the process (Lemma 4.4.2 below) and some moment estimates (Lemma 4.4.1 below). Also, notice that, by comparison with [137, 31], we have already reduced the problem to a compact state space for the position x , the non-compact part of the dynamics only concerns the velocity.*

First, we need a few preliminary lemmas. We start by stating the following Poincaré inequality (with the full gradient) :

Proposition 4.4.1. *For $U^K \in C^\infty(M_K, \mathbb{R})$ there exists $\lambda : \mathbb{R}_+ \rightarrow \mathbb{R}_+$ such that for all $f \in C^\infty(M_K \times \mathbb{R}^d)$ with compact support :*

$$\lambda(\beta) \int_{M_K \times \mathbb{R}^d} \left(f - \int_{M_K \times \mathbb{R}^d} f d\mu_\beta^K \right)^2 d\mu_\beta^K \leq \int_{M_K \times \mathbb{R}^d} |\nabla f|^2 d\mu_\beta^K,$$

and moreover

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(\lambda(\beta)) = -c^*(U^K)$$

where $c^*(U^K)$ is defined as c^* with U replaced by U^K .

Proof. The fact that the Gibbs probability measure $\tilde{\mathcal{Z}}e^{-\beta U^K}$ satisfies a Poincaré inequality with a constant $\lambda(\beta)$ satisfying

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(\lambda(\beta)) = -c^*(U^K)$$

corresponds to [83, Theorem 1.14]. The Gaussian measure $\mathcal{N}(0, \beta I)$ also satisfies a Poincaré inequality with constant β , and we conclude with the tensorization property of the Poincaré inequality, see [6, Proposition 4.3.1]. \square

For μ a probability measure, $H^1(\mu)$ denotes the usual Sobolev space of functions in $L^2(\mu)$ with derivative in $L^2(\mu)$.

Proposition 4.4.2. *There exists $C > 0$ such that for all $\beta > 1$ and $g \in H^1(\mu_\beta^K)$,*

$$\int y^2 g(x, y)^2 \mu_\beta^K(dx dy) \leq C \left(\int g(x, y)^2 \mu_\beta^K(dx dy) + \int |\nabla_y g(x, y)|^2 \mu_\beta^K(dx dy) \right).$$

Proof. This is a particular case of [163, Lemma A.18]. We give a short proof for completeness. Notice that $ye^{-\beta|y|^2/2} = -\beta^{-1}\nabla e^{-\beta|y|^2/2}$. Hence an integration by parts and Young's inequality yield, for any x ,

$$\begin{aligned} & \int_{\mathbb{R}^d} y^2 g^2(x, y) e^{-\beta|y|^2/2} dy \\ &= -\beta^{-1} \int_{\mathbb{R}^d} g^2(x, y) y \cdot \nabla e^{-\beta|y|^2/2} dy \\ &= \beta^{-1} \int_{\mathbb{R}^d} \nabla \cdot (g^2(x, y) y) e^{-\beta|y|^2/2} dy \\ &= d\beta^{-1} \int_{\mathbb{R}^d} g^2(x, y) e^{-\beta|y|^2/2} dy + \beta^{-1} \int_{\mathbb{R}^d} 2g \nabla g(x, y) \cdot y e^{-\beta|y|^2/2} dy \\ &\leq d\beta^{-1} \int_{\mathbb{R}^d} g^2(x, y) e^{-\beta|y|^2/2} dy + \beta^{-2} \int_{\mathbb{R}^d} 2|\nabla g(x, y)|^2 e^{-\beta|y|^2/2} dy \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^d} y^2 g^2(x, y) e^{-\beta|y|^2/2} dy, \end{aligned}$$

and thus

$$\int_{\mathbb{R}^d} y^2 g^2(x, y) e^{-\beta|y|^2/2} dy \leq 2d\beta^{-1} \int_{\mathbb{R}^d} g^2(x, y) e^{-\beta|y|^2/2} dy + 4\beta^{-2} \int_{\mathbb{R}^d} |\nabla g(x, y)|^2 e^{-\beta|y|^2/2} dy.$$

Conclusion follows by integrating with respect to x . \square

The next two lemmas will be used in forthcoming computations to justify that some quantities are finite and therefore allowing to interchange differentiation and integration.

Lemma 4.4.1. *Fix some $K > 0$ and any $c > 0$. Then for all $\alpha > 0$ and initial condition $f_0^K \in C^\infty$ with compact support, there exists $b_{\alpha, K}$ such that if $\beta_0 \geq b_{\alpha, K}$, then*

$$t \mapsto \mathbb{E}_{f_0^K} \left(e^{(\beta_t - \alpha)H_K(Z_t^K)} \right)$$

is finite and locally bounded.

Proof. Write $\tau_N = \inf \{t \geq 0, H_K(Z_t^K) \geq N\}$ and $\phi_t(x, y) = e^{(\beta_t - \alpha)H_K(x, y)}$. For $\beta_0 > \alpha$, we compute for $t \in [0, T]$:

$$\begin{aligned} & \partial_t \phi_t + L_t \phi_t \\ &= \left(\beta_t' H_K + (\beta_t - \alpha) y \cdot \nabla U^K - \gamma_t (\beta_t - \alpha) y \cdot \nabla_y H_K \right. \\ &\quad \left. + \beta_t^{-1} \gamma_t \left((\beta_t - \alpha) \Delta_y H_K + (\beta_t - \alpha)^2 |\nabla_y H_K|^2 \right) \right) \phi_t \\ &\leq \left(\beta_t' \left(\|U^K\|_\infty + \frac{y^2}{2} \right) + (\beta_t - \alpha)^3 \|\nabla U^K\|_\infty + \frac{y^2}{\beta_t - \alpha} - \gamma_t (\beta_t - \alpha) y^2 \right. \\ &\quad \left. + \beta_t^{-1} \gamma_t \left(d(\beta_t - \alpha) + (\beta_t - \alpha)^2 y^2 \right) \right) \phi_t \\ &\leq \left(\beta_0' \|U^K\|_\infty + (\beta_T - \alpha)^3 \|\nabla U^K\|_\infty + Ld(\beta_T - \alpha) + \left(\frac{\beta_t'}{2} + \frac{1}{\beta_t - \alpha} - \frac{\gamma_t \alpha (\beta_t - \alpha)}{\beta_t} \right) y^2 \right) \phi_t. \end{aligned}$$

We can choose β_0 great enough so that $\frac{\beta'_t}{2} + \frac{1}{\beta_t - \alpha} - \frac{\gamma_t \alpha (\beta_t - \alpha)}{\beta_t} \leq 0$ for all $t \geq 0$. We then classically get for $t \in [0, T]$:

$$\mathbb{E} (\phi_{t \wedge \tau_N} (Z_{t \wedge \tau_N}^K)) \leq e^{C_T t} \mathbb{E} (\phi_0 (X_0, Y_0))$$

where $C_T = \beta'_0 \|U^K\|_\infty + (\beta_T - \alpha)^3 \|\nabla U^K\|_\infty + Ld(\beta_T - \alpha)$. The fact that f_0^K has a compact support and Fatou's lemma then yield the result. \square

Lemma 4.4.2. *Fix $K, c > 0$. Then there exists b_K such that if $\beta_0 \geq b_K$, the law f_t^K of the process defined by the Equation (4.7), with an initial condition $f_0^K \in \mathcal{C}^\infty$ with compact support, is smooth, bounded along with its derivative, and satisfies :*

$$\exists \alpha > 0, \forall t \geq 0, \exists C_t \text{ such that } f_t^K + |\nabla f_t^K| \leq C_t e^{-\alpha|y|^2}$$

and $t \mapsto C_t$ is locally bounded.

Proof. First, by Ito's formula, $f_t^K(x, y)$ is a weak measure solution of the forward equation

$$\begin{aligned} \partial_t f_t^K &= -y \cdot \nabla_x f_t^K + \nabla U^K(x) \cdot \nabla_y f_t^K + \gamma_t \nabla_v \cdot (v f_t^K) + \gamma_t \beta_t^{-1} \Delta_v f_t^K \\ &= \tilde{L}_t f_t^K + d\gamma_t f_t^K, \end{aligned} \quad (4.15)$$

where \tilde{L}_t is the generator of the process (\tilde{X}, \tilde{Y}) solving

$$d\tilde{X}_t = -\tilde{Y}_t dt, \quad d\tilde{Y}_t = \nabla U^K(\tilde{X}_t) dt + \gamma_t \tilde{Y}_t dt + \sqrt{2\gamma_t \beta_t^{-1}} dB_t.$$

Using again Ito's formula, we get that the function given by

$$(x, y, t) \mapsto e^{d \int_0^t \gamma_s ds} \mathbb{E}_{x, y} \left(f_0^K \left(\tilde{X}_t, \tilde{Y}_t \right) \right),$$

also solves equation (4.15). Uniqueness of the weak solution of (4.15) is ensured by [18, Theorem 9.8.7], hence

$$f_t^K(x, y) = e^{d \int_0^t \gamma_s ds} \mathbb{E}_{x, y} \left(f_0^K \left(\tilde{X}_t, \tilde{Y}_t \right) \right),$$

from which we immediately get that f_t^K is bounded uniformly over $[0, T]$ for all $T > 0$. Thanks to [85, Theorem 1], f_t^K is smooth for all $t \geq 0$. We can always differentiate (4.15) in a weak sense (i.e. once integrated with respect to a smooth compactly supported function of time and space and formally integrating by parts), from which we get that ∇f_t^K is a weak solution of

$$\partial_t \nabla f_t^K = \tilde{L}_t \nabla f_t^K + J_t \nabla f_t^K,$$

where \tilde{L}_t acts component-wise on ∇f_t^K and

$$J_t(x, y) = \begin{pmatrix} d\gamma_t I_d & \nabla^2 U^K(x) \\ -I_d & 2d\gamma_t I_d \end{pmatrix},$$

which is bounded uniformly over $[0, T]$ for all $T > 0$. For a fixed $T > 0$, considering $(W_t)_{t \geq 0}$ the matrix-valued process solution of $dW_t = W_t J_{T-t}(\tilde{X}_t, \tilde{Y}_t)$ with $W_0 = I_d$ and using again the uniqueness of the weak solution of the PDE, we get the Feynman-Kac representation

$$\nabla f_t^K(x, y) = \mathbb{E}_{x, y} \left(W_t \nabla f_0^K(\tilde{X}_t, \tilde{Y}_t) \right),$$

which can be obtained by Itô's formula for the process $(\tilde{X}_t, \tilde{Y}_t, W_t)_{t \geq 0}$ applied to the test function

$h(x, y, w, t) = w \nabla f_t^K(x, y)$. Hence, ∇f_t^K is uniformly bounded over $[0, T]$, and the same argument applies to all derivatives of f_t^K .

Now, let us prove the Gaussian bound of the statement, starting with f_t^K .

For $z \in \mathbb{R}^{2d}$, let $\epsilon(z) = \min(1, \frac{f_t^K(z)}{2\|\nabla f_t^K\|_\infty})$. If $z' \in B(z, \epsilon(z))$, $f_t^K(z') \geq f_t^K(z) - \|\nabla f_t^K\|_\infty \epsilon(z) \geq \frac{f_t^K(z)}{2}$. Then for any $z = (x_1, y_1) \in \mathbb{R}^{2d}$:

$$\begin{aligned} \mathbb{E}(e^{H_K(Z_t^K)/2}) &= \int_{\mathbb{R}^d \times \mathbb{R}^d} e^{H_K(x,y)/2} f_t^K(x, y) dx dy \\ &\geq \int_{B(z, \epsilon(z))} e^{H_K(x,y)/2} f_t^K(x, y) dx dy \\ &\geq e^{-\frac{\|U\|_\infty}{2}} e^{\frac{|y_1|^2-1}{4}} \frac{f_t^K(z)}{2} \omega_{2d} \epsilon(z)^d \end{aligned}$$

where ω_{2d} is the volume of the unit-sphere in dimension $2d$. Then there are two possibilities. If $f_t^K(x, y) \geq 2\|\nabla f_t^K\|_\infty$, then

$$f_t^K(x, y) \leq \left(2e^{\frac{1}{4}} e^{\frac{\|U\|_\infty}{2}} \frac{\mathbb{E}(e^{H_K(Z_t^K)/2})}{\omega_{2d}} \right) e^{-\frac{y^2}{4}}.$$

Otherwise, $f_t^K(x, y) \leq 2\|\nabla f_t^K\|_\infty$ and

$$f_t^K(x, y) \leq 2\|\nabla f_t^K\|_\infty^{\frac{d}{d+1}} \left(e^{\frac{1}{4}} e^{\frac{\|U\|_\infty}{2}} \frac{\mathbb{E}(e^{H_K(Z_t^K)/2})}{\omega_{2d}} \right)^{\frac{1}{d+1}} e^{-\frac{y^2}{4(d+1)}}.$$

In any case, using the fact that $t \mapsto \mathbb{E}(e^{H_K(Z_t^K)/2})$ is locally bounded for β_0 great enough, we have the result for f_t^K with $\alpha = \frac{1}{4(d+1)}$. Recall the definition of the approximation functions η_m from Proposition 4.3.1. We use them here with U replaced by U^K (or equivalently with H replaced by H_K), but it doesn't change any of their properties since now x is in a compact set. We now turn to ∇f_t^K by using the approximation functions η_m from Section 4.3.1 and integrating by parts:

$$\begin{aligned} \int_{\mathbb{R}^d \times \mathbb{R}^d} \eta_m e^{\frac{H_K}{4}} |\nabla f_t^K|^2 dz &= - \int_{\mathbb{R}^d \times \mathbb{R}^d} \nabla \left(\eta_m e^{\frac{H_K}{4}} \nabla f_t^K \right) f_t^K dz \\ &= - \int_{\mathbb{R}^d \times \mathbb{R}^d} \left(\nabla_y \eta_m \cdot \nabla f_t^K e^{\frac{H_K}{4}} + \frac{\eta_m}{2} e^{\frac{H_K}{4}} \nabla H_K \cdot \nabla f_t^K + \eta_m e^{\frac{H_K}{4}} \Delta f_t^K \right) f_t^K dz \\ &\leq C \int_{\mathbb{R}^d \times \mathbb{R}^d} e^{\frac{H_K}{2}} f_t^K dz = C \mathbb{E} \left(e^{H_K(Z_t^K)/2} \right) \end{aligned}$$

for some constant $C > 0$ independent from m , where we used uniform bounds on the two first derivatives of f_t^K . We can then conclude in the same way as for f_t^K . \square

Setting $\phi_{\beta, \gamma}(h) = |(\nabla_x + \nabla_y)h|^2 + \sigma(\beta, \gamma)h^2$ with $\sigma(\beta, \gamma) = \frac{1}{2} + 2\sqrt{\gamma^{-1}\beta}(1 + \|\nabla U^K\|_\infty + \gamma)^2$, we consider the modified H^1 -norm (and its truncated version for $m \geq 1$):

$$N(t, \beta, \gamma) = \int_{M_K \times \mathbb{R}^d} \phi_{\beta, \gamma} \left(\frac{f_t^K}{\mu_\beta^K} \right) d\mu_\beta^K$$

$$N_m(t, \beta, \gamma) = \int_{M_K \times \mathbb{R}^d} \eta_m \phi_{\beta, \gamma} \left(\frac{f_t^K}{\mu_\beta^K} \right) d\mu_\beta^K$$

as well as

$$I(t, \beta) = \int_{M_K \times \mathbb{R}^d} \left| \nabla \frac{f_t^K}{\mu_\beta^K} \right|^2 d\mu_\beta^K$$

$$I_m(t, \beta) = \int_{M_K \times \mathbb{R}^d} \eta_m \left| \nabla \frac{f_t^K}{\mu_\beta^K} \right|^2 d\mu_\beta^K$$

To study those functionals along the dynamic, write $\tilde{H}_m(t) = H_m(t, \beta_t, \gamma_t)$, $\tilde{H}(t) = H(t, \beta_t, \gamma_t)$, $\tilde{I}_m(t) = I_m(t, \beta_t)$ and $\tilde{I}(t) = I(t, \beta_t)$.

The main technical tool that we will need in order to study the evolution of those functionals will be, given $\phi : \mathcal{C}^\infty \mapsto \mathcal{C}^\infty$, quantities of the form :

$$\Gamma_{\phi, L}(h) = L(\phi(h)) - D_h(\phi)(h)L(h), \quad (4.16)$$

where $D_h(\phi)$ is the pointwise differential of ϕ , see [135]. The reason is that for regular enough h , by writing $L_{\beta, \gamma}^K$ the generator (4.6) on M_K with fixed β and γ , we have

$$\partial_t \int_{M_K \times \mathbb{R}^d} \phi \left(e^{tL_{\beta, \gamma}^K} h \right) d\mu_\beta^K = - \int_{M_K \times \mathbb{R}^d} \Gamma_{\phi, L_{\beta, \gamma}^K} \left(e^{tL_{\beta, \gamma}^K} h \right) d\mu_\beta^K.$$

This kind of quantities has been studied in [135], where the author showed among other things :

Lemma 4.4.3. *Let $\phi(h) = |(\nabla_x + \nabla_y)h|^2 + \sigma h^2$ where $\sigma = \frac{1}{2} + \sqrt{\gamma\beta^{-1}}(1 + \|\nabla U\|_\infty + \gamma)^2$. Then, for all $\beta > 0$, $\gamma > 0$, $h \in \mathcal{C}^\infty$:*

$$\Gamma_{\phi, L_{\beta, \gamma}^{K,*}}(h) \geq \frac{1}{2} |\nabla h|^2 + \Gamma((\nabla_x + \nabla_y)h),$$

where $\Gamma((\nabla_x + \nabla_y)h) = \sum_{i=0}^d \Gamma((\partial_{x_i} + \partial_{y_i})h) = \sum_{i=0}^d \gamma_t \beta_t^{-1} |\nabla_y(\partial_{x_i} + \partial_{y_i})h|^2$.

Proof. This is [135, Example 3]. Let us simply recall the key idea (to alleviate notations we omit the generator in the subscript of Γ). First, Γ is linear in ϕ , hence for ϕ as defined above:

$$\Gamma_\phi = \sigma\Gamma + \Gamma_{|(\nabla_x + \nabla_y)\cdot|^2},$$

where Γ is the classical "carré du champs" $\Gamma(h) = \gamma_t \beta_t^{-1} |\nabla_y h|^2$. We then have the following equality:

$$\Gamma_{|(\nabla_x + \nabla_y)\cdot|^2}(h) = \Gamma((\nabla_x + \nabla_y)h) + (\nabla_x + \nabla_y)h \cdot [L, \nabla_x + \nabla_y]h,$$

where the brackets denotes the commutators of two operators. An elementary computation concludes. \square

Proof of Proposition 4.2.3. First, β_0 must be great enough so that we can apply all previous lemmas of Section 4.4. Let's first justify why \tilde{N}_m , \tilde{N} , \tilde{I}_m and \tilde{I} are finite. They are all finite at time 0 because f_0 has compact support. For $m \in \mathbb{N}$, \tilde{N}_m and \tilde{I}_m are finite for all times as integrals of continuous functions with compact support.

Write $\nabla_t^* = -\nabla + \beta_t \nabla H_K$ the dual of the gradient operator ∇ in $L^2(\mu_{\beta_t}^K)$. Integrating by

parts,

$$\begin{aligned}
\tilde{I}_m &= \int_{M_K \times \mathbb{R}^d} \eta_m \left| \nabla \frac{f_t^K}{\mu_{\beta_t}^K} \right|^2 d\mu_{\beta_t}^K \\
&= \int_{M_K \times \mathbb{R}^d} \nabla_t^* \left(\nabla \eta_m \nabla \frac{f_t^K}{\mu_{\beta_t}^K} \right) f_t^K dz \\
&\leq \int_{M_K \times \mathbb{R}^d} C_t e^{(\beta_t - \alpha) H_K(z)} f_t^K(z) dz = C_t \mathbb{E} \left(e^{(\beta_t - \alpha) H_K(Z_t^K)} \right)
\end{aligned}$$

for some $\alpha > 0$ and $C_t > 0$ locally bounded and independent from m , using Lemma 4.4.2 and that the derivatives of f_t^K are bounded. Lemma 4.4.1 and the monotonous convergence of \tilde{I}_m towards \tilde{I} then implies that \tilde{I} is locally bounded. We conclude that \tilde{N} is also locally bounded thanks to the Poincaré inequality of Proposition 4.4.1. As in (4.12), we have that the dual in $L^2(\mu_{\beta}^K)$ of the generator L_t is

$$L_t^* = -y \cdot \nabla_x + (-\gamma_t y + \nabla_x U^K) \cdot \nabla_y + \gamma_t \beta_t^{-1} \Delta_y$$

and that f_t^K solves $\partial_t f_t^K = L_t^*(f_t^K e^{\beta_t H_K}) e^{-\beta_t H_K}$. With the regularity result from Lemma 4.4.2, and the compactly supported approximation functions η_m , one can differentiate N_m and I_m to get for all m :

$$\begin{aligned}
(\partial_t N_m)(t, \beta_t, \gamma_t) &= \int_{M_K \times \mathbb{R}^d} \eta_m D_h \phi_{\beta_t, \gamma_t}(h_t^K) \frac{\partial_t f_t^K}{\mu_{\beta_t}^K} d\mu_{\beta_t}^K \\
&= \int_{M_K \times \mathbb{R}^d} \eta_m D_h \phi_{\beta_t, \gamma_t}(h_t^K) L_t^*(h_t^K) d\mu_{\beta_t}^K - \int_{M_K \times \mathbb{R}^d} L_t^*(\eta_m \phi_{\beta_t, \gamma_t}(h_t^K)) d\mu_{\beta_t}^K \\
&= - \int_{M_K \times \mathbb{R}^d} \eta_m \Gamma_{\phi_{\beta_t, \gamma_t}}(h_t^K) d\mu_{\beta_t}^K - \int_{M_K \times \mathbb{R}^d} L_t^*(\eta_m) \phi_{\beta_t, \gamma_t}(h_t^K) d\mu_{\beta_t}^K \\
&\quad - 2 \int_{M_K \times \mathbb{R}^d} \Gamma_t(\eta_m, \phi_{\beta_t, \gamma_t}(h_t^K)) d\mu_{\beta_t}^K.
\end{aligned}$$

From Lemma 4.4.3, we get $\Gamma_{\phi_{\beta, \gamma}}(h) \geq \frac{1}{2} |\nabla h|^2 + \Gamma_t((\nabla_x + \nabla_y)h)$, and since

$$\begin{aligned}
&\int_{M_K \times \mathbb{R}^d} \Gamma_t(\eta_m, \phi_{\beta_t, \gamma_t}(h_t^K)) d\mu_{\beta_t}^K \\
&= -\frac{1}{2} \int_{M_K \times \mathbb{R}^d} (\eta_m L_t^* \phi_{\beta_t, \gamma_t}(h_t^K) + L_t^* \eta_m \phi_{\beta_t, \gamma_t}(h_t^K)) d\mu_{\beta_t}^K \\
&= -\frac{1}{2} \int_{M_K \times \mathbb{R}^d} (L_t + L_t^*)(\eta_m) \phi_{\beta_t, \gamma_t}(h_t^K) d\mu_{\beta_t}^K
\end{aligned}$$

and $L_t \eta_m \leq \frac{C \beta_t}{m}$, we get :

$$\begin{aligned}
(\partial_t N_m)(t, \beta_t, \gamma_t) &\leq -\frac{1}{2} \int_{M_K \times \mathbb{R}^d} \eta_m |\nabla h_t^K|^2 d\mu_{\beta_t}^K - \int_{M_K \times \mathbb{R}^d} \Gamma_t((\nabla_x + \nabla_y)h_t^K) d\mu_{\beta_t}^K \\
&\quad + \int_{M_K \times \mathbb{R}^d} L_t(\eta_m) \phi_{\beta_t, \gamma_t}(h_t^K) d\mu_{\beta_t}^K
\end{aligned}$$

$$\begin{aligned} &\leq -\frac{1}{2} \int_{M_K \times \mathbb{R}^d} \eta_m |\nabla h_t^K|^2 d\mu_{\beta_t}^K - \int_{M_K \times \mathbb{R}^d} \Gamma_t ((\nabla_x + \nabla_y) h_t^K) d\mu_{\beta_t}^K \\ &\quad + \frac{C\beta_t}{m} \int_{M_K \times \mathbb{R}^d} \phi_{\beta_t, \gamma_t}(h_t^K) d\mu_{\beta_t}^K. \end{aligned}$$

Now we look at the derivative in β , knowing that $\partial_\beta Z \leq 0$ by writing :

$$N_m(t, \beta, \gamma) = \int_{M_K \times \mathbb{R}^d} \left(\eta_m \left| (\nabla_x + \nabla_y) \ln \left(\frac{f_t^K}{\mu_\beta^K} \right) \right|^2 \frac{f_t^K}{\mu_\beta^K} + \eta_m \sigma(\beta, \gamma) \frac{f_t^K}{\mu_\beta^K} \right) df_t^K.$$

This gives

$$\begin{aligned} &(\partial_\beta N_m)(t, \beta_t, \gamma_t) \\ &\leq \partial_\beta \sigma(\beta_t, \gamma_t) \int_{M_K \times \mathbb{R}^d} \eta_m (h_t^K)^2 d\mu_{\beta_t}^K + \sigma(\beta_t) \int_{M_K \times \mathbb{R}^d} \eta_m (U^K(x) + \frac{y^2}{2}) (h_t^K)^2 d\mu_{\beta_t}^K \\ &\quad + \int_{M_K \times \mathbb{R}^d} \eta_m (U^K(x) + \frac{y^2}{2}) |(\nabla_x + \nabla_y) h_t^K|^2 d\mu_{\beta_t}^K \\ &\quad + \int_{M_K \times \mathbb{R}^d} 2\eta_m (\nabla_x + \nabla_y) \ln(h_t^K) \cdot (\nabla_x + \nabla_y) \partial_\beta (-\ln(\mu_{\beta_t}^K)) h_t^K df_t^K. \end{aligned}$$

We now have to treat all those terms. We will use that $N_m \leq N$. First, since U^K is bounded,

$$\partial_\beta \sigma(\beta_t, \gamma_t) \int_{M_K \times \mathbb{R}^d} \eta_m (h_t^K)^2 d\mu_{\beta_t}^K + \sigma(\beta_t) \int_{M_K \times \mathbb{R}^d} \eta_m U^K(x) (h_t^K)^2 d\mu_{\beta_t}^K \leq C(1 + \beta_t^2) \tilde{N}$$

for some $C > 0$ (in the rest of the proof we denote by C several constants which do not depend on t nor m). From Proposition 4.4.2, applied with $g = h_t^K$, we get :

$$\sigma(\beta_t, \gamma_t) \int_{M_K \times \mathbb{R}^d} \eta_m \frac{y^2}{2} (h_t^K)^2 d\mu_{\beta_t}^K \leq C(1 + \beta_t^2) \tilde{N}.$$

Again, because U^K is bounded :

$$\int_{M_K \times \mathbb{R}^d} U(x) |(\nabla_x + \nabla_y) h_t^K|^2 d\mu_{\beta_t}^K \leq C \tilde{N}.$$

Using again Proposition 4.4.2 we get :

$$\int_{M_K \times \mathbb{R}^d} \eta_m \frac{y^2}{2} |(\nabla_x + \nabla_y) h_t^K|^2 d\mu_{\beta_t}^K \leq C \left(\tilde{N} + \sqrt{\gamma_t^{-1} \beta_t} \int_{M_K \times \mathbb{R}^d} \Gamma_t ((\nabla_x + \nabla_y) h_t^K) d\mu_{\beta_t}^K \right).$$

Finally, using that $a.b \leq \frac{a^2}{2} + \frac{b^2}{2}$ and $-\partial_\beta \ln(\mu_\beta^K) = U^K(x) + \frac{y^2}{2} + \frac{\partial_\beta Z_\beta}{Z_\beta}$, we get :

$$\begin{aligned} &\int_{M_K \times \mathbb{R}^d} \eta_m (\nabla_x + \nabla_y) \ln \left(\frac{f_t^K}{\mu_\beta^K} \right) \cdot (\nabla_x + \nabla_y) \partial_\beta (-\ln(\mu_{\beta_t}^K)) \frac{f_t^K}{\mu_{\beta_t}^K} df_t^K \\ &\leq C \int_{M_K \times \mathbb{R}^d} \eta_m |(\nabla_x + \nabla_y) h_t^K|^2 \left(\frac{f_t^K}{\mu_{\beta_t}^K} \right)^2 d\mu_{\beta_t}^K \end{aligned}$$

$$\begin{aligned}
& + C \int_{M_K \times \mathbb{R}^d} \eta_m |(\nabla_x + \nabla_y)(U(x) + \frac{y^2}{2})|^2 (h_t^K)^2 d\mu_{\beta_t}^K \\
& \leq C \left(N_m + \|\nabla U\|_\infty^2 \int \eta_m (h_t^K)^2 d\mu_{\beta_t}^K + \int y^2 (h_t^K)^2 d\mu_{\beta_t}^K \right)
\end{aligned}$$

and we conclude as the second term. Finally, since γ only appears in the definition of σ , we have :

$$(\partial_\gamma N_m)(t, \beta_t, \gamma_t) = \partial_\gamma \sigma \int_{M_K \times \mathbb{R}^d} \eta_m (h_t^K)^2 d\mu_{\beta_t}^K \leq C \gamma_t \tilde{N}$$

From the previous computation, and from the fact that $\gamma'_t \leq L\beta'_t$, we get :

$$\begin{aligned}
\tilde{N}'_m(t) & = (\partial_t N_m)(t, \beta_t, \gamma_t) + \beta'_t (\partial_\beta N_m)(t, \beta_t, \gamma_t) + \gamma'_t (\partial_\gamma N_m)(t, \beta_t, \gamma_t) \\
& \leq -\frac{1}{2} \tilde{I}_m(t) - \int_{M_K \times \mathbb{R}^d} \eta_m \Gamma_t (Ah_t^K) d\mu_{\beta_t}^K \\
& \quad + C \beta'_t \beta_t \int_{M_K \times \mathbb{R}^d} \Gamma_t (Ah_t^K) d\mu_{\beta_t}^K + \frac{C\beta_t}{m} \tilde{N}_t + C\beta'_t (1 + \beta_t^2) \tilde{N}_t.
\end{aligned}$$

By integration, we get for all $0 \leq s \leq t$:

$$\begin{aligned}
\tilde{N}_m(t) - \tilde{N}_m(s) & \leq \int_s^t \left(-\frac{1}{2} \tilde{I}_m(u) + \frac{C\beta_u}{m} \tilde{N}_u + C\beta'_u (1 + \beta_u^2) \tilde{N}_u \right. \\
& \quad \left. - \int_{M_K \times \mathbb{R}^d} \eta_m \Gamma_t (Ah_t^K) d\mu_{\beta_u}^K + C\beta'_u \beta_u \int_{M_K \times \mathbb{R}^d} \Gamma_t (Ah_t^K) d\mu_{\beta_u}^K \right) du.
\end{aligned}$$

We consider β_0 great enough so that $1 - C\beta'_t \beta_t \geq 0$ for all t . Using monotonous convergence, the fact that $\tilde{I} \geq \tilde{I}_m$, and Fatou's lemma we get :

$$\tilde{N}(t) - \tilde{N}(s) \leq \int_s^t \left(-\frac{1}{2} \tilde{I}(u) + C\beta'_u (1 + \beta_u^2) \tilde{N}_u \right) du.$$

Now, from the Poincaré inequality of Proposition 4.4.1 and the definition of σ ,

$$\tilde{\lambda}(\beta) \tilde{N}(t) \leq \tilde{I}(t)$$

for some $\tilde{\lambda}$ satisfying $\frac{1}{\beta} \ln(\tilde{\lambda}) \rightarrow -c^*$, so that we can find a λ_0 such that

$$\tilde{\lambda}(\beta_t) \geq \lambda_0 e^{-\beta_t \frac{(c+c^*)}{2}} = \frac{\lambda_0}{(e^{c\beta_0} + t)^{1-\alpha}},$$

where $\alpha = (c - c^*)/(2c)$. Taking β_0 large enough so that $C\beta'_t (1 + \beta_t^2) \leq \lambda_0/4(e^{c\beta_0} + t)^{-1+\alpha}$, we have finally obtained that, if $\beta_0 \geq \tilde{b}_K$ for some \tilde{b}_K , then for all $0 \leq s \leq t$

$$\tilde{N}(t) - \tilde{N}(s) \leq \int_s^t \left(-\frac{\lambda_0}{4(e^{c\beta_0} + u)^{1-\alpha}} \tilde{N}(u) \right) du$$

and this concludes (as explained at the beginning of this section). \square

4.5 H^k -hypocoercivity

In all this section, whose goal is to prove Proposition 4.2.7, we use the definitions and notations of Section 4.2.4. In particular, f_t^K stands for the law of the process defined by Equation (4.10), $\mu_\beta^K = e^{-\beta H_K(z)} dz / \mathcal{Z}_\beta^K$ where \mathcal{Z}_β^K makes μ_β^K a probability density on M_K , and $h_t^K = f_t^K / \mu_{\beta_t}^K$. According to [159], f_t^K is a smooth function and solves

$$\partial_t f_t^K = L_t^{K,*} \left(\frac{f_t^K}{\mu_{\beta_t}^K} \right) \mu_{\beta_t}^K,$$

but here the dual in $L^2(\mu_{\beta_t})$ of the generator of the process is

$$L_t^{K,*} = -\beta_t^{-1} \sigma(y) \nabla_x^* \nabla_x - \gamma_t \beta_t^{-1} \nabla_y^* \nabla_y + \beta_t^{-1} (\nabla_x^* \nabla_y - \nabla_y^* \nabla_x),$$

where the dual are taken in $L^2(\mu_\beta^K)$:

$$\begin{aligned} \nabla_x^* &= -\nabla_x \cdot + \beta \nabla U^K. \\ \nabla_y^* &= -\nabla_y \cdot + \beta \nabla W \cdot. \end{aligned}$$

Indeed, the additional diffusive part in x has been designed to be reversible. In order to prove Proposition 4.2.7, we introduce for $m \in \mathbb{N}$ the classical H^m -Sobolev norms on (M_K^2, μ_β^K) given by

$$\|h\|_{H^m(\mu_\beta^K)} = \sum_{\alpha \in \mathbb{N}^{2d}, |\alpha| \leq m} \int_{M_K^2} |\partial^\alpha h|^2 d\mu_\beta^K.$$

The general strategy is similar to the L^2 case of Section 4.4, namely we will prove that $\|h_t^K - 1\|_{H^m}$ goes to zero for all m , and conclude by a Sobolev embedding for m large enough. The constant in the Sobolev embedding depends on the time t which should be compensated by the fact $\|h_t^K - 1\|_{H^m}$ goes to zero fast enough. As in L^2 case, we need to introduce some modified Sobolev norm to deal with the lack of dissipativity in the x variable in some part of the space. Following [170], for $m \in \mathbb{N}$, we consider a modified H^m -Sobolev norm of the form

$$\begin{aligned} N_m(t, \beta) = & \int_{M_K \times M_K} \left(\frac{f_t^K}{\mu_\beta^K} - 1 \right)^2 + \sum_{k=1}^m \left(\sum_{i=0}^k \omega_{i,k}(\beta) \left| \nabla_x^i \nabla_y^{k-i} \frac{f_t^K}{\mu_\beta^K} \right|^2 + \omega_k(\beta) \nabla_x^{k-1} \nabla_y \frac{f_t^K}{\mu_\beta^K} \cdot \nabla_x^m \frac{f_t^K}{\mu_\beta^K} \right) d\mu_\beta^K \end{aligned} \quad (4.17)$$

for some weights ω to be fixed later on. Recall the definition

$$\mathcal{M} = \{y \in M_K; \nabla^2 W(y) = I_d\}.$$

If $y \in \mathcal{M}$, then we obtain ∇_x in the derivative of

$$\int_{M_K \times M_K} \nabla_x^{k-1} \nabla_y \frac{f_t^K}{\mu_\beta^K} \cdot \nabla_x^m \frac{f_t^K}{\mu_\beta^K} d\mu_\beta^K$$

using the commutator $[\nabla_y, \nabla W \cdot \nabla_x]$, and for $y \notin \mathcal{M}$, it comes from the $\sigma(y)\nabla_x^* \nabla_x$ part of $L_t^{K,*}$. Here we used the notations

$$\begin{aligned} |\nabla_x^i \nabla_y^{k-i} h|^2 &= \sum_{|\alpha_1|=i; |\alpha_2|=k-i} |\partial_x^{\alpha_1} \partial_y^{\alpha_2} h|^2 \\ \nabla_x^{k-1} \nabla_y h \cdot \nabla_x^m h &= \sum_{|\alpha|=k-1} \sum_{j=1}^d \partial_x^\alpha \partial_{y_j} h \partial_x^\alpha \partial_{x_j} h. \end{aligned}$$

We also define $\tilde{N}_m(t) = N_m(t, \beta_t)$. Since the process is now in a compact set, we do not need the approximation functions η_m , and the subscript here indicates the order of the Sobolev norm in contrast to the previous section. Besides, in Section 4.4, we had to keep track of the dependency of the constant in β_0 , as some uniformity in time was necessary in Proposition 4.2.5 for the renewal argument of the proof of Proposition 4.2.6. This is no longer the case here.

In order to study the evolution of N_m , we need first to have some commutation results and control over the derivative of the L^2 -norm of $\nabla_x^{m_1} \nabla_y^{m_2} h$ as in Lemma 4.4.3. Here, $\nabla_x^{m_1} \nabla_y^{m_2} h$ denotes the vector of all derivative of h of order m_1 on x and m_2 on y :

$$\nabla_x^{m_1} \nabla_y^{m_2} h = \{ \partial_x^{\alpha_1} \partial_y^{\alpha_2} h \mid |\alpha_1| = m_1, |\alpha_2| = m_2 \}$$

The method used here is adapted from [170] to take into account the time-inhomogeneity and the new dynamic. Recall the notation (4.16) for generalized Γ operators.

Lemma 4.5.1. *Let $m_1, m_2 \in \mathbb{N}$, then there exists some constant $\theta > 0$ such that for all $h \in \mathcal{C}^\infty(M_K^2)$:*

$$\begin{aligned} \Gamma_{t, |\nabla_x^{m_1} \nabla_y^{m_2} \cdot|^2}(h) &\geq \beta_t^{-1} (\gamma_t |\nabla_x^{m_1} \nabla_y^{m_2+1} h|^2 + \sigma |\nabla_x^{m_1+1} \nabla_y^{m_2} h|^2) \\ &\quad - \theta(1 + \gamma_t) \sum_{\substack{k=1, l=1 \\ k+l \leq m_1+m_2}}^{m_1+1, m_2+1} |\nabla_x^k \nabla_y^l h|^2 - \theta \mathbb{1}_{m_2 \geq 1} \sum_{l=1}^{m_2} |\nabla^l \sigma|^2 |\nabla_x^{m_1+2} \nabla_y^{m_2-l} h|^2. \end{aligned}$$

Proof. As in [137, Lemma 10], we have for smooth h :

$$\Gamma_{t, |\nabla_x^{m_1} \nabla_y^{m_2} \cdot|^2}(h) = \Gamma_t(\nabla_x^{m_1} \nabla_y^{m_2} h) + \nabla_x^{m_1} \nabla_y^{m_2} h \cdot \left[L_t^{K,*}, \nabla_x^{m_1} \nabla_y^{m_2} \right] h.$$

Then first :

$$\Gamma_t(\nabla_x^{m_1} \nabla_y^{m_2} h) = \beta_t^{-1} (\gamma_t |\nabla_x^{m_1} \nabla_y^{m_2+1} h|^2 + \sigma |\nabla_x^{m_1+1} \nabla_y^{m_2} h|^2).$$

Then, we can write $L_t^{K,*} = v \cdot \nabla + \beta_t^{-1} \sigma \Delta_x + \beta_t^{-1} \gamma_t \Delta_y$ with the drift

$$v(x, y) = \begin{pmatrix} -\nabla W(y) - \sigma(y) \nabla U^K(x) \\ \nabla U^K(x) - \gamma_t \nabla W(y) \end{pmatrix}.$$

First,

$$[\beta_t^{-1} \gamma_t \Delta_y, \nabla_x^{m_1} \nabla_y^{m_2}] = 0.$$

Then, using Cauchy-Schwarz inequality,

$$\nabla_x^{m_1} \nabla_y^{m_2} h \cdot [\beta_t^{-1} \sigma \Delta_x, \nabla_x^{m_1} \nabla_y^{m_2}] h = \nabla_x^{m_1} \nabla_y^{m_2} h \cdot \beta_t^{-1} \sum_{l=1}^{m_2} \binom{m_2}{l} \nabla_y^l \sigma \cdot \nabla_y^{m_2-l} \nabla_x^{m_1} \Delta_x h$$

$$\geq -\beta_t^{-1} \left(|\nabla_x^{m_1} \nabla_y^{m_2} h|^2 + \theta \sum_{l=1}^{m_2} |\nabla^l \sigma|^2 |\nabla_x^{m_1+2} \nabla_y^{m_2-l} h|^2 \right).$$

Notice that if $m_2 = 0$, then $\nabla_x^m h \cdot [\beta_t^{-1} \sigma \Delta_x, \nabla_x^m] h = 0$. The next term is:

$$\begin{aligned} [(-\nabla W - \sigma \nabla U^K) \nabla_x, \nabla_x^{m_1} \nabla_y^{m_2}] h &= \sum_{l=1}^{m_2} \binom{m_2}{l} \nabla_y^{l+1} W \nabla_x^{m_1+1} \nabla_y^{m_2-l} h \\ &\quad + \sum_{\substack{k \leq m_1 \\ l \leq m_2 \\ (k,l) \neq (0,0)}} \binom{m_1}{k} \binom{m_2}{l} \nabla_y^l \sigma \nabla_x^{k+1} U \nabla_x^{m_1-k+1} \nabla_y^{m_2-l} h \end{aligned}$$

and

$$\begin{aligned} [(-\gamma_t \nabla W + \nabla U^K) \nabla_y, \nabla_x^{m_1} \nabla_y^{m_2}] h &= \gamma_t \sum_{l=1}^{m_2} \binom{m_2}{l} \nabla_y^{l+1} W \nabla_x^{m_1} \nabla_y^{m_2-l+1} h \\ &\quad - \sum_{k=1}^{m_1} \binom{m_1}{k} \nabla_x^{k+1} U^K \nabla_x^{m_1-k} \nabla_y^{m_2+1} h. \end{aligned}$$

Putting those last two lines together and using Cauchy-Schwarz we get :

$$\begin{aligned} \nabla_x^{m_1} \nabla_y^{m_2} h \cdot [v \cdot \nabla, \nabla_x^{m_1} \nabla_y^{m_2}] h \\ \geq -\theta(1 + \gamma_t) \left(\sum_{l=1}^{m_2} |\nabla_x^{m_1+1} \nabla_y^{m_2-l} h|^2 + \sum_{\substack{1 \leq k \leq m_1 \\ 1 \leq l \leq m_2}} |\nabla_x^{m_1-k+1} \nabla_y^{m_2-l} h|^2 \right. \\ \left. + \sum_{l=1}^{m_2} |\nabla_x^{m_1} \nabla_y^{m_2-l+1} h|^2 + \sum_{k=1}^{m_1} |\nabla_x^{m_1-k} \nabla_y^{m_2+1} h|^2 \right). \end{aligned}$$

This concludes the proof. \square

Lemma 4.5.2. *For all $m \in \mathbb{N}$ there exists some constant $\theta > 0$ such that for all smooth h , denoting $P^m(t, \beta) = \int_{M_K \times M_K} \nabla_x^{m-1} \nabla_y \frac{f_t^K}{\mu_\beta^K} \cdot \nabla_x^m \frac{f_t^K}{\mu_\beta^K} d\mu_\beta^K$:*

$$\begin{aligned} (\partial_t P^m)(t, \beta_t) &\leq \int_{M_K \times M_K} - \left(\frac{1}{2} \mathbb{1}_{\mathcal{M}} - \theta \mathbb{1}_{\mathcal{M}^c} \right) |\nabla_x^m h_t^K|^2 \\ &\quad + \theta(1 + \gamma_t) \left(\sum_{k=1}^{m-2} |\nabla_x^k h_t^K|^2 + (|\nabla \sigma|^2 + \sigma) |\nabla_x^{m+1} h_t^K|^2 + \sum_{k=1}^{m-1} |\nabla_x^k \nabla_y h_t^K|^2 \right) d\mu_{\beta_t}^K. \end{aligned}$$

Proof. The derivative of P^m is given by :

$$(\partial_t P^m)(t, \beta_t) = \int_{M_K \times M_K} \left(\nabla_x^{m-1} \nabla_y L_t^{K,*} h_t^K \cdot \nabla_x^m h_t^K + \nabla_x^{m-1} \nabla_y h_t^K \cdot \nabla_x^m L_t^{K,*} h_t^K \right) d\mu_{\beta_t}^K.$$

We then have to study the two terms in the integral separately at first, by using commutators.

For any smooth h :

$$\begin{aligned}
\nabla_x^{m-1} \nabla_y L_t^{K,*} h \cdot \nabla_x^m h &= \nabla_x^{m-1} \left[\nabla_y, L_t^{K,*} \right] h \cdot \nabla_x^m h \\
&+ \sum_{k=1}^{m-1} \nabla_x^{k-1} \left[\nabla_x, L_t^{K,*} \right] \nabla_x^{m-k} \nabla_y h \cdot \nabla_x^m h + L_t^{K,*} \nabla_x^{m-1} \nabla_y h \cdot \nabla_x^m h \\
&= \nabla_x^{m-1} \left(-\nabla W \nabla_x - \nabla \sigma \nabla U^K \cdot \nabla_x - \gamma_t \nabla W \nabla_y + \beta_t \nabla \sigma \Delta_x \right) h \cdot \nabla_x^m h \\
&+ \sum_{k=1}^{m-1} \nabla_x^{k-1} \left(\nabla^2 U^K \nabla_y - \sigma \nabla^2 U^K \nabla_x \right) \nabla_x^{m-k} \nabla_y h \cdot \nabla_x^m h + L_t^{K,*} \nabla_x^{m-1} \nabla_y h \cdot \nabla_x^m h \\
&\leq - \left(\frac{1}{2} \mathbb{1}_{\mathcal{M}} - \theta \mathbb{1}_{\mathcal{M}^c} \right) |\nabla_x^m h|^2 + \theta \sum_{k=1}^{m-1} |\nabla_x^k h|^2 + \theta(1 + \gamma_t) \sum_{k=1}^{m-1} |\nabla_x^k \nabla_y h|^2 \\
&\quad + \theta |\nabla \sigma|^2 |\nabla_x^{m+1} h|^2 + L_t^{K,*} \nabla_x^{m-1} \nabla_y h \cdot \nabla_x^m h
\end{aligned}$$

where we used that $|\nabla \sigma \nabla U^K| \leq \frac{1}{2}$. Similarly, we have :

$$\nabla_x^{m-1} \nabla_y h \cdot \nabla_x^m L_t^{K,*} h \leq \theta \sum_{k=1}^{m-1} |\nabla_x^k \nabla_y h|^2 + \theta \sum_{k=1}^{m-1} |\nabla_x^k h|^2 + \nabla_x^{m-1} \nabla_y h \cdot L_t^{K,*} \nabla_x^m h.$$

We conclude with the fact that :

$$\begin{aligned}
&\int_{M_K \times M_K} L_t^* \nabla_x^{m-1} \nabla_y h_t^K \cdot \nabla_x^m h_t^K + \nabla_x^{m-1} \nabla_y h_t^K \cdot L_t^* \nabla_x^m h_t^K \, d\mu_{\beta_t}^K \\
&= \int_{M_K \times M_K} \Gamma_t(\nabla_x^{m-1} \nabla_y h_t^K, \nabla_x^m h_t^K) \, d\mu_{\beta_t}^K \\
&\leq \int_{M_K \times M_K} \theta(1 + \gamma_t) \left(|\nabla_x^m \nabla_y h_t^K|^2 + |\nabla_x^{m-1} \nabla_x h_t^K|^2 + |\nabla_x^m \nabla_y|^2 \right) + \beta_t^{-1} \sigma |\nabla_x^{k+1} h|^2 \, d\mu_{\beta_t}^K.
\end{aligned}$$

□

In order to state the main lemma, we introduce the following set :

$$\mathcal{P} = \left\{ g : \mathbb{R}_+ \mapsto \mathbb{R}_+ \text{ smooth, } \exists a, C > 0 \text{ s.t. } \beta^{-a}/C \leq g(\beta), |g'(\beta)| \leq C\beta^a \right\},$$

where \mathcal{P} stands for polynomial. The main step in order to prove an analogous to Proposition 4.2.3 in higher Sobolev norms is then the following dissipation result.

Lemma 4.5.3. *For all $m \geq 1$, there exist $q_m, r_m, (\omega_{i,m})_{i \leq m}$ and ω_m some functions of β , all in \mathcal{P} , such that if $f_0^K \in \mathcal{C}^\infty(M_K \times M_K)$ then, for all $t \geq 0$,*

$$\|h_t^K - 1\|_{H^m(\mu_{\beta_t}^K)} \leq q_m(\beta_t) \tilde{N}_m(t)$$

and :

$$(\partial_t N_m)(t, \beta_t)$$

$$\leq -r_m(\beta_t) \int_{M_K \times M_K} \left(\sigma |\nabla_x^{m+1} h_t^K|^2 + \sum_{i=0}^m |\nabla_x^i \nabla_y^{m+1-i} h_t^K|^2 + \sum_{1 \leq i+j \leq m} |\nabla_x^i \nabla_y^j h_t^K|^2 \right) d\mu_{\beta_t}^K. \quad (4.18)$$

Proof. The proof is by induction. In fact we start at $m = 0$, setting simply

$$N_0(t, \beta) = \int_{M_K \times M_K} \left(\frac{f_t^K}{\mu_\beta^K} - 1 \right)^2 d\mu_\beta^K.$$

Hence,

$$\begin{aligned} (\partial_t N_0)(t, \beta_t) &= - \int_{M_K \times M_K} \Gamma_t \left(\frac{f_t^K}{\mu_{\beta_t}^K} \right) d\mu_{\beta_t}^K \\ &= - \int_{M_K \times M_K} \beta_t^{-1} (\gamma_t |\nabla_y h_t^K|^2 + \sigma |\nabla_x h_t^K|^2) d\mu_{\beta_t}^K \end{aligned}$$

which is the result for $m = 0$ and $r_0(\beta_t) = \beta_t^{-1} \min(1, \kappa)$. One could also have initialized the induction for $m = 1$ as in Proposition 4.2.3. Now, let's fix $m \in \mathbb{N}$ and suppose we have the result for $m - 1$:

$$\begin{aligned} (\partial_t N_{m-1})(t, \beta_t) &\leq \\ &- r_{m-1}(\beta_t) \int_{M_K \times M_K} \left(\sigma |\nabla_x^m h_t^K|^2 + \sum_{i=0}^{m-1} |\nabla_x^i \nabla_y^{m-i} h_t^K|^2 + \sum_{i+j \leq m-1} |\nabla_x^i \nabla_y^j h_t^K|^2 \right) d\mu_{\beta_t}^K. \end{aligned}$$

We set

$$N_m = N_{m-1} + \int_{M_K \times M_K} \left(\sum_{i=0}^m \omega_{i,m}(\beta) \left| \nabla_x^i \nabla_y^{k-i} \frac{f_t^K}{\mu_\beta^K} \right|^2 + \omega_m(\beta) \nabla_x^{m-1} \nabla_y \frac{f_t^K}{\mu_\beta^K} \cdot \nabla_x^m \frac{f_t^K}{\mu_\beta^K} \right) d\mu_\beta^K$$

with weights to be determined later on, so that

$$\begin{aligned} (\partial_t N_m)(t, \beta_t) &= (\partial_t N_{m-1})(t, \beta_t) - \int_{M_K \times M_K} \sum_{i=0}^m \omega_{i,m}(\beta) \Gamma_{|\nabla_x^i \nabla_y^{k-i}|^2} (h_t^K) d\mu_{\beta_t}^K + \omega_m(\beta) (\partial_t P^m)(t, \beta_t). \end{aligned}$$

In this equality, using the two previous lemmas, the terms of order $m + 1$ are bounded by:

$$\begin{aligned} \int_{M_K \times M_K} (\omega_{m-1,m} |\nabla \sigma|^2 + \omega_m (\sigma + |\nabla \sigma|^2)) |\nabla_x^{m+1} h_t^K|^2 \\ - \beta_t^{-1} \sum_{i=0}^m \omega_{i,m}(\beta_t) (\gamma_t |\nabla_x^i \nabla_y^{m+1-i} h_t^K|^2 + \sigma |\nabla_x^{i+1} \nabla_y^{m-i} h_t^K|^2) d\mu_{\beta_t}^K \end{aligned}$$

In order to get (4.18), we would like this to be less than

$$-r_m(\beta_t) \int_{M_K \times M_K} \left(\sigma |\nabla_x^{m+1} h_t^K|^2 + \sum_{i=0}^m |\nabla_x^i \nabla_y^{m+1-i} h_t^K|^2 \right) d\mu_{\beta_t}^K.$$

Using that $|\nabla \sigma|^2 \leq \sigma$, this is indeed the case if we impose the conditions $\omega_{m,m}(\beta) \geq 4\beta\omega_m(\beta) + \beta\omega_{m+1,m}$ and $\omega_{i,m}(\beta) \geq r_m\beta \max(\kappa^{-1}, \frac{1}{2})$. Next, the terms of order at most $m-1$ are bounded by :

$$\int_{M_K \times M_K} \theta(1 + \gamma_t) \max_{0 \leq i \leq m} \omega_{i,m} \sum_{i+j \leq m-1} |\nabla_x^i \nabla_y^j h_t^K|^2 - r_{m-1} \sum_{i+j \leq m-1} |\nabla_x^i \nabla_y^j h_t^K|^2 d\mu_{\beta_t}^K$$

which means, similarly, in order to get (4.18), we want to impose the conditions

$$\max_{0 \leq i \leq m} \omega_{i,m} \theta(1 + \gamma_t) \leq \frac{1}{2} r_{m-1}, \quad r_{m-1} \geq 2r_m.$$

Finally, the terms of order exactly m are bounded by

$$\begin{aligned} - \int_{M_K \times M_K} \left(r_{m-1} \sum_{i=1}^{m-1} |\nabla_x^i \nabla_y^{m-i} h_t^K|^2 + \left(r_{m-1} \sigma + \omega_m \frac{1}{2} \mathbb{1}_{\mathcal{M}} - \omega_m \theta \mathbb{1}_{\mathcal{M}^c} \right) |\nabla_x^m h_t^K|^2 \right. \\ \left. - \max_i \omega_{i,m} \theta(1 + \gamma_t) \sum_{i=0}^m |\nabla_x^i \nabla_y^{m-i} h_t^K|^2 \right) d\mu_{\beta_t}^K \end{aligned}$$

which leads to the conditions: $r_m \leq \frac{1}{2}\omega_m$, $\omega_m \theta \leq \frac{1}{2}r_{m-1}\sigma_*$ and $\frac{1}{2}r_{m-1}\sigma_* \geq r_m$.

Now, fix the $\omega_{i,m}$ to be equal to $\frac{r_{m-1}}{4\theta(1+L\beta)}$ except $\omega_{m,m}$ equal to $\frac{r_{m-1}}{2\theta(1+L\beta)}$, then $\omega_m = \min(\frac{\sigma_* r_{m-1}}{2\theta}, \frac{\omega_{m,m}}{4\beta}, \omega_{m,m})$, and finally set $r_m = \min(\frac{r_{m-1}}{2}, \frac{r_{m-1}\sigma_*}{2}, \frac{\omega_m}{2}, \beta^{-1} \min(\kappa, 2)\omega_{i,m})$. These choices ensures that all the conditions in the computations above are met, which means that (4.18) holds. Moreover, all these functions are in \mathcal{P} , which concludes. \square

Similarly to Proposition 4.4.1 but now in the fully (position and velocity) compact case, we have the following Poincaré inequality:

Proposition 4.5.1. *If $U^K : M_K \mapsto \mathbb{R}$ is a C^∞ function, W is as constructed in Section 4.2.4, and μ_β^K is the probability measure on $M_K \times M_K$ proportional to $e^{-\beta H_K}$, then there exists $\lambda : \mathbb{R}_+ \mapsto \mathbb{R}_+$ such that for all $f \in C^\infty(M_K \times M_K)$:*

$$\lambda(\beta) \int_{M_K \times M_K} \left(f - \int_{M_K \times M_K} f d\mu_\beta^K \right)^2 d\mu_\beta \leq \int_{M_K \times M_K} |\nabla f|^2 d\mu_\beta^K$$

and

$$\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(\lambda(\beta)) = -c^*(U^K)$$

where $c^*(U^K)$ is defined as c^* with U replaced by U^K .

Proof. Using that $c^*(H_K) = c^*(U^K)$ since W has only one minimum, this is [83, Theorem 1.14]. \square

We are now ready to prove Proposition 4.2.7.

Proof of Proposition 4.2.7. Let $m = d+1$. We first show that there exist some constants $C_1, C_2 > 0$ such that $\tilde{N}_m(t) \leq C_1 e^{-C_2 t^\alpha}$ for all $t \geq 0$, where $\alpha = \frac{c-c^*}{2c}$. Indeed, we have :

$$\tilde{N}'_m(t) = \partial_t N_m(t, \beta_t) + \beta'_t \partial_\beta N_m(t, \beta_t).$$

From Lemma 4.5.3 and Proposition 4.5.1,

$$\partial_t N_m \leq -\frac{\tilde{\lambda}(\beta_t) r_m}{2} N_m.$$

where $\tilde{\lambda}$ satisfies $\lim_{\beta \rightarrow \infty} \frac{1}{\beta} \ln(\tilde{\lambda}(\beta)) = -c^*(U^K)$ and $r_m \geq \beta^{-a}/C$ for some $a > 0$. Hence, we have some constant $C > 0$ such that $\lambda(\beta_t) r_m / 2 \geq C e^{-\frac{c+c^*}{2} \beta_t} = C(e^{c\beta_0} + t)^{-1+\alpha}$. On the other hand, from the conditions on the ω 's and since $\partial_\beta e^{\beta H_K} \leq \|H_K\|_\infty e^{\beta H}$, there exist some $a, C' > 0$ such that $\partial_\beta N_m \leq C' \beta_t^a N_m$ yielding $\beta'_t \partial_\beta N_m \leq C'(1+t)^{-1+\frac{a}{2}} N_m$ for some other constant $C' > 0$, and thus :

$$\tilde{N}'_m \leq \left(-\frac{C}{(1+t)^{1-\alpha}} + \frac{C'}{(1+t)^{1-\frac{a}{2}}} \right) \tilde{N}_m,$$

yielding our first claim.

From the Sobolev embedding, there exists $C > 0$ such that for any smooth h on $M_K \times M_K$, we have $\|h\|_{L^\infty} \leq C \|h\|_{H^m(\mu_{\beta_0}^K)}$. Then we have :

$$\|h\|_{L^\infty} \leq 1 + \|h - 1\|_{L^\infty} \leq 1 + C \|h - 1\|_{H^m(\mu_{\beta_0}^K)} \leq 1 + C e^{\beta_t \|H\|_\infty} \|h - 1\|_{H^m(\mu_{\beta_t}^K)}.$$

Applying this with $h = h_t^K$ and using that $\|h_t^K - 1\|_{H^m(\mu_{\beta_t}^K)} \leq C \beta_t^a \tilde{N}_m(t)$ for some $a, C > 0$, we get constants $C, b > 0$ such that :

$$\|h_t^K\|_{L^\infty} \leq 1 + C(1+t)^b e^{-C_2 t^\alpha},$$

yielding the result. □

4.6 Faster than logarithmic schedules

Proof of Theorem 4.1.3. Some parts of the proof follow the proof of Theorem 4.1.2, to which we refer for details, focusing on the new arguments in the present settings.

Up to a translation we assume without loss of generality that $x_* = 0$.

As in the proof of Theorem 4.1.2, it is in fact sufficient to prove that for all $\delta > 0$

$$\mathbb{P}_{f_0} (|Z_t| \leq \min(\delta, \sqrt{\varepsilon_t}) \forall t \geq t_0) > 0$$

for a given fixed initial condition f_0 and for t_0 large enough and then use a controlability argument based on Lemma 4.2.8 and the Markov property to get the claimed result. Besides, it is sufficient to prove this result for δ small enough and, since the times in $[0, t_0]$ are treated with the controlability argument, focusing on the times larger than t_0 , we are interested in an event under which the process stays in a small ball around 0, and we can thus modify U outside such a ball without modifying the result.

The Jacobian matrix of the drift $b(z) = (y, -\nabla U(x) - \gamma y)$ of the process at $z = (x, y)$ is

$$J(z) = \begin{pmatrix} 0 & I \\ -\nabla^2 U(x) & -\gamma I \end{pmatrix}.$$

Since $\nabla^2 U(0)$ is positive semi-definite, a simple calculation shows that the eigenvalues of $J(0)$ all have a negative real part, and thus there exist a positive definite symmetric matrix M of size $2d$ and $r > 0$ such that

$$u \cdot MJ(0)u \leq -2ru \cdot Mu$$

for all $u \in \mathbb{R}^{2d}$, see e.g. [4, Lemma 4.3]. Write $\|u\|_M = \sqrt{u \cdot Mu}$ and let $\delta > 0$ be sufficiently small so that

$$u \cdot MJ(z)u \leq -r\|u\|_M^2 \quad (4.19)$$

for all $u \in \mathbb{R}^{2d}$ and all $z \in \mathbb{R}^{2d}$ with $\|z\|_M \leq \delta$. As discussed above, up to a modification of U outside the ball $\mathcal{B}(0, \delta)$, without loss of generality we can modify the potential U outside this ball and assume that in fact (4.19) holds for all $z \in \mathbb{R}^{2d}$. Similarly we assume that $\nabla^3 U$ is bounded.

Using that $b(0) = 0$, we get that for all $z \in \mathbb{R}^{2d}$

$$z \cdot Mb(z) = z \cdot M(b(z) - b(0)) = \int_0^1 z \cdot MJ(pz)z dp \leq -r\|z\|_M^2. \quad (4.20)$$

Let Z and \tilde{Z} be two solutions of (4.1) with the same initial condition and driven by the same Brownian motion, but with two different potentials, Z being associated to U and \tilde{Z} to $\tilde{U}(z) = z \cdot \nabla^2 U(0)z/2$. In particular, \tilde{Z} is a Gaussian process. Then

$$\begin{aligned} d\|Z_t - \tilde{Z}_t\|_M^2 &\leq -2r\|Z_t - \tilde{Z}_t\|_M^2 dt + 2\|Z_t - \tilde{Z}_t\|_M |M^{1/2}| |\nabla U(\tilde{Z}_t) - \nabla^2 U(0)\tilde{Z}_t| dt \\ &\leq -r\|Z_t - \tilde{Z}_t\|_M^2 dt + \frac{1}{4r} \|\nabla^3 U\|_\infty^2 |M| |\tilde{Z}_t|^4 dt. \end{aligned}$$

Let $(\alpha_t)_{t \geq 0}$ be a positive non-increasing function, vanishing at infinity, to be chosen later on. Then the event $\mathcal{G} = \{|\tilde{Z}_t| \leq \alpha_t \forall t \geq 0\}$ implies that for all $t \geq 0$

$$|Z_t| \leq |\tilde{Z}_t| + |M^{-1/2}| \|Z_t - \tilde{Z}_t\|_M \leq \alpha_t + C \left(\int_0^t \alpha_s^2 e^{r(s-t)} ds \right)^{1/2} := \tilde{\alpha}_t$$

with $C^2 = |M||M^{-1}| \|\nabla^3 U\|_\infty / (2\sqrt{r})$. Notice that $\tilde{\alpha}_t$ vanishes at infinity, more precisely $\tilde{\alpha}_t \leq \alpha_t + C(\alpha_{3t/4}/\sqrt{r} + \alpha_0 \sqrt{te^{-rt/8}})$. As a consequence, it only remains to prove that \mathcal{G} has a positive probability for some suitable function $t \mapsto \alpha_t$. Again, following the proof of Theorem 4.1.2, we see that it is sufficient to prove that $t \mapsto \mathbb{P}(|\tilde{Z}_t| \geq \alpha_t)$ is integrable for a given fixed initial condition. Since \tilde{Z} is a Gaussian process, we simply have to control its second moment. We chose an initial condition such that $\mathbb{E}(\tilde{Z}_0) = 0$, so that $\mathbb{E}(\tilde{Z}_t) = 0$ for all $t \geq 0$.

Remark that the drift of \tilde{Z}_t also satisfies (4.20), since its Jacobian matrix at any $z \in \mathbb{R}^{2d}$ is equal to $J(0)$. Thus we get, for all $t \geq 0$,

$$\partial_t \mathbb{E} \left(\|\tilde{Z}_t\|_M^2 \right) \leq -r \mathbb{E} \left(\|\tilde{Z}_t\|_M^2 \right) + \frac{d|M|}{\beta_t},$$

so that, writing $C' = |M||M^{-1}|(\mathbb{E}|\tilde{Z}_0|^2 + d)$,

$$\mathbb{E}\left(|\tilde{Z}_t|^2\right) \leq |M^{-1}|\mathbb{E}\left(\|\tilde{Z}_t\|_M^2\right) \leq C' \left(e^{-rt} + \int_0^t \frac{e^{r(s-t)}}{\beta_s} ds \right) := C' \kappa_t,$$

Using that the law of \tilde{Z}_t is Gaussian with zero mean, we get that there exist $K, h > 0$ such that for all $t \geq 0$

$$\mathbb{P}(|\tilde{Z}_t| \geq \alpha_t) \leq K \exp\left(-h \frac{\alpha_t^2}{\kappa_t}\right).$$

This is integrable in time if we chose $\alpha_t^2 = \sup_{s \geq t} 2 \ln(s) \kappa_s / h$ (which is non-increasing). Since $\ln(t) = o(\beta_t)$ and $\kappa_t \leq \sup_{s \geq 2t/3} 1/(r\beta_s) + e^{-rt/3}(1 + t \sup_{u \geq 0} 1/\beta_u)$, we get that $\kappa_t = o(1/\ln(t))$, in other words $\alpha_t \rightarrow 0$. We conclude by using the previous bounds on $\tilde{\alpha}_t$ and κ_t and the fact that

$$\sup_{s \geq 3t/4} \ln(s) \sup_{u \geq 2s/3} \beta_u^{-1} \leq \sup_{s \geq t/2} \ln(s) \beta_s^{-1}$$

to get the quantitative convergence speed ε_t stated in the theorem. \square

Remark: in order to adapt the previous proof in a case where γ_t is not constant, we can still find M and r such that (4.19) holds with the Jacobian matrix of the drift at time t , but they depend on γ_t , hence when differentiating $\|Z_t - \tilde{Z}_t\|_M^2$ there is an additional term involving $\partial_t M$ which has to be sufficiently small to be absorbed by the contraction at rate r . Moreover, r scales as γ_t when $\gamma_t \rightarrow 0$ and as $1/\gamma_t$ when $\gamma_t \rightarrow +\infty$, which means for the proof to be valid, γ_t or $1/\gamma_t$ should not be too small depending on β_t .

Chapter 5

Switched diffusion processes for non-convex optimization and saddle points search

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Abstract : We introduce and investigate stochastic processes designed to find local minimizers and saddle points of non-convex functions, exploring the landscape more efficiently than the standard noisy gradient descent. The processes switch between two behaviours, a noisy gradient descent and a noisy saddle point search. It is proven to be well-defined and to converge to a stationary distribution in the long time. Numerical experiments are provided on low-dimensional toy models and for Lennard-Jones clusters.

5.1 Introduction

5.1.1 Overview

This work addresses the issue of finding the local minimizers and the saddle points of a given non-convex potential $U : \mathbb{R}^d \rightarrow \mathbb{R}_+$. These questions are ubiquitous in a wide range of scientific

fields. In particular, in molecular dynamics, U being the energy of a molecular system, the minimizers are the metastable state of the system, while the saddle points are the transition states between the former. As we will see, we will design a stochastic algorithm which targets both local minimizers and saddle points, in such a way that each of this task benefits from the other. In particular, the algorithm is suitable even as an optimisation tool, when the goal is only to find the global minimizers of U .

In high dimension, this problem is challenging, as an exhaustive search is impossible and running local search algorithms started from random initial conditions only works when it is possible to sample starting points that have a reasonable probability to hit the basin of attraction of the points of interest (for a gradient descent or a saddle point search), which is often not the case when these basins are concentrated around an unknown manifold of dimension much smaller than d .

A classical solution in order to visit the whole space while taking into account the energy landscape (hence focusing on low-energy areas) is to follow the overdamped Langevin diffusion process, which is the Markov process solving

$$dX_t = -\nabla U(X_t)dt + \sqrt{2\varepsilon}dB_t, \quad (5.1)$$

where B is a d -dimensional Brownian motion and $\varepsilon > 0$ is a temperature parameter. When ε is small, this is a noisy perturbation of a deterministic gradient descent (contrary to the stochastic gradient descent algorithm, here the noise is voluntarily added, it has a constant intensity and does not come from a Monte Carlo approximation of ∇U). Under standard growth conditions on U at infinity, the process is ergodic with respect to the measure

$$\mu_\varepsilon(dx) = \frac{e^{-U(x)/\varepsilon}dx}{\int_{\mathbb{R}^d} e^{-U(y)/\varepsilon}dy},$$

i.e. the time spent in any given domain is asymptotically proportional to its probability with respect to μ_ε . Hence, the temperature ε has to be taken small enough to counteract the entropic effect due to the high dimension d and ensure that the vicinity of minimizers have a high probability. Then, one can use the point of the trajectory with the lowest energy as a starting point for a local gradient descent (or a variant, like the stochastic gradient descent). However, as ε vanishes, it is well known that (5.1) is metastable, since transitions between different potential wells occur in a time of order roughly $e^{c/\varepsilon}$ for some $c > 0$, due to the energy barriers induced by low-probability regions interspersing high-probability ones. This makes the convergence of the law of the process towards its equilibrium, and thus the exploration, very slow, which makes this method fail in practice.

Besides, according to large deviations theory, more precisely to the Freidlin-Wentzell results on the low noise behaviour of diffusion processes, it is known that, as ε vanishes, the process (5.1) is likely to exit from a potential well through the saddle point with the lowest energy level on the boundary of the well. Instead of waiting for an unlikely deviation of the Brownian motion to lead the process (5.1) to this saddle point, this naturally motivates the definition of a process which actively looks for it. More precisely, the main object of this work is a process which switches randomly between two dynamics, the noisy gradient descent (5.1) and a noisy saddle points search.

The rest of this work is organized as follows. In the remainder of the introduction, we present two saddle point search algorithm in Section 5.1.2, and we define the stochastic processes we are going to investigate. In Section 5.2, we conduct a theoretical study of the processes, and in Section 5.3 a numerical study.

5.1.2 Deterministic saddle point algorithms

Since saddle point search is less standard than optimization, let us first present some existing deterministic algorithms on this topic. A first class of methods, based on reaction paths, requires the knowledge of two local minimizers, and then finds a path of minimal elevation between them, which passes through a saddle point see e.g. [70, 53]. This doesn't correspond to our context, where the local minimizers are unknown. A second class of methods, considered e.g. in [54, 121, 66, 115, 151, 17, 75] and references within and which will be the one of interest for us, relies on local walkers, analogous of the gradient descent for optimization, i.e. solutions of some ODEs for which saddle points of U are stable equilibrium. Given some $x \in \mathbb{R}^d$, write:

$$\lambda_1(x) \leq \lambda_2(x) \leq \dots \leq \lambda_d(x)$$

for the ordered eigenvalues of $\nabla^2 U(x)$, and suppose that we are given $v_1(x), \dots, v_d(x) \in \mathbb{R}^d$ such that $v_i(x)$ is an eigenvector of $\nabla^2 U(x)$ associated to $\lambda_i(x)$ (in other words, when the eigenvalues are not all simple, we assume that we have an arbitrary rule to select a given eigenbasis, for instance we take the basis obtained as the limit of the Jacobi algorithm). The idealised saddle dynamic (ISD) is the solution of

$$\dot{x}_t = - (I - 2v_1(x_t)v_1(x_t)^T) \nabla U(x_t).$$

In other words, x_t follows a gradient descent, except in the direction $v_1(x_t)$ where a reflection is performed, i.e. the process follows a gradient ascent in this direction. Notice that in general $x \mapsto v_1(x)$ is not continuous so the existence of this process is unclear and may be restricted to some parts of the space or to a finite time interval.

A variation of the ISD is the so-called Gentlest Ascent Dynamic (GAD) $(x_t, v_t) \in \mathbb{R}^d \times \mathbb{S}^{d-1}$ solving

$$\begin{cases} \dot{x}_t &= - (I - 2v_t v_t^T) \nabla U(x_t) \\ \eta \dot{v}_t &= -(I - v_t v_t^T) \nabla^2 U(x_t) v_t, \end{cases}$$

where $\eta > 0$ is a fixed parameter. If $\nabla^2 U(x_t)$ were fixed in the second equation, this would be a gradient descent on \mathbb{S}^{d-1} for the Rayleigh quotient $v \mapsto -v^T \nabla^2 U(x_t) v$. As η vanishes, formally, we recover the ISD. Contrary to the later, the GAD is always well-defined for all initial conditions and all times.

The following results on the ISD and GAD are from [115, Theorems 2 and 3] and [54].

Proposition 5.1.1. • *Any critical point of U is an equilibrium points for the ISD. It is stable if and only if it is a index-1 saddle point.*

- *Any $(x, v) \in \mathbb{R}^d \times \mathbb{S}^{d-1}$ with x a critical point of U and v an eigenvalue of $\nabla^2 U$ is an equilibrium point of the Gentlest Ascent dynamic. It is stable if and only if x is a index-1 saddle point and v is associated to the negative eigenvalue.*
- *If $\Omega \subset \mathbb{R}^d$ satisfies that for all $x \in \Omega$, we have $\lambda_1(x) < 0 < \lambda_2(x)$, then there exists a unique saddle point z_* in Ω , and for all $x_0 \in \Omega$, there exists a unique solution to the ISD which converges exponentially fast towards z_* .*
- *Under the same assumption, there is $\delta > 0$ such that if $(x_0, v_0) \in \Omega \times \mathbb{S}^{d-1}$, and $|v_0 - v_1(x_0)| < \delta$, then there exists a unique solution to the GAD which converges exponentially fast towards $(z_*, v_1(z_*))$.*

The convergence results are only local, and one cannot expect more in general since the ISD may have attracting singularities [115]. In the case of the GAD, with a potential of the form

$\sum_{i=1}^d U_i(x_i)$, and an initial condition $v_0 \in \text{vect}(e_1, \dots, e_i)$, v_t will stay orthogonal to e_j , $j > i$, and hence the process will never get close to an equilibrium point with an eigenvector not in $\text{vect}(e_1, \dots, e_i)$. As in the optimization case where the overdamped Langevin diffusion (5.1) allows for a global exploration while the gradient descent only converges locally, it is thus natural to add a small Brownian noise to the deterministic ISD and GAD. The resulting processes will explore eventually the whole space but, thanks to Proposition 5.1.1, will still be attracted locally by saddle points (notice that the Freidlin-Wentzell theory on random perturbation of ODE does not apply directly in the ISD case because of the discontinuity of $x \mapsto v_1(x)$).

5.1.3 The stochastic processes

For simplicity, from now on, we will restrict ourselves to the case of a function defined on compact manifold (specifically the periodic torus). Indeed, in practical situation, local minima and saddle points are located in a compact set. Most of the definitions and arguments below would be easily adapted to \mathbb{R}^d provided suitable modifications outside a given compact, in particular to ensure the stability of the processes.

Write \mathbb{T}^d for the d -dimensional torus and fix some function $U \in \mathcal{C}^2(\mathbb{T}^d, \mathbb{R}_+)$. As in the previous section, we write $\lambda_i(x)$ the ordered eigenvalues of $\nabla^2 U(x)$, and we consider functions $x \mapsto v_i(x)$ such that $v_i(x)$ is an eigenvector of $\nabla^2 U(x)$ associated to $\lambda_i(x)$ for all $x \in \mathbb{T}^d$ and $i \in \llbracket 1, d \rrbracket$. Moreover, we assume that the functions v_i are measurable for all $i \in \llbracket 1, d \rrbracket$, which is indeed possible:

Lemma 5.1.1. *For all $i \in \llbracket 1, d \rrbracket$ there exists a measurable function $v_i : \mathbb{T}^d \rightarrow \mathbb{S}^{d-1}$ such that $v_i(x)$ is and eigenvector of $\nabla^2 U(x)$ associated to $\lambda_i(x)$ for all $x \in \mathbb{T}^d$.*

Proof. Given a symmetric matrix H and (e_1, \dots, e_d) the canonical basis of \mathbb{R}^d , the function $H \mapsto (u_1, \mu_1, \dots, u_d, \mu_d)$, where u_i is the limit of the gradient descent for the Rayleigh quotient starting from e_i and μ_i is the associated eigenvalue, is measurable. At least one of the μ_i is the smallest eigenvalue of H , hence we may just select the smallest indices i_0 such that it is the case and consider the associated vector. We can then iterate by applying the same procedure to $(I - u_{i_0} u_{i_0}^T)H(I - u_{i_0} u_{i_0}^T) + (|H| + 1)u_{i_0} u_{i_0}^T$, and similarly by induction. We conclude with the fact that $x \mapsto \nabla^2 U(x)$ is continuous, hence measurable. \square

As in \mathbb{R}^d , for $\varepsilon > 0$ the overdamped Langevin process is defined on \mathbb{T}^d as the solution of (5.1). It is ergodic with respect to μ_ε the probability measure with density proportional to $e^{-U/\varepsilon}$ on the torus. Similarly, we define the noisy ISD as the solution on \mathbb{T}^d of

$$dX_t = - (I - 2v_1(X_t)v_1(X_t)^T) \nabla U(X_t) dt + \sqrt{2\varepsilon} dB_t, \quad (5.2)$$

which, contrary to its deterministic counterpart, is always well-defined (see Proposition 5.2.1 below). Concerning the noisy version of GAD, we may wonder whether it is necessary to add noise to both coordinates, and thus in general we can consider the noisy GAD as the solution on $\mathbb{T}^d \times \mathbb{S}^{d-1}$ of

$$\begin{cases} dX_t &= - (I - 2V_t V_t^T) \nabla U(X_t) dt + \sqrt{2\varepsilon} dB_t, \\ dV_t &= (I - V_t V_t^T) \left[-\frac{1}{\eta} \nabla^2 U(X_t) V_t dt + \sqrt{2\varepsilon'} dB_t' \right] - d\varepsilon' dt, \end{cases} \quad (5.3)$$

where $\eta > 0$, $\varepsilon' \geq 0$ and B, B' are independent d -dimensional Brownian motions. The second line is such that if $\nabla^2 U(X_t)$ is constant then this is an overdamped Langevin diffusion on the sphere with potential given by the Rayleigh quotient (see e.g. [110, Section 3.2.3] or [2]). In particular, according to [110, Lemma 3.18], $V_t \in \mathbb{S}^{d-1}$ for all $t \geq 0$. In fact, by contrast with

the deterministic case, since the noisy ISD is well defined, we will not insist much on the noisy GAD, and simply discuss the case $\varepsilon' = 0$ in Section 5.2.1.

Next, we define the idealised switched process (ISP) as the Markov process $(X_t, I_t)_{t \geq 0}$ on $\mathbb{T}^d \times \{0, 1\}$ where $(I_t)_{t \geq 0}$ is a Markov process on $\{0, 1\}$ with constant jump rate $\nu > 0$ and X solves

$$dX_t = H_{I_t}(X_t)dt + \sqrt{2\varepsilon}dB_t, \quad (5.4)$$

with $(B_t)_{t \geq 0}$ a Brownian motion independent from $(I_t)_{t \geq 0}$ and, for all $x \in \mathbb{T}^d$,

$$H_0(x) = -\nabla U(x), \quad H_1(x) = -(I - 2v_1(x)v_1(x)^T)\nabla U(x).$$

In other words, the process alternates between the overdamped Langevin dynamics and the noisy ISD, the time being two switching events between independent and distributed according to an exponential law of parameter ν . Likewise, we can define the gentle switched process (GSP) as the Markov process $(X_t, V_t, I_t)_{t \geq 0}$ on $\mathbb{T}^d \times \mathbb{S}^{d-1} \times \{0, 1\}$ where

$$\begin{cases} dX_t &= \bar{H}_{I_t}(X_t, V_t) + \sqrt{2\varepsilon}dB_t, \\ dV_t &= (I - V_tV_t^T) \left[-\frac{1}{\eta}\nabla^2 U(X_t)V_t dt + \sqrt{2\varepsilon'}dB'_t \right] - d\varepsilon' dt, \end{cases} \quad (5.5)$$

where $(I_t)_{t \geq 0}$ is as in the ISP, independent from B, B' , and

$$\bar{H}_0(x, v) = -\nabla U(x), \quad \bar{H}_1(x, v) = -(I - 2vv^T)\nabla U(x).$$

Finally, let us introduce slight variations of the processes defined above. Consider

$$\mathcal{S} = \{x \in \mathbb{T}^d, \lambda_1(x) = \lambda_2(x)\},$$

which is the set of singularities of the deterministic ISD flow. As pointed out in [115], some points of \mathcal{S} may be attracting singularities for this flow, and thus they will also locally attract the noisy ISD when ε is small, or the noisy GAD when ε and η are small. This behaviour may be mitigated as follows. Fix some non-decreasing $f : \mathbb{R}_+ \rightarrow [1, 2]$ such that $f(0) = 1$ and $f(r) = 2$ for all r larger than some small threshold $r_* > 0$. Then, setting $a(x) = f(\lambda_2(x) - \lambda_1(x))$ the drift H_1 in the noisy ISD may be replaced by

$$\hat{H}_1(x) = -(I - a(x)v_1(x)v_1(x)^T - (2 - a(x))v_2(x)v_2(x)^T)\nabla U(x).$$

In other words, when $\lambda_1(x)$ and $\lambda_2(x)$ are clearly distinguished, then we recover the previous noisy ISD, however, on \mathcal{S} , rather than undergoing an orthogonal reflection with respect to $v_1(x)$, $\nabla U(x)$ is orthogonally projected on the orthogonal of the space spanned by $v_1(x), v_2(x)$, which means that, in these two directions, the process behave like a Brownian motion. Natural choices for f would be piecewise constant (with $f(r) = 1$ for $r < r_*$) or piecewise linear (with $f(r) = 1 + r/r_*$ for $r < r_*$). In the second case, the drift \bar{H}_1 is continuous.

An analogous modification can be applied to the drift \bar{H}_1 of the noisy GAD, in which case the process is then (X, V_1, V_2) where V_1, V_2 are orthogonal vectors of \mathbb{S}^{d-1} whose evolution is given, in the case $\varepsilon' = 0$, by

$$\begin{aligned} dV_{1,t} &= -\frac{1}{\eta} (I - V_{1,t}V_{1,t}^T) \nabla^2 U(X_t)V_{1,t} dt \\ dV_{2,t} &= -\frac{1}{\eta} (I - V_{2,t}V_{2,t}^T - 2V_{1,t}V_{1,t}^T) \nabla^2 U(X_t)V_{2,t} dt. \end{aligned}$$

(we refer to [110, Section 3.2.3] to derive the case $\varepsilon' > 0$, where the constraints are now that $|v_1|^2 = |v_2|^2 = 1$ and $v_1^T v_2 = 0$).

This variation can be generalised to any degree of degeneracy of the smallest eigenvalue, i.e. for $k \geq 2$ modifying the drift H_1 in the vicinity of the set where $\lambda_1(x) = \dots = \lambda_k(x)$ (generically these sets are empty for $k > 2$, but in many practical cases they are not, due to some symmetries in the problem).

5.2 Theoretical analysis

Before turning to numerical experiment, we are interested in the existence of the different processes, and some of their properties, mainly in the long time limit. For the well-known Langevin process, we refer to [110, 112].

A valuable tool to study long time behavior of a process is the Doeblin condition. A Markov kernel $\mathcal{P} : \mathbb{T}^d \rightarrow \mathcal{M}^1(\mathbb{T}^d)$ is said to satisfy a Doeblin condition if there exist $c > 0$ and a probability measure μ such that for all $x \in \mathbb{T}^d$, $\mathcal{P}(x) \geq c\mu$. This implies that $(\mathcal{P}^n)_n$ converges in total variation to the unique probability measure μ_∞ such that $\mu_\infty \mathcal{P} = \mu_\infty$, see for example [79]. In the continuous-time setting, this can be written as follow: there exists $t_0, c > 0$ and a probability measure μ , such that $\delta_x P_{t_0} \geq c\mu$ for all $x \in \mathbb{T}^d$, with P_t the semi-group of the process, and $\delta_x P_{t_0}$ is hence the law of the process starting from x a time t_0 .

5.2.1 Noisy ISD and Noisy GAD

Since we work on the compact torus and the drift of the noisy ISD (5.2) is measurable and bounded, the well-posedness and long-time behavior follows from classical results on diffusion processes. We summarize these results on the next proposition. Apart from the continuous-time equation (5.2), we are also interested in the corresponding Euler-Maruyama scheme. The noisy ISD is covered by the following:

Proposition 5.2.1. *Consider $\sigma > 0$, $b : \mathbb{T}^d \rightarrow \mathbb{R}^d$ measurable and bounded, and X solution to*

$$dX_t = b(X_t)dt + \sigma dB_t. \quad (5.6)$$

Strong existence: for any initial condition $x_0 \in \mathbb{T}^d$, and Brownian motion B , there exists a unique Markov process X^{x_0} solution to equation (5.6), with Brownian motion B and initial condition x_0 .

Moreover, this process admits a unique invariant probability measure which admits a density with respect to the Lebesgue measure, and the law of the process converges exponentially fast towards this stationary measure in the total variation distance.

The Euler-Maruyama scheme defined for $\delta > 0$ by

$$X_{n+1} = X_n + \delta b(X_n) + \sqrt{\delta} G_n$$

with $(G_n)_n$ a sequence of standard Gaussian variables, admits as well a unique stationary measure μ^δ , and there exists $c, C, \delta_0 > 0$ independent from δ such that for all $0 < \delta < \delta_0$, $x_0 \in \mathbb{T}^d$:

$$\|\mathcal{L}aw(X_n) - \mu^\delta\|_{TV} \leq C e^{-c\delta n}.$$

Proof. The existence of a unique solution X^{x_0} to Equation (5.6) with initial condition x_0 comes from [154, Corrolary 7.1.7 and 8.1.7]. By Itô's formula, the law M^{x_0} of $(X_t^{x_0})_{t \in [0, T]}$ (a probability

measure on $\mathcal{C}([0, T], \mathbb{T}^d)$ is a measure solution to the Kolmogorov equation

$$\partial_t M^{x_0} = L^* M^{x_0},$$

where L^* is the dual in $L^2(\mathbb{R}^d)$ of the generator

$$L\varphi = b(x) \cdot \nabla \varphi + \frac{\sigma^2}{2} \Delta \varphi,$$

in the sense that for all function $\varphi \in \mathcal{C}^2([0, T] \times \mathbb{T}^d, \mathbb{R})$

$$\int_{[0, T] \times \mathbb{T}^d} (\partial_t - L)\varphi(t, x) M^{x_0}(dt, dx) = 0.$$

Thus, according to [18, Proposition 6.5.1], $\mathcal{L}aw(X_t^{x_0})$ (the time-marginal of M^{x_0}) admits a density $h^{x_0}(t, \cdot)$ with respect to the Lebesgue measure, for all $t > 0$, and for any compact interval $J \subset \mathbb{R}_+$

$$h^{x_0} \in \mathbb{H}^{p,1}(J) := \left\{ u : \mathbb{R}_+ \times \mathbb{T}^d \rightarrow \mathbb{R}, \int_J \|u(t, \cdot)\|_{H^{p,1}} dt < \infty \right\},$$

where $\|\cdot\|_{H^{p,1}}$ is the classical Sobolev norm, for some $p > d + 2$. Since we are in a compact set, $h^{x_0} \in \mathbb{H}^{2,1}$, and [18, Proposition 6.2.7] yields that h^{x_0} satisfies an Harnack inequality for t great enough: there exists $C, \tau > 0$ such that for all $x_0 \in \mathbb{T}^d$ and t great enough:

$$\sup_{\mathbb{T}^d} h^{x_0}(t - \tau, \cdot) \leq C \inf_{\mathbb{T}^d} h^{x_0}(t, \cdot).$$

Since $h^{x_0}(t - \tau, \cdot)$ is a probability density, we have $\sup_{\mathbb{T}^d} h^{x_0}(t - \tau, \cdot) \geq \text{Leb}(\mathbb{T}^d)$, where Leb stands for the Lebesgue measure. In particular, there exists $t_0 > 0$ such that:

$$\inf_{x_0 \in \mathbb{T}^d} \inf_{\mathbb{T}^d} h^{x_0}(t_0, \cdot) > 0.$$

This is a Doeblin condition for the law of the process, with reference measure the Lebesgue measure, and in particular it classically implies the existence of a unique stationary measure for the process (5.2) and the exponential convergence of the law at time t toward this equilibrium.

For the Euler-Maruyama scheme, fix $n = \lfloor t/\delta \rfloor$, and write:

$$X_n^{x_0} = x_0 + \delta \sum_{k=0}^{n-1} b(X_k^{x_0}) + \sqrt{\delta} \sum_{k=0}^{n-1} G_k,$$

and

$$G = n^{-1/2} \sum_{k=0}^{n-1} G_k.$$

We have $\delta \sum_{k=0}^{n-1} b(X_k^{x_0}) \leq t \|b\|_\infty$. If $A \subset \mathbb{T}^d$ is a measurable set, we are looking for a lower bound on $\mathbb{P}(X_n^{x_0} \in A)$. Let $\bar{X}_n^{x_0}$ be the Euler scheme seen on \mathbb{R}^d rather than \mathbb{T}^d (considering b as a periodic function), with initial condition given as the representant of x_0 in $[0, 1)^d$ and let \bar{A} be the intersection of $[0, 1)^d$ with the pre-image of A by the periodic quotient $\mathbb{R}^d \rightarrow \mathbb{T}^d$. Then,

$\mathbb{P}(X_n^{x_0} \in A) \geq \mathbb{P}(\bar{X}_n^{x_0} \in \bar{A})$, and

$$\begin{aligned} \mathbb{P}(\bar{X}_n^{x_0} \in \bar{A}) &= \mathbb{P}\left(\sqrt{n\delta}G \in \bar{A} - x_0 - \delta \sum_{k=0}^{n-1} b(X_k)\right) \\ &\geq \inf_{|a| \leq 2\pi d + t \|b\|_\infty} \int_{\bar{A}-a} e^{-|y|^2/(t-\delta)} dy \\ &\geq e^{-2(4\pi d + t \|b\|_\infty)/t} \text{Leb}(A). \end{aligned}$$

In other words, the n -step transition kernel of the Euler scheme satisfies a Doeblin condition with constant independent from the step size δ . This implies the existence of a unique stationary measure μ^δ such that for all $k \in \mathbb{N}$,

$$\|\mathcal{L}aw(X_{k\lfloor t/\delta \rfloor}) - \mu^\delta\|_{TV} \leq \alpha^k \|\mathcal{L}aw(X_0) - \mu^\delta\|_{TV}.$$

This gives for all $n \in \mathbb{N}$

$$\begin{aligned} \|\mathcal{L}aw(X_n) - \mu^\delta\|_{TV} &\leq \|\mathcal{L}aw(X_{\lfloor t/\delta \rfloor \lfloor n/\lfloor t/\delta \rfloor \rfloor}) - \mu^\delta\|_{TV} \\ &\leq \alpha^{\lfloor n/\lfloor t/\delta \rfloor \rfloor} \|\mathcal{L}aw(X_0) - \mu^\delta\|_{TV} \leq Ce^{-c\delta n}, \end{aligned}$$

which concludes the proof. \square

We now turn to the analysis of the noisy GAD (5.3). When $\varepsilon' > 0$, we get an elliptic diffusion with bounded drift on a smooth compact manifold with no boundary, so essentially the adaptation of Proposition 5.2.1 in this more general context apply. In the following we focus on the case $\varepsilon' = 0$. Indeed, one may think that it is only necessary to have noise on the position in order to visit the whole space, and then the auxiliary vector V will go to the associated eigenvectors. The question is whether the process is hypoelliptic and controllable. However, it is clear that it cannot be the case in general, simply by considering counter-examples of the form

$$U(x) = \sum_{i=1}^d U_i(x_i).$$

Indeed, in these cases, if e.g. $v_0 = (1, 0, \dots, 0)$, then $v_t = v_0$ for all $t \geq 0$, hence there are no hope of having a unique stationary measure, and convergences towards it for all initial conditions. Let us discuss some additional conditions that ensure this result. First, notice that if $(X_t, V_t)_{t \geq 0}$ is a noisy GAD then so is $(X_t, -V_t)_{t \geq 0}$. In fact the relevant variable to define the process is not V_t but the class $\{V_t, -V_t\}$ on the projective sphere $\mathbb{P}^d = \mathbb{S}^{d-1}/\mathcal{R}$ with the equivalence relation given by $v\mathcal{R}u$ iff $u = -v$ or $u = v$, and we identify the process with its projection on $\mathbb{T}^d \times \mathbb{P}^d$ (which is still a Markov process, solution of the same SDE (5.3) but where the drift of V_t is seen as a vector field on \mathbb{P}^d).

Proposition 5.2.2. *If U is \mathcal{C}^3 , then the noisy GAD is well-defined in the sense that there exists a unique strong solution to Equation (5.3). If in addition, we suppose that the potential U satisfies the following:*

- *There exists $(\tilde{x}, \tilde{v}) \in \mathbb{T}^d \times \mathbb{P}^d$ such that:*

$$(\partial_{x_i} \nabla^2 U(\tilde{x}) \tilde{v})_{1 \leq i \leq d}$$

spans \tilde{v}^\perp .

- For all $v \in \mathbb{P}^d$, there exists H in the convex hull of the set

$$\{\nabla^2 U(x), x \in \mathbb{T}^d\}$$

such that, denoting by $(\tilde{\lambda}_i)$ the ordered eigenvalues of H and (\tilde{v}_i) the associated eigenvectors,

$$\begin{cases} v &= \tilde{v}_1, \\ \tilde{\lambda}_1 &< \tilde{\lambda}_2. \end{cases}$$

Then the noisy GAD admits a unique stationary measure μ_{GAD} on $\mathbb{T}^d \times \mathbb{P}^d$ with a positive density with respect to the Lebesgue measure. Moreover, for any initial condition, the law at time t of the process converges exponentially fast to μ_{GAD} in total variation.

Remark 5.2.1. The second condition is implied by: For all $v \in \mathbb{P}^d$, there exists $x \in \mathbb{T}^d$ such that

$$\begin{cases} v &= v_1(x), \\ \lambda_1(x) &< \lambda_2(x). \end{cases}$$

Proof. If U is \mathcal{C}^3 , then the noisy GAD is an SDE with Lipschitz coefficient, hence its well-posedness. The first additional assumption ensures that the generator of the noisy GAD

$$\mathcal{L} = -(I - 2vv^t)\nabla U(x) \cdot \nabla_x + \varepsilon\Delta_x - \frac{1}{\eta}(I - vv^t)\nabla^2 U(x)v \cdot \nabla_v$$

satisfies a weak Hörmander condition at (\tilde{x}, \tilde{v}) , see [152].

Next, we want to establish the controllability of the process, in the following sense: fix $(x_{ini}, v_{ini}), (x_f, v_f) \in \mathbb{T}^d \times \mathbb{P}^d$, $\delta > 0$. We want to show that there exists $T > 0$ and a control $u \in \mathcal{C}^0([0, T], \mathbb{R}^d)$ such that the solution of

$$\begin{cases} x'(t) &= -(I - 2v(t)v(t)^T)\nabla U(x(t)) + u(t), \\ v'(t) &= -\frac{1}{\eta}(I - v(t)v(t)^T)\nabla^2 U(x(t))v(t), \end{cases} \quad (5.7)$$

with $(x(0), v(0)) = (x_{ini}, v_{ini})$, satisfies $\|(x(1), v(1)) - (x_f, v_f)\| \leq \delta$.

We first suppose that v_{ini} and v_f are not orthogonal. Fix H such that the second condition of Proposition 5.2.2 is satisfied with $v = v_f$, and x_1, \dots, x_p , and $\alpha_1, \dots, \alpha_p$ such that

$$H = \sum_{i=1}^p \alpha_i \nabla^2 U(x_i), \quad \sum_{i=1}^p \alpha_i = 1.$$

Fix $T > 0$, $n \in \mathbb{N}$, and $\gamma > 0$ such that $T = n(\gamma + \gamma^2 + 2\gamma^4) + \gamma^2 + \gamma^4$. Write $\beta_i = \alpha_1 + \dots + \alpha_i$, and for $k \in \llbracket 0, n \rrbracket$:

$$u(t) = \begin{cases} (-x_{ini} + x_1)/(\alpha_1\gamma^2) & \text{if } 0 < t < \alpha_1\gamma^2, \\ (I - 2v(t)v(t)^t)\nabla U(x_1) & \text{if } \alpha_1(\gamma^2 + \gamma^4) < t < \alpha_1(\gamma + \gamma^2 + \gamma^4), \\ (x_{i+1} - x_i)/(\alpha_{i+1}\gamma^2) & \text{if } (k + \beta_i)(\gamma + \gamma^2 + 2\gamma^4) \\ & < t < (k + \beta_i)(\gamma + \gamma^2 + 2\gamma^4) + \alpha_{i+1}\gamma^2, \\ (I - 2v(t)v(t)^t)\nabla U(x_i) & \text{if } (k + \beta_i)(\gamma + \gamma^2 + 2\gamma^4) + \alpha_{i+1}(\gamma^2 + \gamma^4) \\ & < t < (k + \beta_{i+1})(\gamma + \gamma^2 + 2\gamma^4) - \alpha_{i+1}\gamma^4, \\ (x_f - x_p)/\gamma^2 & \text{if } T - \gamma^2 < t < T, \end{cases}$$

and u is linear on the remaining intervals of size γ^4 . Write as well

$$\bar{x}(t) = x_i \text{ for } (k + \beta_{i-1})\gamma < t < (k + \beta_i)\gamma, \quad k \in \mathbb{N}.$$

As γ goes to 0, v converges towards the solution to

$$\bar{v}'(t) = -\frac{1}{\eta}(I - \bar{v}(t)\bar{v}(t)^T)\nabla^2 U(\bar{x}(t))\bar{v}(t)$$

which is itself close to

$$w'(t) = -\frac{1}{\eta}(I - w(t)w(t)^T)Hw(t).$$

For clarity, we only show the second point which is the more complex one. We may write for all $0 \leq u \leq T$:

$$\begin{aligned} & \left\| \int_0^u (I - \bar{v}_s \bar{v}_s^t) \nabla^2 U(\bar{x}) \bar{v}_s ds - \int_0^u (I - \bar{v}_s \bar{v}_s^t) H \bar{v}_s ds \right\| \\ & \leq \left\| \int_0^u (I - \bar{v}_s \bar{v}_s^t) \nabla^2 U(\bar{x}) \bar{v}_s ds - \sum_{k=0}^{m-1} \sum_{i=1}^p (I - \bar{v}_{k\gamma} \bar{v}_{k\gamma}^t) \nabla^2 U(x_i) \bar{v}_{k\gamma} \alpha_i \gamma \right\| \\ & + \left\| \sum_{k=0}^{m-1} \sum_{i=1}^p (I - \bar{v}_{k\gamma} \bar{v}_{k\gamma}^t) \nabla^2 U(x_i) \bar{v}_{k\gamma} \alpha_i \gamma - \sum_{k=0}^{m-1} \sum_{i=1}^p (I - \bar{v}_{k\gamma} \bar{v}_{k\gamma}^t) H \bar{v}_{k\gamma} \gamma \right\| \\ & + \left\| \sum_{k=0}^{m-1} \sum_{i=1}^p (I - \bar{v}_{k\gamma} \bar{v}_{k\gamma}^t) H \bar{v}_{k\gamma} \gamma - \int_0^u (I - \bar{v}_s \bar{v}_s^t) H \bar{v}_s ds \right\|. \end{aligned}$$

where $m = \lfloor u/\gamma \rfloor$. By hypothesis on H , the second term is 0. \bar{v} depends on γ by definition, but it is $\|\nabla U\|_\infty$ -Lipschitz for all $\gamma > 0$, hence the first and third term are going to 0 as $\gamma \rightarrow 0$, uniformly on $0 \leq u \leq T$. The map $v \mapsto (I - vv^t)Hv$ is \mathcal{C}^1 on a compact set, hence is Lipschitz. Thus we have:

$$\|\bar{v}(u) - w(u)\| \leq L \int_0^u \sup_{r < s} \|\bar{v}(r) - w(r)\| ds + \left\| \int_0^u (I - \bar{v}_s \bar{v}_s^t) \nabla^2 U(\bar{x}) \bar{v}_s ds - \int_0^u (I - \bar{v}_s \bar{v}_s^t) H \bar{v}_s ds \right\|,$$

and

$$\sup_{0 \leq u \leq T} \|\bar{v}(u) - w(u)\| \leq e^{LT} \sup_{0 \leq u \leq T} \left\| \int_0^u (I - \bar{v}_s \bar{v}_s^t) \nabla^2 U(\bar{x}) \bar{v}_s ds - \int_0^u (I - \bar{v}_s \bar{v}_s^t) H \bar{v}_s ds \right\| \xrightarrow{\gamma \rightarrow 0} 0.$$

Now, all it remains to do is to fix $T > 0$ great enough so that $w(T)$ is in the δ -neighborhood of v_f , then γ small enough so that $v(T)$ is as well, and n accordingly.

If v_{ini} and v_f are orthogonal, writing π for the canonical projection from \mathbb{S}^{d-1} to \mathbb{P}^d , there exists an intermediate v_{inter} which is not orthogonal to neither v_{ini} or v_f , and the same control allows to go from (x_{ini}, v_{ini}) to (x_{ini}, v_{inter}) in a time T , and from (x_{ini}, v_{inter}) to (x_f, v_f) in another time T .

We conclude with [152, Theorem 2.1] for the existence of the stationary measure and the convergence, and with [120, Theorem 5.2] for the positive density. \square

5.2.2 Switched processes

When the mode $(I_t)_{t \geq 0}$ is an autonomous Markov chain on a finite set $\llbracket 0, m-1 \rrbracket$, $m \in \mathbb{N}$ (i.e., as it is the case in the processes we have considered in Section 5.1.3, if its jump rate does not depend on X) then the well-posedness of switched processes of the form

$$dX_t = H_{I_t}(X_t)dt + \sigma_{I_t}(X_t)dB_t, \quad (5.8)$$

with some drifts H_0, \dots, H_{m-1} immediately follows from the well-posedness of the corresponding diffusion processes for each $i \in \llbracket 0, m-1 \rrbracket$, since the process is then simply defined by induction along the jump times of I . In particular, in view of the previous section, the ISP (5.4) is well defined.

Moreover, in general, it is sufficient that one of the diffusion processes satisfies a Doeblin condition to imply the same for the switched process:

Proposition 5.2.3. *If I is irreducible and there exists i_0 such that the diffusion (5.8) with $I_t = i_0$ satisfies a Doeblin condition (see the introduction of Section 5.2), then the switched process admits a unique invariant probability measure, and the law of the switched process converges exponentially fast towards this stationary measure.*

Proof. The existence results from the previous construction. Fix $t_0 > 0$ such that for all $t > t_0$, $x \in \mathbb{R}^d$, $A \subset \mathbb{T}^d$ measurable,

$$\mathbb{P}_x(\bar{X}_t \in A) \geq cl(A)$$

where $c > 0$ and \bar{X} is a solution to equation (5.8) with $I_0 = i_0$. Since I is an irreducible Markov process, we have for $t > 0$

$$\mathbb{P}(I_s = i_0, \forall s \in [t, 2t]) > 0.$$

Hence we have:

$$\begin{aligned} \mathbb{P}(X_{2t} \in A, I_{2t} = i_0) &\geq \mathbb{P}(X_{2t} \in A, I_s = i_0, \forall s \in [t, 2t]) \\ &= \mathbb{E}(\mathbb{P}_{X_t}(\bar{X}_t \in A) \mathbb{1}_{I_s = i_0, \forall s \in [t, 2t]}) \\ &\geq cl(A)\mathbb{P}(I_s = i_0, \forall s \in [t, 2t]) \\ &= \tilde{c}l(A), \end{aligned}$$

which is a Doeblin condition with reference measure $l \otimes \delta_{i_0}$, and this concludes the proof. \square

Corollary 5.2.1. *The ISP is well-defined, admit stationary measure, and its laws converge as t goes to infinity exponentially fast towards its unique stationary measure in the total variation distance.*

5.3 Numerical experiments

The main goal of the present work is to gain some empirical insights on the qualitative behavior of the processes introduced in Section 5.1.3 on simple models. Some questions that we have in particular are the following: what happens if the direction of the gentlest ascend starting from a local minimum does not correspond to the direction the process has to take eventually to find a saddle point? How does the process behave in front of attractive singularities of the ISD flow? How does the efficiency of the process (in terms of exploration) depend on the switching rate? How does it compare to a basic overdamped Langevin process?

We will consider three models. The first one is a mixture of Gaussian, for which we can easily choose where are the minima and the saddle point and what are the gentlest ascend directions at the minima. The second one is the function studied in [115], for which the unique saddle point is separated from the two minima by singular lines. Finally, the third example, in higher dimension and closer to a genuine application, is the Lennard-Johns cluster model with 7 particles.

Contrary to the theoretical analysis, most processes here live on \mathbb{R}^d , which may raise a stability issue. This can be seen in dimension 1, where the process switch between a gradient descent and a gradient ascent, and thus can be non recurrent, or even explosive e.g. for potential of the form $|x|^4$ at infinity. This can be solved by a suitable modification of the dynamics outside some compact set, for instance replacing H_1 in (5.4) by $\tilde{H}_1(x) = H_1(x)1_{|x| \leq R} + H_0(x)1_{|x| > R}$ or a smooth interpolation, or adding a deterministic jump from $I_t = 1$ to $I_t = 0$ when $|X_t| \geq R$. Then, classical Lyapunov conditions on U implies that the process remains stable. However, this will not be necessary in our simple numerical experiments.

5.3.1 First 2D model: a mixture of Gaussians

We consider here a mixture of Gaussian in dimension 2. The potential is of the form:

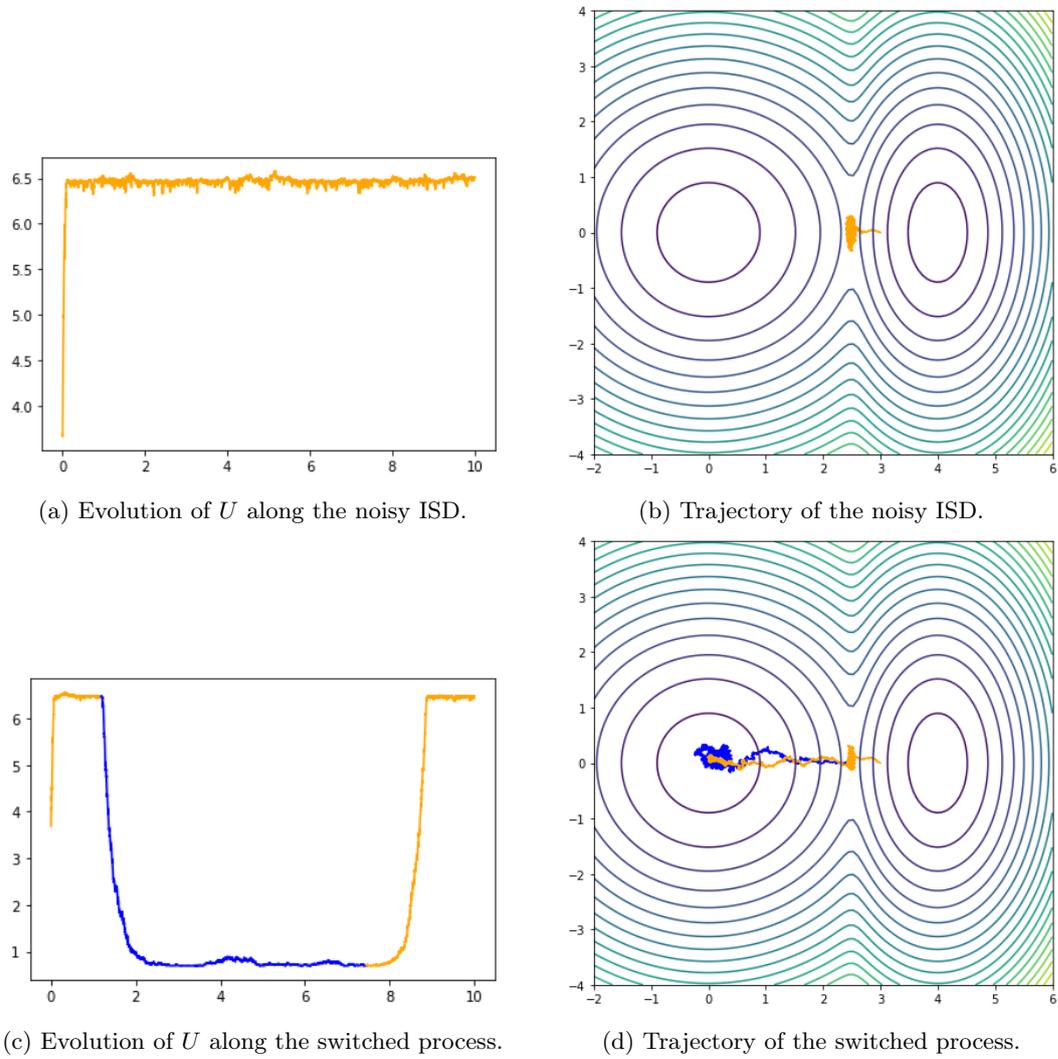
$$U_1(x, y) = -\ln \left(\frac{1}{2} e^{-(x^2+y^2)} + \frac{1}{2} e^{-s_x(x-m_x)^2 - s_y(y-m_y)^2} \right),$$

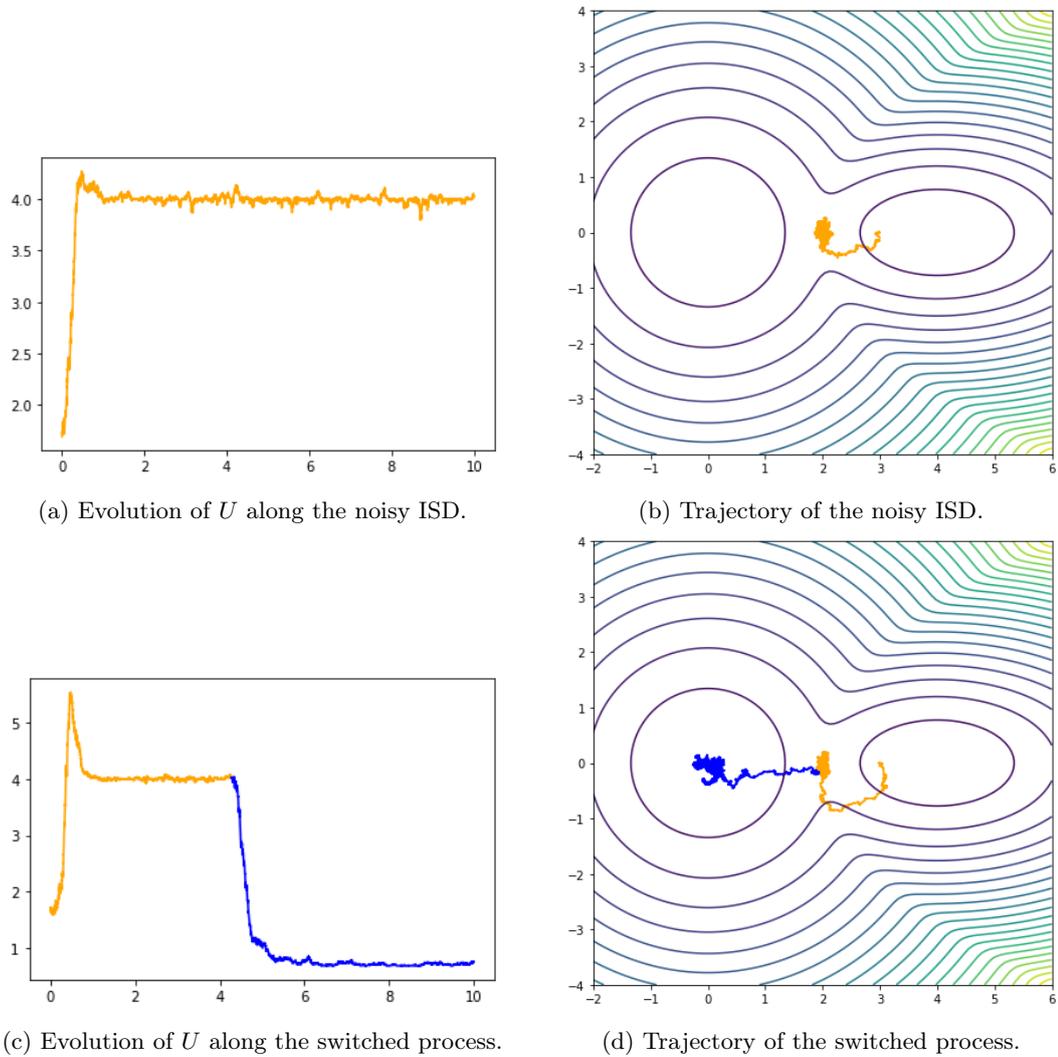
with some parameters $m_x, m_y \in \mathbb{R}$, $s_x, s_y > 0$. This is a classical model in statistics for multimodal problems. Here we take $(m_x, m_y) = (4, 0)$ and consider two cases, either $(s_x, s_y) = (3, 1)$ or $(s_x, s_y) = (1, 3)$, see Figure 5.1 and 5.2. In those figures, we represent a typical trajectory of the noisy ISD and of the ISP, with $\varepsilon = 0.03$, the final time $T = 10$, and $\nu = 0.2$ in the case of the ISP, as well as the level lines of the potential. In these two cases, there are two local minimizers $(\tilde{x}_1, 0)$ and $(\tilde{x}_2, 0)$ separated by a unique saddle point $(\tilde{z}, 0)$, where $\tilde{x}_1 < \tilde{z} < \tilde{x}_2$, but they differ by the direction taken by the saddle search in the well from the left. The yellow part represent the trajectories of the noisy ISD, or the part of the ISP where $I_t = 1$, and in blue the part of the ISP where $I_t = 0$ (corresponding to a gradient descent).

According to the Large Deviation Principle, for a small ε , if the initial condition corresponds to the right local minima $(\tilde{x}_2, 0)$, the overdamped Langevin process (5.1) will typically stays in the vicinity of this minimizer for a time exponentially long with ε , and will likely go from there to the other minimizer by following in reverse the trajectory of a gradient descent starting from a point arbitrarily close to the saddle point (which in the present case is a straight line from the minimum to the saddle point), see [65, Chapter 4, Theorem 2.1] as well as their computation of the quasi-potential.

In the case $(s_x, s_y) = (3, 1)$, with some initial condition $(x_0, 0)$, $\tilde{z} < x_0 < \tilde{x}_2$, the noisy (and deterministic) ISD will follow the same reactive trajectory as the overdamped Langevin process, the gentlest way to go to the saddle point being here along the gradient, but it happens much earlier (since this is the behaviour of the deterministic system at $\varepsilon = 0$ and not a large deviation from it). However, in the case, $(s_x, s_y) = (1, 3)$, the gentlest way to leave the right minima is to start along the directions $(0, 1)$ and $(0, -1)$, see figure 5.2. Nevertheless, independently from this difference in the beginning of the trajectory, in both cases the saddle point is found by the deterministic dynamics for initial condition between \tilde{x}_1 and \tilde{x}_2 .

For initial condition (x_0, y_0) with $x_0 > \tilde{x}_2$, the ISD goes to infinity. Hence, the dynamics has to be modified outside some compact set, as explained in the introduction of this section, so that the process does not escape to infinity. In that case, one only need to wait for the process to enter the domain of attraction of the saddle point for the deterministic ISD.

Figure 5.1: Case $(s_x, s_y) = (3, 1)$

Figure 5.2: Case $(s_x, s_y) = (1, 3)$.

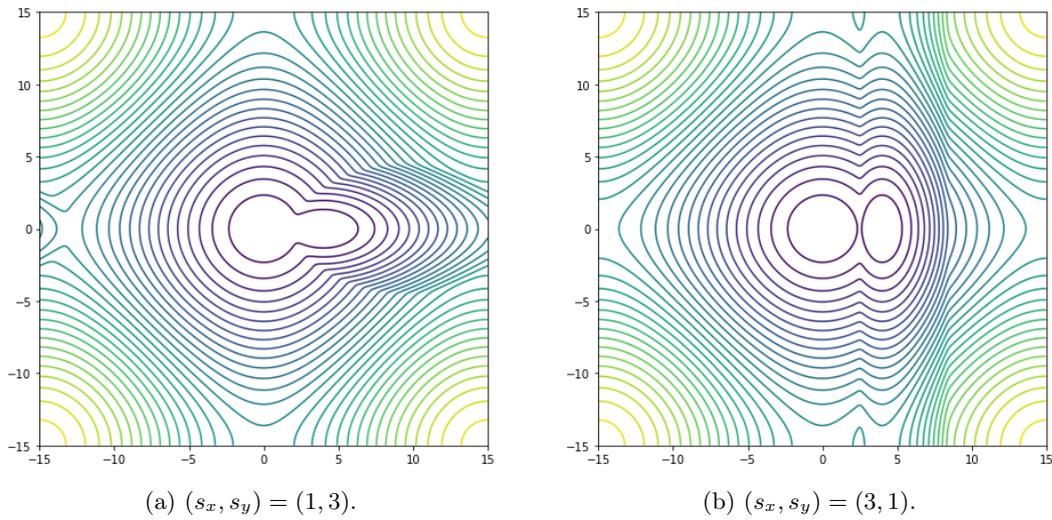
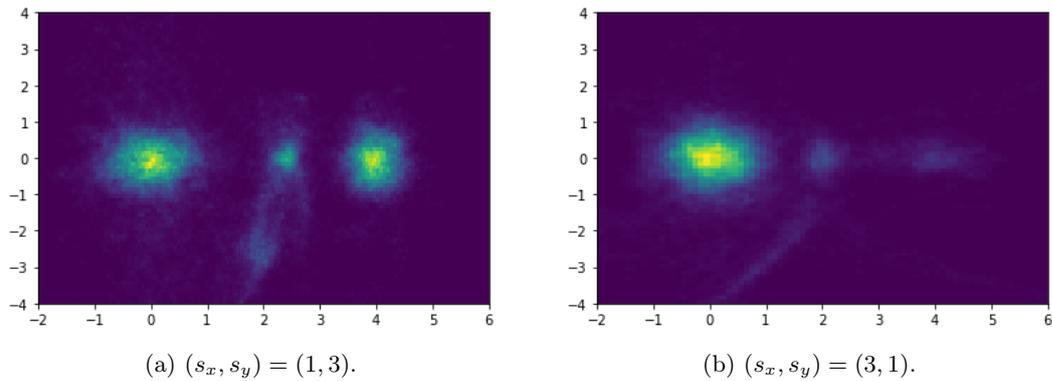


Figure 5.3: Periodized potential.

Figure 5.4: Invariant measure of the ISP for $\nu = 0.1$, $\varepsilon = 0.05$.

However, as an alternative way to enforce stability in order to get quantitative results, in the present case with a simple illustrative purpose, we simply use a periodized version of the potential. Denote

$$\tilde{U}_1(x, y) = -\ln \left(\frac{1}{2} e^{-L^2(\sin^2(x/L) + \sin^2(y/L))} + \frac{1}{2} e^{-L^2(s_x \sin^2((x-m_x)/L) + s_y \sin^2((y-m_y)/L))} \right),$$

where $L > 0$ is a parameter, see Figure 5.3. This periodized potential has two supplementary saddle point, but for all $(x, y) \in \mathbb{R}^2$, $\lim_{L \rightarrow \infty} \tilde{U}_1(x, y) = U_1(x, y)$, and we may defined the ISP on $(\pi L\mathbb{T})^2$.

Using a 2-D histogram, $\nu = 0.1$, $\varepsilon = 0.05$, we get a representation of the invariant measure in Figure 5.4. We see that the invariant measure charges both minima, as well as the saddle point between the two.

Now, if the goal is to find both minima, then one can find one of them using a gradient descent, and the second one using the ISP. Since the ISD allows to find the saddle point, then

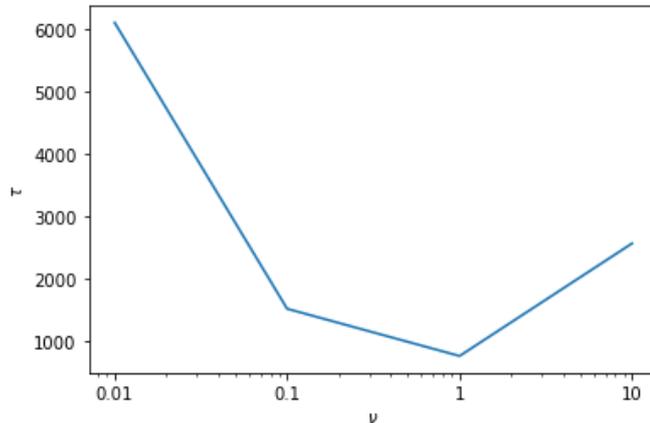


Figure 5.5: Time to reach a minima from the other one on the periodized potential.

if the switching rate is low enough, the switched process will do as well, and thanks to the Brownian noise, after a first switch, will have a positive probability to be in the domain of attraction for the gradient descent of the second minima, and thus will find it. If it was not in the right domain of attraction, then the process will go back to the first well, and repeat the same kind of trajectories. The success of the algorithm is then the same as the one of a rigged coin flip. For a small ε , as long as the transitions from one well to another are driven by this switching behaviour, the transition time behaves much better than the exponentially long time of the overdamped Langevin dynamics (with Brownian-driven rare transitions). At a fixed ε , when the switching rate becomes too small, the process has to wait for switching events to cross the saddle (and eventually when it becomes very small the process behaves like the overdamped Langevin dynamics and the transitions are driven by the small Brownian noise); on the other hand, a large switching rate induces an averaging phenomenon (the drift along the gentlest ascend direction vanishes), which impairs the efficiency. Thus, there should be an optimal switching rate in terms of mean transition time. This is indeed what we observed, see Figure 5.5. The numerical experiment were conducted with $\varepsilon = 0.03$, $(x_0, y_0) = (4, 0)$, $I_0 = 0$, and the time was estimated by Monte-Carlo with $n = 15$ repetitions.

5.3.2 A 2D model with singular lines

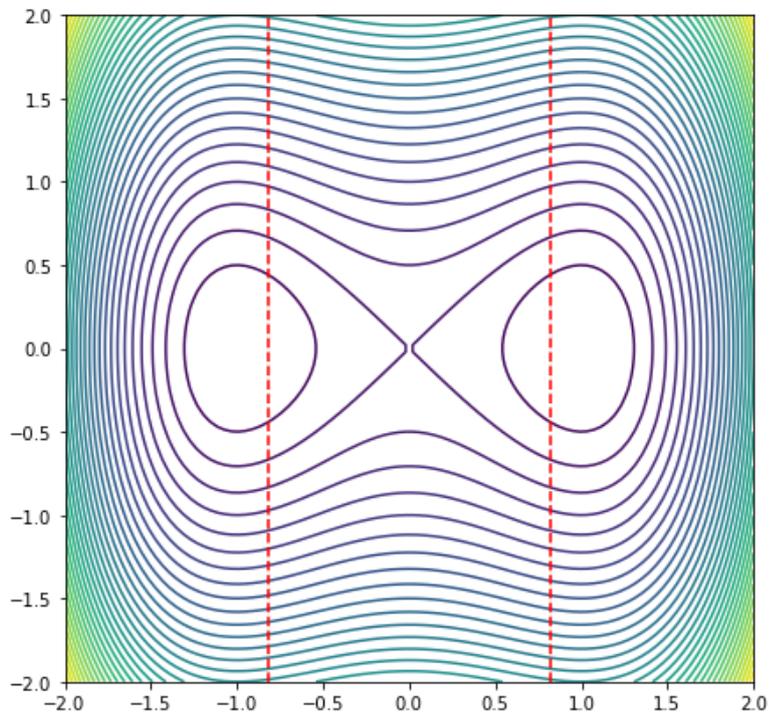
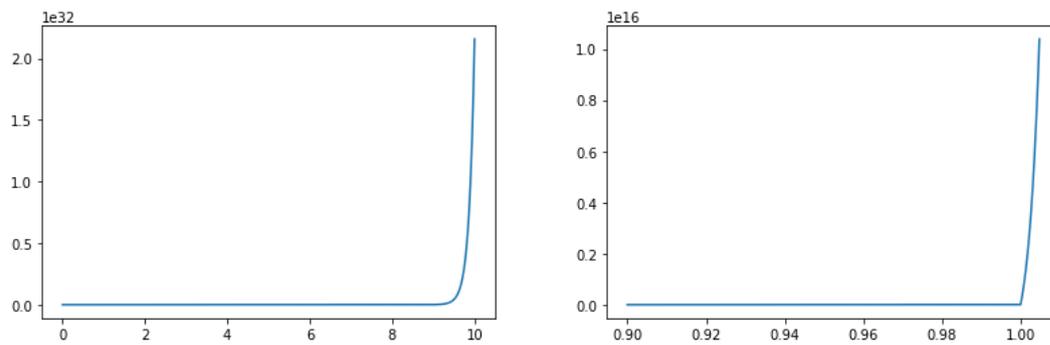
Now we are interested in the following potential:

$$U_2(x, y) = (1 - x^2)^2 + 2y^2,$$

for $(x, y) \in \mathbb{R}^2$, see Figure 5.6.

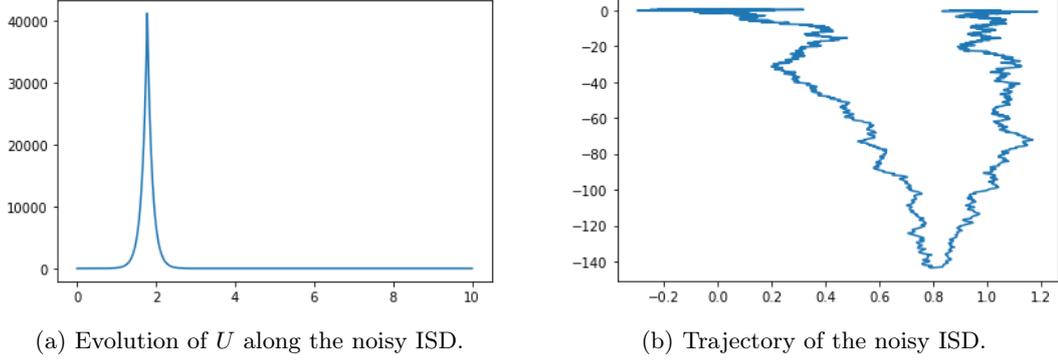
The deterministic ISD and GAD have been studied for this potential in [115]. This potential has two minima, $(-1, 0)$ and $(1, 0)$, and one saddle point $(0, 0)$. However, there are two lines, $\{x = \pm\sqrt{4/6}\}$, for which the Hessian of U has two equal eigenvalues. The deterministic GAD and ISD cannot cross those lines, and go to infinity, see Figure 5.7. In the noisy case, the Brownian motion may allow the process to cross the line, see Figure 5.8.

As seen in figure 5.8, the Brownian motion allow to cross the set of singularities, but for small ε , this crossing may happen far from the set of minima and saddle point, because the deterministic process satisfies $\lim_{t \rightarrow \infty} y_t = +\infty$ for $x_0 > \sqrt{4/6}$ and $y_0 > 0$, where (x_t, y_t) is the

Figure 5.6: Level line of the potential U_2 .(a) Evolution of U along the deterministic ISD.

(b) Trajectory of the deterministic ISD.

Figure 5.7: $\varepsilon = 0.0$.

Figure 5.8: $\varepsilon = 0.05$.

ISD. The singular lines are repulsive, and for $x > \sqrt{4/6}$, the process is attracted to the line $\{x = 1\}$. Concretely, for the process to cross the singular line, the noise must be great enough so that this occurs before the simulation stops due to numerical limits.

Since the existence of this singularity results from a crossing between the eigenvalues of the Hessian of the potential U_2 , we study the solution to solve the issue of singularities proposed in Section 5.1.3, to see in particular if it allows a faster convergences towards the saddle point in our example here. Recall the set of singularities:

$$\mathcal{S} = \{(x, y) \in \mathbb{R}^2, \lambda_1(x, y) = \lambda_2(x, y)\},$$

and the modified noisy ISD (writting $z = (x, y)$ and Z_t the process):

$$Z_t = - (I - 2g(Z_t)v_1(Z_t)^t v_1(Z_t) - (2 - g(Z_t)v_2(Z_t)^t v_2(Z_t))) \nabla U_2(Z_t) dt + \sqrt{2\varepsilon} dB_t,$$

with $g(z) = f(\lambda_2(z) - \lambda_1(z))$ for some function $f: \mathbb{R}_+ \rightarrow \mathbb{R}_+$ such that $f(0) = 1$, and $f(r) = 2$ for $r \geq r_*$, and some small $r_* > 0$. As explained, the idea is to replace the reflection with respect to $v_1(x)^\perp$ by a projection on $\text{vect}(v_1(x), v_2(x))^\perp$.

In dimension 2, the process simply becomes a Brownian motion near \mathcal{S} . For numerical study we consider:

$$f_1(r) = 1 + \mathbb{1}_{r > r_*},$$

and

$$f_2(r) = 1 + \frac{r}{r_*} \mathbb{1}_{r \leq r_*} + \mathbb{1}_{r > r_*},$$

where $r_* > 0$ is a fixed parameter. An example of trajectory with f_1 , is given in Figure 5.9.

We compare the speed at which the process reaches the saddle point with the different cut function $f_0 = 2$, f_1 , and f_2 . We chose as parameter $r_* = 2$, $x_0 = (0.9, 0)$, and $n = 500$ trials. The average of

$$\tau = \inf \{t \geq 0, |X_t| < 0.1\},$$

over the n trials is displayed in Figure 5.10 for $\varepsilon \in \{0.03, 0.04, 0.05, 0.06\}$.

We can see that the regularised dynamics reach the saddle point faster than the initial dynamic with f_0 . Moreover, as explained before, for smaller values of ε , there is a positive probability that the process doesn't reach the saddle point before hitting numerical limits. For a given temperature ε , this probability is lower for the processes defined from f_1 or f_2 . This possible failure was not observed in the experiments displayed in Figure 5.10, but for $\varepsilon = 0.02$, we

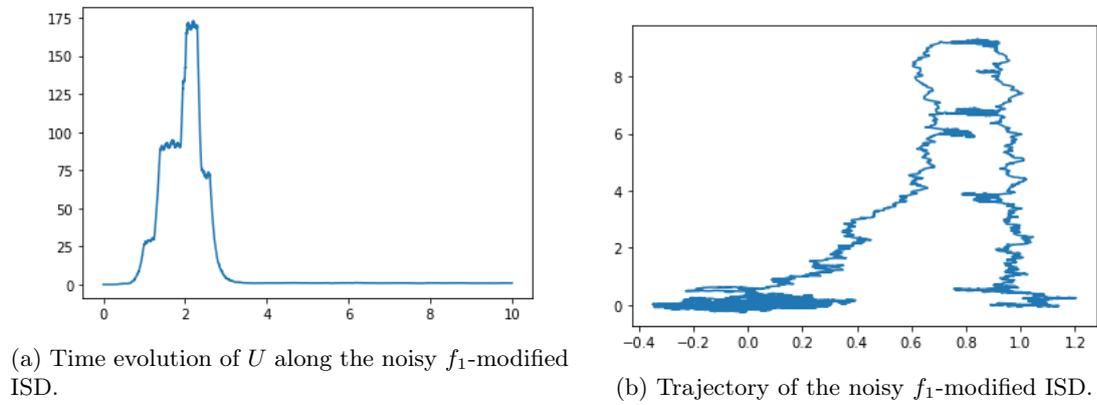
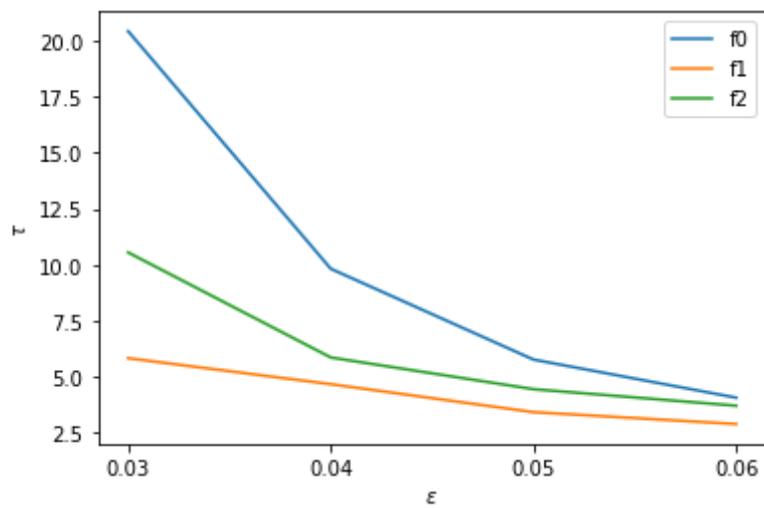
Figure 5.9: f_1 -modified ISD, $\varepsilon = 0.05$.

Figure 5.10: Time to reach the saddle point.

estimated the probability of failure with 500 trials for each process. We get 0.394 for f_0 , and 0.046 for f_2 . Even at $\varepsilon = 0.02$, no failure was observed for f_1 .

Here we haven't used any of the modifications discussed at the beginning of Section 5.3 to enforce stability, in order to study the effects of the singular line on the time needed to find the saddle point.

5.3.3 Lennard-Jones clusters

We now study numerically the process for a potential in higher dimension. Consider the Lennard-Jones potential for $N = 7$ particles in dimension 2, given by

$$U_3(x_1, \dots, x_N) = \sum_{i < j} W(|x_i - x_j|),$$

where $x_i \in \mathbb{R}^2$ for all $1 \leq i \leq N$, and for $r > 0$:

$$W(r) = 4 \left(\frac{1}{r^{12}} - \frac{1}{r^6} \right).$$

The potential U is invariant by rotation and translation of the full system and by permutation of the particles. Once these symmetries are ruled out, it has three non-global local minima, and an additional global one, represented in Figure 5.11. Lennard-Jones clusters in dimension 2 or 3 are classical models in physics and have been extensively, see e.g. [141, 40] and references within.

We use as initial condition the local minimum such that $U \approx -11, 47$, and we compute the time necessary for the process to visit all minima for different values of ν and ε , estimated over 20 experiments. The average time is given in Figure 5.12. These results confirm the interpretation of Figure 5.5 discussed in Section 5.3.1. We see that the sensibility of the exploration time to the switching rate increases as the temperature ε decreases, as should be expected: in the high frequency regime, the drift along the gentlest ascent direction averages to zero so that, in that direction, the process moves at the speed of a Brownian motion with variance ε ; in the low frequency regime, the transitions between different wells are driven by the Brownian noise and thus follow an Eyring-Kramers formula, so that the mean transition time is exponentially large with ε^{-1} .

Since U_3 is invariant by global translations and rotations of the system, 0 is always an eigenvalue of its Hessian, associated to eigenvectors which are orthogonal to ∇U_3 . As a consequence, at points x where $\nabla^2 U_3(x)$ has no negative eigenvalue, the ISD dynamics is the same as the gradient descent dynamics. For a real application, these known symmetries should be taken into account in order to avoid this. However, as we saw, even without addressing this issue, the ISP still finds all minima faster than the Langevin process: even though the gentle ascend behaviour plays no role in the vicinity of minimizers, it still makes saddle points locally attractive for the dynamics, which is a key point for the efficiency of the exploration.

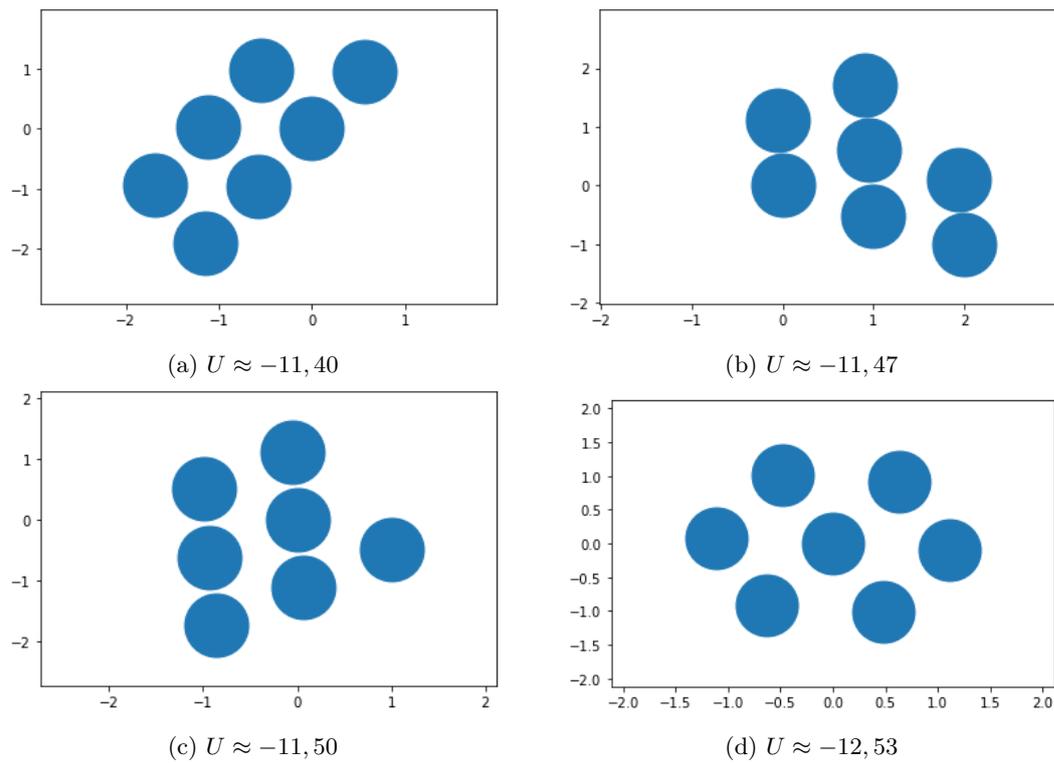
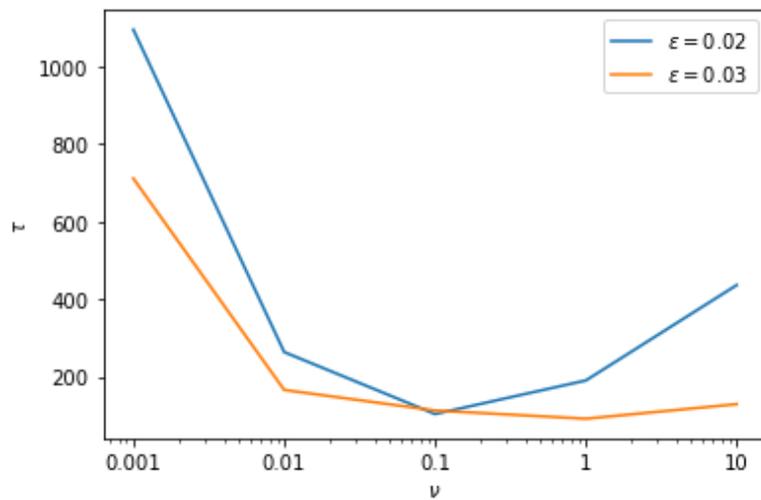
Figure 5.11: List of minimizers of U 

Figure 5.12: Time to visit all minima of the Lennard-Jones cluster.

Part III

Fleming-Viot processes

Chapter 6

Convergence of a particle approximation for the quasi-stationary distribution of a diffusion process: uniform estimates in a compact soft case.

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Abstract : We establish the convergences (with respect to the simulation time t ; the number of particles N ; the timestep γ) of a Moran/Fleming-Viot type particle scheme toward the quasi-stationary distribution of a diffusion on the d -dimensional torus, killed at a smooth rate. In these conditions, quantitative bounds are obtained that, for each parameter ($t \rightarrow \infty$, $N \rightarrow \infty$ or $\gamma \rightarrow 0$) are independent from the two others.

6.1 Introduction

6.1.1 The problem

Start from the diffusion on the d -dimensional periodic flat torus \mathbb{T}^d

$$dZ_t = b(Z_t)dt + dB_t \quad (6.1)$$

with $b \in \mathcal{C}^1(\mathbb{T}^d)$, where $(B_t)_{t \geq 0}$ is a d -dimensional Brownian motion. Add a killing rate $\lambda \in \mathcal{C}(\mathbb{T}^d)$ and, given a standard exponential random variable E independent from $(Z_t)_{t \geq 0}$, define the death time

$$T = \inf \left\{ t \geq 0, E \leq \int_0^t \lambda(Z_s) ds \right\}. \quad (6.2)$$

Then a probability measure ν on \mathbb{T}^d is said to be a quasi-stationary distribution (QSD) associated to the SDE (6.1) and the rate λ if

$$\mathcal{L}aw(Z_0) = \nu \quad \Rightarrow \quad \forall t \geq 0, \mathcal{L}aw(Z_t | T > t) = \nu.$$

In our case, there exists a unique QSD ν_* and, whatever the initial distribution η_0 of Z_0 ,

$$\mathcal{L}aw(Z_t | T > t) \xrightarrow[t \rightarrow \infty]{} \nu_*$$

see e.g. [32, Theorem 2.1]) or Corollary 6.2.8 below.

The present work is dedicated to the proof of convergence of an algorithm designed to approximate ν_* . This is classically done through a system of N interacting particles whose empirical measure converges to $\mathcal{L}aw(Z_t | T > t)$ as $N \rightarrow \infty$, where killed particles are resurrected in a suitable way in order to keep constant the size of the system (while a naive Monte Carlo simulation would see the sample shrink along time). This question has already been addressed by many authors in various contexts, see the discussion in Section 1.3.3. Before introducing the algorithm, stating our results and comparing them with previous works, for now, let us simply highlight the main specificities of the present work.

The first novelty is that we take into account the time-discretization of the continuous-time diffusion. That way, we establish error bounds between the theoretical target QSD and the empirical measure indeed obtained with an actual implementation of the algorithm. There are three sources of errors: first, the continuous-time SDE (6.1) has to be discretized with some time-step parameter $\gamma > 0$. Second, as will be detailed below, a non-linearity in the theoretical algorithm has to be approximated by a system of N particles. This leads to the definition of an ergodic Markov chain whose invariant measure is close, in some sense, for large N , to the QSD of the time-discretization of the diffusion. But then this Markov chain is only run for a finite simulation time $t = m\gamma$, $m \in \mathbb{N}$. A third error term then comes from the fact that stationarity is not fully achieved. We will obtain quantitative error bounds in γ , N and t .

A second specificity is that the bound obtained for each parameter will be uniform in the other two. For instance, the only other work in which the long-time convergence of the chain is proven to be, under some (restrictive) conditions, uniform in N , is [38] in a finite state space. Besides, our work is quite close in spirit to this work of Cloez and Thai.

Finally, although it was not the primary motivation of the present work, it seems that the particular definition of the system of interacting particles considered here, in particular the rebirth mechanism, was not considered in previous works (where, basically, killed particles are

resurrected at the position of one of the other particles). Our variant is initially motivated by the property stated in Proposition 6.1.1 below, which has been indicated to the second author by Bertrand Cloez. Yet, this variant has the unintended advantage to be both discrete in time and non-failable, in the sense that it is well-defined for all times, even though all particles die simultaneously from time to time (see also [142] on this question).

Note that we restrict the study to a compact state space. Moreover, we only consider soft killing at some continuous rate, and no hard killing which would correspond to the case where T is the escape time from some sub-domain (see e.g. [11, 48]). Finally, as will be seen below, as far as the long-time behaviour of the process is concerned we will work in a perturbative regime, namely we will assume that the variations of λ are small with respect to the mixing time of the diffusion (6.1) (while $\|\lambda\|_\infty$ itself is not required to be small). These very restrictive conditions, which rule out many cases of practical interest, have to be considered in light of our very strong results (Theorems 6.1.1 and 6.1.2 below and all the corollaries of Section 6.2.5, gathered in Figure 6.1). In fact, although already interesting by itself, this restricted framework can be thought as a toy model motivated in particular by the case that arises in the parallel replica algorithm [104]. In that case, T is the escape time for (6.1) from a bounded metastable domain, so that the lifespan of the process is expected to be larger than its mixing time (and to depend little from the initial condition, given it is far enough from the boundary). Hence, the compact and perturbative assumptions are consistent with this objective. The restriction to smooth killing rate, however, is made to avoid additional difficulties in the hard case where, even in the metastable case, the probability to leave the domain is high (and exhibits high variations) when the process is close to its boundary. The initial motivation of the present study was to test the general strategy of the proof (via coupling arguments) in a first simple case, with the goal of extending it later on to the metastable hard case by combining it with some Lyapunov arguments to control the variations of the killing rate near the boundary. This is postponed for future work.

This chapter is organized as follows. The algorithm and main results are presented in Section 6.1.2. Section 6.2 contains the proofs, and more precisely: a general coupling argument, which is the central tool for all our results, is presented in Section 6.2.1; the basic bounds in terms of $t \rightarrow +\infty$, $N \rightarrow +\infty$ and $\gamma \rightarrow 0$ are then stated and proven respectively in Sections 6.2.2, 6.2.3 and 6.2.4; finally, these basic results are combined in Section 6.2.5, concluding the proofs of the main theorems and inducing a number of corollaries.

Notations and conventions

We respectively denote $\mathcal{P}(F)$ and $\mathcal{B}(F)$ the set of probability measures and of Borel sets of a Polish space F . Functions on \mathbb{T}^d are sometimes identified to $[0, 1]^d$ -periodic functions, and similar non-ambiguous identifications are performed, for instance if $x \in \mathbb{T}^d$ and G is a d -dimensional standard gaussian random variable, $x + G$ has to be understood in \mathbb{T}^d , etc. A Markov kernel Q on F is indiscriminately understood as, first, a function from F to $\mathcal{P}(F)$, in which case we denote $Q : x \mapsto Q(x, \cdot)$ (where $Q(x, \cdot)$ denotes the probability $A \in \mathcal{B}(F) \mapsto Q(x, A) \in [0, 1]$); second, a Markov operator on bounded measurable functions on F , in which case we denote $Q : f \mapsto Qf$ (where $Qf(x) = \int f(w)Q(x, dw)$); third, by duality, a function on $\mathcal{P}(F)$, in which case we denote $Q : \mu \mapsto \mu Q$ (so that $\mu(Qf) = (\mu Q)f$). In particular, $Q(x, \cdot) = \delta_x Q$ for $x \in F$. If $\mu \in \mathcal{P}(F)$ and $k \in \mathbb{N}_*$, we denote $\mu^{\otimes k} \in \mathcal{P}(F^k)$ the law of a k -uplet of independent random variables with law μ . Similarly, if Q is a Markov kernel on F , we denote $Q^{\otimes k}$ the kernel on F^k such that $Q^{\otimes k}(x, \cdot) = Q(x_1, \cdot) \otimes \cdots \otimes Q(x_k, \cdot)$ for all $x = (x_1, \dots, x_k) \in F^k$. We denote $\mathcal{E}(1)$ the exponential law with parameter 1, $\mathcal{U}(I)$ the uniform law on a set I and $\mathcal{N}(m, \Sigma)$ the

Gaussian law with mean m and variance matrix Σ . We use bold letters for random variables in \mathbb{T}^{dN} and decompose them in d -dimensional coordinates, like $\mathbf{X} = (X_1, \dots, X_N)$ with $X_i \in \mathbb{T}^d$, or $\mathbf{X}_1 = (X_{1,1}, \dots, X_{N,1})$.

6.1.2 The algorithm and main result

Starting from the diffusion (6.1) killed at time T given by (6.2), we introduce two successive approximations. The first is time discretization. For a given time step $\gamma > 0$ and a sequence $(G_k)_{k \in \mathbb{N}}$ of independent random variables with law $\mathcal{N}(0, I_d)$, we consider the Markov chain on \mathbb{T}^d given by $\tilde{Z}_0 = Z_0$ and

$$\forall k \in \mathbb{N}, \quad \tilde{Z}_{k+1} = \tilde{Z}_k + \gamma b(\tilde{Z}_k) + \sqrt{\gamma} G_k \quad (6.3)$$

and, given $E \sim \mathcal{E}(1)$ independent from $(G_k)_{k \in \mathbb{N}}$ and Z_0 ,

$$\tilde{T} = \inf \left\{ t = n\gamma, n \in \mathbb{N}_*, E \leq \gamma \sum_{k=1}^n \lambda(\tilde{Z}_k) \right\}.$$

From classical results for Euler schemes of diffusions (see e.g. [131]), it is quite clear that, for any $A \in \mathcal{B}(\mathbb{T}^d)$ and all $t \geq 0$,

$$\mathbb{P} \left(\tilde{Z}_{\lfloor t/\gamma \rfloor} \in A, \tilde{T} < t \right) \xrightarrow{\gamma \rightarrow 0} \mathbb{P} (Z_t \in A, T < t),$$

from which, for all $t \geq 0$,

$$\mathcal{L}aw \left(\tilde{Z}_{\lfloor t/\gamma \rfloor} \mid \tilde{T} < t \right) \xrightarrow{\gamma \rightarrow 0} \mathcal{L}aw (Z_t \mid T < t)$$

(we will prove this, see Corollary 6.2.4 below). Note that, from the memoryless property of the exponential law, given a sequence $(U_k)_{k \in \mathbb{N}}$ of independent variables uniformly distributed over $[0, 1]$ and independent from $(G_k)_{k \in \mathbb{N}}$ and Z_0 , then $((\tilde{Z}_n)_{n \in \mathbb{N}}, \tilde{T})$ has the same joint distribution as $((\tilde{Z}_n)_{n \in \mathbb{N}}, \hat{T})$ with

$$\hat{T} = \inf \left\{ t = n\gamma, n \in \mathbb{N}_*, U_n \leq p(\tilde{Z}_n) \right\}$$

where $p(z) = 1 - \exp(-\gamma \lambda(z))$ is the probability that, arriving at state z , the chain is killed.

A naive Monte Carlo sampler for the QSD would be to simulate N independent copies of the chain (6.3) killed with probability $z \mapsto p(z)$ and to consider after a large number of iterations the distribution of the copies that have survived. However, after a long time, most copies (possibly all) would have died and the estimator would be very bad. To tackle this issue, we have to introduce a rebirth mechanism to reincorporate dead particles in the system.

Denote $K : \mathbb{T}^d \rightarrow \mathcal{P}(\mathbb{T}^d)$ the Markov kernel associated with the transition (6.3), i.e.

$$Kf(x) = (2\pi)^{-d/2} \int_{\mathbb{R}^d} f(x + \gamma b(x) + \sqrt{\gamma}y) e^{-\frac{1}{2}|y|^2} dy.$$

For $\mu \in \mathcal{P}(\mathbb{T}^d)$, let Q_μ be the Markov kernel such that, for all $x \in \mathbb{T}^d$, $Q_\mu(x, \cdot)$ is the law of the random variable X defined as follows. Let $(X_k, U_k)_{k \in \mathbb{N}}$ be a sequence of independent random variables such that, for all $k \in \mathbb{N}$, X_k and U_k are independent, $U_k \sim \mathcal{U}([0, 1])$ and $X_0 \sim K(x, \cdot)$ while, for $k \geq 1$, $X_k \sim \mu K$. Let $H = \inf \{ k \in \mathbb{N}, U_k \geq p(X_k) \}$, and set $X = X_H$. Since λ is bounded, p is uniformly bounded away from 1 and thus H is almost surely finite, so that Q_μ is

well-defined.

In other words, a random variable $X \sim Q_\mu(x, \cdot)$ may be constructed through the following algorithm (in which *new* means: independent from all the variables previously drawn).

1. Draw $X_0 \sim \mathcal{N}(x + \gamma b(x), \gamma I_d)$ and a new $U_0 \sim \mathcal{U}([0, 1])$.
2. If $U_0 \geq p(X_0)$, set $X = X_0$ in \mathbb{T}^d (in that case, we say the particle has moved from x to X_0 without dying).
3. If $U_0 < p(X_0)$ then set $i = 1$ and, while X is not defined, do:
 - (a) Draw a new X'_i distributed according to μ , a new $X_i \sim \mathcal{N}(X'_i + \gamma b(X'_i), \gamma I_d)$ and a new $U_i \sim \mathcal{U}([0, 1])$.
 - (b) If $U_i \geq p(X_i)$, set $X = X_i$ in \mathbb{T}^d (in that case, we say the particle has died, resurrected at X'_i , moved to X_i and survived).
 - (c) If $U_i < p(X_i)$, set $i \leftarrow i + 1$ (in that case, we say the particle has died, resurrected at X'_i , moved to X_i and died again) and go back to step (a).

From this, we define a chain $(Y_k)_{k \in \mathbb{N}}$ as follows. Set $Y_0 = Z_0$ and suppose that Y_k has been defined for some $k \in \mathbb{N}$. Let $\eta_k = \mathcal{L}aw(Y_k)$, and draw a new $Y_{k+1} \sim Q_{\eta_k}(Y_k, \cdot)$. This somewhat intricate definition is motivated by the following results (whose proof is postponed to Section 6.2):

Proposition 6.1.1. *For all $n \in \mathbb{N}$*

$$\eta_n = \mathcal{L}aw\left(\tilde{Z}_n \mid \tilde{T} > n\gamma\right).$$

In particular, as $n \rightarrow \infty$, the law η_n of Y_n converges toward the QSD of \tilde{Z} . Unfortunately, it is impossible to sample $(Y_k)_{k \in \mathbb{N}}$ in practice since this would require to sample according to η_k for any $k \in \mathbb{N}$. This is a classical case of a time-inhomogeneous Markov chain which is interacting with its own law or, similarly, of a measure-valued sequence $(\eta_k)_{k \in \mathbb{N}}$ with a non-linear evolution. Such processes arise in many applications, see e.g. [43, 42] and references within. Motivated by the Law of Large Numbers, we are lead to a second approximation, which is to use mean-field interacting particles. For a fixed $N \in \mathbb{N}_*$ and for $x = (x_i)_{i \in \llbracket 1, N \rrbracket} \in \mathbb{T}^{dN}$, we denote

$$\pi(x) := \frac{1}{N} \sum_{i=1}^N \delta_{x_i} \in \mathcal{P}(\mathbb{T}^d)$$

the associated empirical distribution. Then we define the Markov operator R on \mathbb{T}^{dN} as

$$R(x, \cdot) = Q_{\pi(x)}(x_1, \cdot) \otimes \cdots \otimes Q_{\pi(x)}(x_N, \cdot).$$

In other words, a random variable $\mathbf{Y} \sim Q(x, \cdot)$ is such that the Y_i 's are independent with $Y_i \sim Q_{\pi(x)}(x_i, \cdot)$. In order to specify the parameters involved, we will sometimes write $R_{N, \gamma}$ for R .

Let us informally describe the transitions of such a Markov chain $(\mathbf{X}_k)_{k \in \mathbb{N}}$: the i^{th} particle follows the transition given by (6.3) independently from the other particles until it dies. If it dies at a step $k \in \mathbb{N}_*$, then it is resurrected on another particle $X_{J, k-1}$ with J uniformly distributed over $\llbracket 1, N \rrbracket$ (in particular and contrary to most previous works on similar algorithms, $J = i$ is not excluded, although it doesn't change much since its probability vanishes as $N \rightarrow \infty$) and

immediatly performs a step of (6.3); if it dies again after this unique step, it is resurrected again and performs a new step, and so on until it is not killed after a resurrection and an Euler scheme step. Then this is the new value $X_{i,k}$ from which the particle follows again the transitions (6.3) until its next death, etc.

Note that there is no problem of simultaneous death since at step k the particles are resurrected on positions at step $k - 1$, which are well-defined even if all particles die at once at step k .

It is easily seen that R admits a unique invariant measure toward which the law of the associated Markov chain converges exponentially fast (in the total variation sense for instance), but a naive argument yields a convergence rate that heavily depends on N (and possibly γ). Similarly, classical studies can be conducted for the limits $N \rightarrow \infty$ and $\gamma \rightarrow 0$ but again with estimates that are typically exponentially bad with respect to the total simulation time. In the following we will focus on a somewhat perturbative regime under which we will establish estimates for each of these limits that are uniform with respect to the other parameters. Even for the continuous-time process (corresponding to $\gamma = 0$, see Section 6.2.4 for the definition), such uniform results are new (see Corollaries 6.2.3 and 6.2.5).

Recall that the \mathcal{W}_1 Wasserstein distance between $\mu, \nu \in \mathcal{P}(\mathbb{T}^d)$ is defined by

$$\mathcal{W}_1(\mu, \nu) = \inf \{ \mathbb{E}(|X - Y|) : X \sim \mu, Y \sim \nu \} .$$

More generally, for ρ a distance on some Polish space F , denote \mathcal{W}_ρ the corresponding Wasserstein distance on $\mathcal{P}(F)$, defined by

$$\mathcal{W}_\rho(\mu, \nu) = \inf \{ \mathbb{E}(\rho(X, Y)) : X \sim \mu, Y \sim \nu \} . \tag{6.4}$$

If $X \sim \mu$ and $Y \sim \nu$, we call (X, Y) a coupling of μ and ν . If (X, Y) is a coupling for which the infimum in (6.4) is attained, we say that it is an optimal coupling. From [164, Corollary 5.22], such an optimal coupling always exists.

Our first main result is a long-time convergence rate uniform in N :

Theorem 6.1.1. *There exist $c_1, c_2, \gamma_0 > 0$ and a distance ρ on \mathbb{T}^d equivalent to the Euclidean distance, that depend only on the drift b and the dimension d , such that, if λ is Lipschitz with a constant L_λ and*

$$\kappa := c_1 - c_2 L_\lambda e^{\gamma \|\lambda\|_\infty} , \tag{6.5}$$

then the following holds: for all $\gamma \in (0, \gamma_0]$, $N \in \mathbb{N}$ and all $\mu, \nu \in \mathcal{P}(\mathbb{T}^{dN})$, considering the distance $\rho_N(x, y) = \sum_{i=1}^N \rho(x_i, y_i)$ for $x, y \in \mathbb{T}^{dN}$,

$$\mathcal{W}_{\rho_N}(\mu R_{N,\gamma}, \nu R_{N,\gamma}) \leq (1 - \gamma \kappa) \mathcal{W}_{\rho_N}(\mu, \nu) .$$

As a consequence, there exists $C > 0$ that depends only on b and d such that for all $\gamma \in (0, \gamma_0]$, $m, N \in \mathbb{N}$ and all $\mu, \nu \in \mathcal{P}(\mathbb{T}^{dN})$,

$$\mathcal{W}_1(\mu R_{N,\gamma}^m, \nu R_{N,\gamma}^m) \leq CN (1 - \gamma \kappa)^m .$$

This means that, with respect to the metric ρ_N , $R_{N,\gamma}$ has a Wasserstein curvature of $\gamma \kappa$ in the sense of [93].

Theorem 6.1.1 is proven in Section 6.2.2. From this first result, similar bounds can be obtained for large N and small γ (see Sections 6.2.3 and 6.2.4). Combining all these results eventually yields a quantitative bound on the error made in practice by approximating ν_* by the empirical

distribution of the particular particle system:

Theorem 6.1.2. *Under the conditions of Theorem 6.1.1, suppose that κ given by (6.5) is positive. There exists $C > 0$ such that for all $N \in \mathbb{N}$, $\gamma \in (0, \gamma_0]$, $t \geq 0$ and $\mu_0 \in \mathcal{P}(\mathbb{T}^{dN})$, if $(\mathbf{X}_k)_{k \in \mathbb{N}}$ is a Markov chain with initial distribution μ_0 and transition kernel $R_{N, \gamma}$,*

$$\mathbb{E} [\mathcal{W}_1 (\pi(\mathbf{X}_{\lfloor t/\gamma \rfloor}), \nu_*)] \leq C (\sqrt{\gamma} + \alpha(N) + e^{-\kappa t}),$$

where

$$\alpha(N) = \begin{cases} N^{-1/2} & \text{if } d = 1, \\ N^{-1/2} \ln(1 + N) & \text{if } d = 2, \\ N^{-1/d} & \text{if } d > 2. \end{cases}$$

All the constants in Theorems 6.1.1 and 6.1.2 (and all other results stated in this work) are explicit. More precisely, c_1 and γ_0 come from [122, Corollary 2.2] (see Proposition 6.2.1 below) where an explicit value is given, and all the other constants involved in our results can be tracked by following the explicit computations.

In Theorem 6.1.2, the speeds of the different convergences (exponential in the simulation time, with the square-root of the timestep and with α of the number of particles) are optimal since they are optimal for non-interacting diffusions (i.e. the case $\lambda = 0$), see in particular [62] for the large N asymptotic.

Other intermediary results will be established in the rest of the paper that are interesting by themselves: propagation of chaos (i.e. $N \rightarrow \infty$) and continuous-time limit at a fixed time (even without the condition $\kappa > 0$) respectively in Propositions 6.2.4 and 6.2.5. From that, results for the continuous-time process ($\gamma = 0$), the equilibria ($t = \infty$) or the non-linear process ($N = \infty$), or when two parameters among three are sent to their limits, are then simple corollaries, see Section 6.2.5. All these results are summarised in Figure 6.1 at the end of this work.

Note that $\exp(-\gamma\lambda(x))$ is the probability that the chain is not killed when it arrives at state x . The time step γ should be chosen in such a way that this probability is relatively large, say at least one half. In that case, $\exp(\gamma\|\lambda\|_\infty)$ is typically close to 1. In other words, the positivity of κ given by (6.5) is mostly a condition about L_λ being small enough.

This perturbation condition is different from the one considered in [133], where $\|\lambda\|_\infty$ rather than L_λ is supposed to be small (while our main arguments are a direct adaptation of the coupling arguments of [133]). This difference comes from the fact that, in the present study, we work with the \mathcal{W}_1 distance rather than the total variation one (which is a Wasserstein distance but associated to the discrete metric $d(x, y) = \mathbb{1}_{x \neq y}$). Indeed, in our coupling arguments, we need to control $|\lambda(x) - \lambda(y)|$ the difference between the death rates of two processes at different locations, which is bounded here by $L_\lambda|x - y|$ and in [133] by $2\|\lambda\|_\infty \mathbb{1}_{x \neq y}$. In fact our argument for the long-time convergence may easily be adapted to the total variation distance framework, following [133]. Nevertheless this would be more troublesome in the study of the limit $N \rightarrow \infty$. Then, one needs to couple η_k (that admits a density with respect to the Lebesgue measure) with $\pi(\mathbf{X}_k)$ (which is a sum of Dirac masses), so that the total variation distance is not adapted. This may be solved by considering $\mathcal{W}_1 \rightarrow$ total variation regularization results for (Euler schemes of) diffusions, that can be established by coupling arguments again. Nevertheless, in order to focus on the other difficulties of the problem and for the sake of clarity, we decided to stick to the \mathcal{W}_1 distance in all the different results of this work. Similar Wasserstein coupling arguments have been used in [38] on a similar problem (see next section) and in [167] for a different kind of mean-field interacting particle system (also with a similar perturbative condition corresponding to the fact σ in [167, Proposition 3.1] has to be positive, i.e. the interaction should be small with respect to the independent mixing).

Notice that, among all possible discretization schemes, we only considered the explicit Euler-Maruyama one. This choice was made for simplicity, but the proofs could be extended to other usual schemes. The main ingredient required is a Wasserstein curvature of order γ for a modified \mathcal{W}_1 distance (see Proposition 6.2.1, based on [122, Corollary 2.2]). Similarly, we only considered the case of an elliptic diffusion process with a constant diffusion matrix for simplicity (since we use [122, Corollary 2.2] which covers this case), although a similar Wasserstein contraction certainly holds in a much more general framework (even hypoelliptic non-elliptic, as in continuous-time settings [56]). As stated in the introduction, the present paper does not aim at the broadest generality, and by avoiding technicalities we want to highlight the main issue (i.e. the question of the uniformity of bounds in the various parameters).

6.2 Proofs

Let us first establish the preliminary result stated in the introduction:

Proof of Proposition 6.1.1. For $n \in \mathbb{N}$, denote

$$\eta_n = \mathcal{L}aw(Y_n), \quad \nu_n = \mathcal{L}aw\left(\tilde{Z}_n \mid \tilde{T} \geq n\gamma\right).$$

Since $\nu_0 = \eta_0$, suppose by induction that $\nu_n = \eta_n$ for some $n \in \mathbb{N}$. Keeping the notations introduced in the definition of the kernel Q_μ , consider the events $B_k = \{U_k \geq p(X_k)\}$. Then, for all bounded measurable f ,

$$\begin{aligned} Q_\mu f(x) &= \mathbb{E}(f(X)) \\ &= \mathbb{E}\left(f(X) \sum_{k \in \mathbb{N}} \mathbb{1}_{B_k \cap (\bigcap_{j=0}^{k-1} B_j^c)}\right) \\ &= \mathbb{E}(f(X_0) \mathbb{1}_{U_0 \geq p(X_0)}) + \sum_{k \geq 1} \mathbb{E}(f(X_k) \mathbb{1}_{U_k \geq p(X_k)}) \prod_{j=0}^{k-1} \mathbb{P}(B_j^c) \\ &= K[f(1-p)](x) + \sum_{k \geq 1} \mu K[f(1-p)](\mu K p)^{k-1} K p(x). \end{aligned}$$

In particular, integrating with respect to μ , we obtain

$$\mu Q_\mu f = \mu K[f(1-p)] \sum_{k \in \mathbb{N}} (\mu K p)^k = \frac{\mu K[f(1-p)]}{\mu K[1-p]}.$$

Applied with $\mu = \eta_n$, this reads

$$\eta_{n+1} f = \mathbb{E}(f(Y_{n+1})) = \mathbb{E}(\mathbb{E}(f(Y_{n+1}) \mid Y_n)) = \eta_n Q_{\eta_n} f = \frac{\eta_n K[f(1-p)]}{\eta_n K[1-p]}.$$

On the other hand,

$$\begin{aligned} \mathbb{E}\left(f(\tilde{Z}_{n+1}) \mathbb{1}_{\tilde{T} > (n+1)\gamma}\right) &= \mathbb{E}\left(f(\tilde{Z}_{n+1}) \mathbb{1}_{\tilde{T} > n\gamma} \mathbb{1}_{U_n \geq p(\tilde{Z}_{n+1})}\right) \\ &= \mathbb{E}\left(f(\tilde{Z}_{n+1}) \left(1 - p(\tilde{Z}_{n+1})\right) \mathbb{1}_{\tilde{T} > n\gamma}\right) \end{aligned}$$

$$= \mathbb{P}(\tilde{T} > n\gamma) \nu_n K[f(1-p)],$$

from which

$$\nu_{n+1} f = \frac{\mathbb{E}\left(f(\tilde{Z}_{n+1}) \mathbb{1}_{\tilde{T} > (n+1)\gamma}\right)}{\mathbb{P}(\tilde{T} > (n+1)\gamma)} = \frac{\mathbb{P}(\tilde{T} > n\gamma) \nu_n K[f(1-p)]}{\mathbb{P}(\tilde{T} > n\gamma) \nu_n K[1-p]} = \frac{\nu_n K[f(1-p)]}{\nu_n K[1-p]},$$

which concludes. \square

6.2.1 The basic coupling

The long-time estimates needed to prove convergence toward equilibrium and uniform in time estimates in N and γ are based on the fact that, as long as particles don't die, they follow the chain (6.3) which, like its continuous-time counterpart (6.1), have some mixing properties. In order to quantify the latters, we start by stating [122, Corollary 2.2] in a suitable way in our context.

Proposition 6.2.1. *There exists $c_1, a, \gamma_0 > 0$ (that all depend only on the drift b of (6.1) and on the dimension d) such that, denoting $\rho(x, y) = (1 - \exp(-a|x - y|))/a$ for $x, y \in \mathbb{T}^d$, then ρ is a metric on \mathbb{T}^d with*

$$\forall \gamma \in (0, \gamma_0], \forall \mu, \nu \in \mathcal{P}(\mathbb{T}^d), \quad \mathcal{W}_\rho(\mu K, \nu K) \leq (1 - c_1 \gamma) \mathcal{W}_\rho(\mu, \nu).$$

Proof. This is [122, Corollary 2.2] applied to a diffusion with smooth drift on the torus, in which case the distance on \mathbb{T}^d for which the contraction holds is ρ . \square

In the rest of the paper, ρ is the metric and c_1, a, γ_0 are the constants given by Proposition 6.2.1. Remark that ρ is equivalent to the Euclidian metric, with

$$\beta|x - y| \leq \rho(x, y) \leq |x - y| \quad \text{for} \quad \beta = 2(1 - e^{-a\sqrt{d}/2})/(a\sqrt{d}),$$

where we used that the diameter of \mathbb{T}^d is $\sqrt{d}/2$ and that $r \mapsto (1 - \exp(-ar))/a$ is a concave function with derivative 1 at zero. In particular, \mathcal{W}_1 and \mathcal{W}_ρ are equivalent.

Now, in this particle system, the contraction property of the chain (6.3) may be counterbalanced by the death/resurrection mechanism through which particles interact. Indeed, considering two systems of N interacting particles, for $i \in \llbracket 1, N \rrbracket$ the previous result means that we can couple the i^{th} particles of both systems to get closer one to the other (on average), as long as they don't die. But then, one of the two particle can die and resurrect far from the other, or even if they die simultaneously they may resurrect far apart one from the other. That being said, first, the closer they get, the easier it is to couple them in order to die simultaneously, and second, when they die simultaneously, keeping the particles close one to the other amount to do a suitable coupling of the laws from which the particles are resurrected. This is quantified in the following proposition.

In all the rest of the paper, we suppose that λ is L_λ -Lipschitz (but not necessarily that κ given by (6.5) is positive).

Proposition 6.2.2. *Let $\mu_0, \mu_1, \mu'_0, \mu'_1 \in \mathcal{P}(\mathbb{T}^d)$ and let (X_0, X'_0) (resp. (X_1, X'_1)) be a coupling of $\mu_0 K$ and $\mu'_0 K$ (resp. $\mu_1 K$ and $\mu'_1 K$). Then*

$$\mathcal{W}_\rho(\mu_0 Q_{\mu_1}, \mu'_0 Q_{\mu'_1}) \leq h \left(\mathbb{E}(\rho(X_0, X'_0)) + \frac{q_0}{1 - q_1} \mathbb{E}(\rho(X_1, X'_1)) \right)$$

where

$$h = 1 - \min p + (a\beta)^{-1} \gamma L_\lambda$$

and, considering $U \sim \mathcal{U}([0, 1])$ independent from (X_0, X'_0, X_1, X'_1) ,

$$q_i = \mathbb{P}(U < p(X_i) \wedge p(X'_i)), \quad i = 0, 1.$$

Proof. Let $(X_k, X'_k, U_k)_{k \in \mathbb{N}}$ be a sequence of independent triplet of random variables such that, for all $k \in \mathbb{N}$, $U_k \sim \mathcal{U}([0, 1])$ is independent from (X_k, X'_k) , which are such as defined in the proposition for $k = 0$ and 1 and, for $k > 1$, have the same distribution as (X_1, X'_1) . Set $H = \inf\{n \in \mathbb{N}, U_n < p(X_n)\}$ and $H' = \inf\{n \in \mathbb{N}, U_n < p(X'_n)\}$. Then, by considering the law of $(X_k, U_k)_{k \in \mathbb{N}}$ alone, it is clear that $X_H \sim \mu_0 Q_{\mu_1}$ and, similarly, $X'_{H'} \sim \mu'_0 Q_{\mu'_1}$, so that

$$\mathcal{W}_\rho(\mu_0 Q_{\mu_1}, \mu'_0 Q_{\mu'_1}) \leq \mathbb{E}(\rho(X_H, X'_{H'})).$$

Different cases are distinguished depending on the value of H and H' . In the simplest case, none of the particles dies:

$$\begin{aligned} \mathbb{E}(\rho(X_H, X'_{H'}) \mathbb{1}_{H=H'=0}) &= \mathbb{E}(\rho(X_0, X'_0) \mathbb{1}_{U_0 \geq p(X_0) \vee p(X'_0)}) \\ &\leq \mathbb{E}(\rho(X_0, X'_0) \mathbb{1}_{U_0 \geq \min p}) \\ &\leq (1 - \min p) \mathbb{E}(\rho(X_0, X'_0)), \end{aligned}$$

where we used the independence between U_0 and (X_0, X'_0) . In the second case, only one particle dies: using that $\|\rho\|_\infty \leq 1/a$,

$$\begin{aligned} \mathbb{E}(\rho(X_H, X'_{H'}) \mathbb{1}_{H \wedge H'=0 < H \vee H'}) &\leq a^{-1} \mathbb{P}(U_0 \in [p(X_0) \wedge p(X'_0), p(X_0) \vee p(X'_0)]) \\ &= a^{-1} \mathbb{E}(|p(X_0) - p(X'_0)|) \\ &\leq a^{-1} \gamma L_\lambda \mathbb{E}(|X_0 - X'_0|) \\ &\leq (a\beta)^{-1} \gamma L_\lambda \mathbb{E}(\rho(X_0, X'_0)). \end{aligned}$$

In the third case, both particles die $k \geq 1$ times:

$$\begin{aligned} \mathbb{E}(\rho(X_H, X'_{H'}) \mathbb{1}_{H=H'=k}) &= \mathbb{E} \left(\rho(X_k, X'_k) \mathbb{1}_{U_k \geq p(X_k) \vee p(X'_k)} \prod_{j=0}^{k-1} \mathbb{1}_{U_j < p(X_j) \wedge p(X'_j)} \right) \\ &\leq q_0 q_1^{k-1} \mathbb{E}(\rho(X_k, X'_k) \mathbb{1}_{U_k \geq \min p}) \\ &\leq q_0 q_1^{k-1} (1 - \min p) \mathbb{E}(\rho(X_1, X'_1)). \end{aligned}$$

Finally, combining the computations of the last two cases, the fourth one reads, for $k \geq 1$,

$$\begin{aligned} \mathbb{E}(\rho(X_H, X'_{H'}) \mathbb{1}_{H \wedge H'=k < H \vee H'}) &\leq a^{-1} q_0 q_1^{k-1} \mathbb{P}(U_k \in [p(X_k) \wedge p(X'_k), p(X_k) \vee p(X'_k)]) \\ &\leq (a\beta)^{-1} q_0 q_1^{k-1} \gamma L_\lambda \mathbb{E}(\rho(X_1, X'_1)). \end{aligned}$$

Summing these four cases concludes. \square

6.2.2 Long-time convergence

For $N \in \mathbb{N}_*$ denote ρ_N the metric on \mathbb{T}^{dN} given by

$$\rho_N(x, y) = \sum_{i=1}^N \rho(x_i, y_i).$$

The following result is similar to the results of [133, 167, 38] and based on the same coupling argument.

Proposition 6.2.3. *There exists $c_2 > 0$ (that depends only on the drift b of (6.1) and on the dimension d) such that for all $\gamma \in (0, \gamma_0]$ $N \in \mathbb{N}$, and all $\mu, \nu \in \mathcal{P}(\mathbb{T}^{dN})$,*

$$\mathcal{W}_{\rho_N}(\mu R_{N,\gamma}, \nu R_{N,\gamma}) \leq (1 - \gamma\kappa) \mathcal{W}_{\rho_N}(\mu, \nu).$$

with κ given by (6.5).

Proof. It is in fact sufficient to prove this for $\mu = \delta_x$ and $\nu = \delta_y$ for any $x, y \in \mathbb{T}^{dN}$. Indeed, assuming the result proven for Dirac masses, in the general case, considering $(\mathbf{X}_0, \mathbf{Y}_0)$ an optimal coupling of μ and ν and $(\mathbf{X}_1, \mathbf{Y}_1)$ an optimal coupling of $R(\mathbf{X}_0, \cdot)$ and $R(\mathbf{Y}_0, \cdot)$, then $\mathbf{X}_1 \sim \mu R$ and $\mathbf{Y}_1 \sim \nu R$, so that

$$\begin{aligned} \mathcal{W}_{\rho_N}(\mu R, \nu R) &\leq \mathbb{E}(\rho_N(\mathbf{X}_1, \mathbf{Y}_1)) \\ &= \mathbb{E}(\mathbb{E}(\rho_N(\mathbf{X}_1, \mathbf{Y}_1) \mid (\mathbf{X}_0, \mathbf{Y}_0))) \\ &= \mathbb{E}(\mathbb{E}(\mathcal{W}_{\rho_N}(\delta_{\mathbf{X}_0} R, \delta_{\mathbf{Y}_0} R) \mid (\mathbf{X}_0, \mathbf{Y}_0))) \\ &\leq (1 - \gamma\kappa) \mathbb{E}(\rho_N(\mathbf{X}_0, \mathbf{Y}_0)) \\ &= (1 - \gamma\kappa) \mathcal{W}_{\rho_N}(\mu, \nu). \end{aligned}$$

Hence, in the following, we fix $x, y \in \mathbb{T}^{dN}$. Let $(X_i, Y_i)_{i \in \llbracket 1, N \rrbracket}$ be independent pairs of random variables in \mathbb{T}^d where, for all $i \in \llbracket 1, N \rrbracket$, (X_i, Y_i) is an optimal coupling of $Q_{\pi(x)}(x_i, \cdot)$ and $Q_{\pi(y)}(y_i, \cdot)$. Then (\mathbf{X}, \mathbf{Y}) is a coupling of $R(x, \cdot)$ and $R(y, \cdot)$, so that

$$\begin{aligned} \mathcal{W}_{\rho_N}(\delta_x R, \delta_y R) &\leq \mathbb{E}(\rho_N(\mathbf{X}, \mathbf{Y})) = \sum_{i=1}^N \mathbb{E}(\rho(X_i, Y_i)) \\ &= \sum_{i=1}^N \mathcal{W}_\rho(Q_{\pi(x)}(x_i, \cdot), Q_{\pi(y)}(y_i, \cdot)). \end{aligned}$$

We want to apply Proposition 6.2.2 with $\mu_1 = \pi(x)$, $\mu_0 = \delta_{x_i}$, $\mu'_1 = \pi(y)$ and $\mu'_0 = \delta_{y_i}$. To do so, for all $i \in \llbracket 1, N \rrbracket$, we consider $(\tilde{X}_i, \tilde{Y}_i)$ an optimal coupling of $K(x_i, \cdot)$ and $K(y_i, \cdot)$. From Proposition 6.2.1,

$$\mathbb{E}(\rho(\tilde{X}_i, \tilde{Y}_i)) \leq (1 - c_1\gamma) \rho(x_i, y_i). \quad (6.6)$$

Moreover, if $J \sim \mathcal{U}(\llbracket 1, N \rrbracket)$ is independent from the $(\tilde{X}_i, \tilde{Y}_i)$'s, we remark that $(\tilde{X}_J, \tilde{Y}_J)$ is a coupling of $\pi(x)K$ and $\pi(y)K$. Proposition 6.2.2 applied with these couplings reads, for all

$i \in \llbracket 1, N \rrbracket$,

$$\mathcal{W}_\rho(Q_{\pi(x)}(x_i, \cdot), Q_{\pi(y)}(y_i, \cdot)) \leq h \left(\mathbb{E} \left(\rho(\tilde{X}_i, \tilde{Y}_i) \right) + \frac{q_i}{1 - q_*} \mathbb{E} \left(\rho(\tilde{X}_J, \tilde{Y}_J) \right) \right) \quad (6.7)$$

where, if $U \sim \mathcal{U}([0, 1])$ is independent from the previous variables,

$$q_i := \mathbb{P} \left(U < p(\tilde{X}_i) \wedge p(\tilde{Y}_i) \right)$$

and, conditioning on the value of J ,

$$q_* := \mathbb{P} \left(U < p(\tilde{X}_J) \wedge p(\tilde{Y}_J) \right) = \frac{1}{N} \sum_{i=1}^N q_i.$$

Summing (6.7) over $i \in \llbracket 1, N \rrbracket$ and applying (6.6) yields

$$\mathcal{W}_{\rho_N}(\delta_x R, \delta_y R) \leq h \left((1 - c_1 \gamma) \sum_{i=1}^N \rho(x_i, y_i) + \frac{Nq_*}{1 - q_*} \mathbb{E} \left(\rho(\tilde{X}_J, \tilde{Y}_J) \right) \right).$$

Applying Proposition 6.2.1 again,

$$\mathbb{E} \left(\rho(\tilde{X}_J, \tilde{Y}_J) \right) = \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left(\rho(\tilde{X}_i, \tilde{Y}_i) \right) \leq \frac{1}{N} (1 - c_1 \gamma) \sum_{i=1}^N \rho(x_i, y_i),$$

and the previous inequality becomes

$$\mathcal{W}_{\rho_N}(\delta_x R, \delta_y R) \leq \frac{h(1 - c_1 \gamma)}{1 - q_*} \rho_N(x, y).$$

Bounding $1 - q_* \geq 1 - \max p \geq \exp(-\gamma \|\lambda\|_\infty)$ and $\max p - \min p \leq \sqrt{d/2} \gamma L_\lambda$ yields

$$\begin{aligned} \frac{h(1 - c_1 \gamma)}{1 - q_*} &\leq (1 - c_1 \gamma) \frac{1 - \max p + \max p - \min p + (a\beta)^{-1} \gamma L_\lambda}{1 - \max p} \\ &\leq 1 - c_1 \gamma + \gamma L_\lambda e^{\gamma \|\lambda\|_\infty} \left((a\beta)^{-1} + \sqrt{d} \right), \end{aligned}$$

which concludes. \square

As a direct consequence, Proposition 6.2.3 gives

$$\forall m \in \mathbb{N}, \quad \mathcal{W}_{\rho_N}(\mu R^m, \nu R^m) \leq e^{-\kappa m \gamma} \mathcal{W}_{\rho_N}(\mu, \nu),$$

with κ that does not depends on N nor γ . Provided $\kappa > 0$, and since $\mathcal{P}(\mathbb{T}^{dN})$ is complete for \mathcal{W}_1 (hence for \mathcal{W}_{ρ_N}) the Banach fixed-point theorem implies then that R admits a unique invariant measure toward which it converges at rate $\gamma \kappa$.

In the rest of the paper, κ is given by (6.5) (but is not necessarily assumed positive).

Proof of Theorem 6.1.1. The first part of the theorem has already been proven in Proposition 6.2.3. The last statement then follows from the first part, the equivalence between the Euclidean distance and ρ_N and the fact $\mathcal{W}_{\rho_N}(\nu, \mu) \leq \|\rho_N\|_\infty = N\sqrt{d}/2$ for all $\nu, \mu \in \mathcal{P}(\mathbb{T}^{dN})$. \square

6.2.3 Propagation of chaos

Recall that η_k is the law at time k of the non-homogeneous Markov chain $(Y_k)_{k \in \mathbb{N}}$ on \mathbb{T}^d introduced in Section 6.1.2 with transition kernels Q_{η_k} and initial condition η_0 , and that $R = R_{N,\gamma}$ is the transition kernel of the Markov chain $(\mathbf{X}_k)_{k \in \mathbb{N}}$ on \mathbb{T}^{dN} .

Lemma 6.2.1. *There exist $C_1 > 0$ such that for all $N \in \mathbb{N}$, $\gamma \in (0, \gamma_0]$, $\eta \in \mathcal{P}(\mathbb{T}^d)$ and $\mu \in \mathcal{P}(\mathbb{T}^{dN})$,*

$$\mathcal{W}_{\rho_N}(\mu R, \mu Q_\eta^{\otimes N}) \leq \gamma N C_1 \int_{\mathbb{T}^{dN}} \mathcal{W}_\rho(\pi(x), \eta) \mu(dx).$$

Proof. Similarly to the proof of Proposition 6.2.3, we start with the case $\mu = \delta_x$ for some $x \in \mathbb{T}^{dN}$. Let $(X_i, Y_i)_{i \in \llbracket 1, N \rrbracket}$ be N independent pairs of random variables such that for all $i \in \llbracket 1, N \rrbracket$, (X_i, Y_i) is an optimal coupling of $Q_{\pi(x)}(x_i, \cdot)$ and $Q_\eta(x_i, \cdot)$. Then (\mathbf{X}, \mathbf{Y}) is a coupling of $R_N(x, \cdot)$ and $Q_\eta^{\otimes N}(x, \cdot)$, so that

$$\begin{aligned} \mathcal{W}_{\rho_N}(\delta_x R_N, \delta_x Q_\eta^{\otimes N}) &\leq \mathbb{E}(\rho_N(X, Y)) \\ &= \sum_{i=1}^N \mathbb{E}(\rho(X_i, Y_i)) = \sum_{i=1}^N \mathcal{W}_\rho(\delta_{x_i} Q_{\pi(x)}, \delta_{x_i} Q_\eta). \end{aligned}$$

From Proposition 6.2.2 (bounding $q_0 \leq \max p \leq \gamma \|\lambda\|_\infty$ and $1 - q_1 \geq 1 - \max p \geq \exp(-\gamma_0 \|\lambda\|_\infty)$)

$$\begin{aligned} \mathcal{W}_\rho(\delta_{x_i} Q_{\pi(x)}, \delta_{x_i} Q_\eta) &\leq \gamma \|\lambda\|_\infty (1 + (a\beta)^{-1} \gamma_0 L_\lambda) e^{\gamma_0 \|\lambda\|_\infty} \mathcal{W}_\rho(\pi(x), \eta) \\ &:= \gamma C_1 \mathcal{W}_\rho(\pi(x), \eta). \end{aligned}$$

Now in the general case where μ is not a Dirac mass, considering $Z_0 \sim \mu$, and (Z_1, Z_2) an optimal coupling of $R(Z_0, \cdot)$ and $Q_\eta^{\otimes N}(Z_0, \cdot)$ and conditioning with respect to Z_0 ,

$$\mathcal{W}_{\rho_N}(\mu R_N, \mu Q_\eta^{\otimes N}) \leq \mathbb{E}(\rho_N(Z_1, Z_N)) \leq \gamma N C_1 \mathbb{E}(\mathcal{W}_\rho(\pi(Z_0), \eta)).$$

□

Proposition 6.2.4. *There exist $C_2, C_3 > 0$ such that for all $N \in \mathbb{N}$, $\gamma \in (0, \gamma_0]$, $m \in \mathbb{N}$ and $\eta_0 \in \mathcal{P}(\mathbb{T}^d)$, first,*

$$\mathcal{W}_{\rho_N}(\eta_0^{\otimes N} R^m, \eta_m^{\otimes N}) \leq C_2 N \alpha(N) \gamma \sum_{s=1}^m (1 - \gamma \kappa)^{s-1}, \quad (6.8)$$

and second, if $(\mathbf{X}_k)_{k \in \mathbb{N}}$ is a Markov chain with initial distribution $\eta_0^{\otimes N}$ and transition kernel R , then

$$\mathbb{E}(\mathcal{W}_\rho(\pi(\mathbf{X}_m), \eta_m)) \leq C_3 \alpha(N) \left(1 + \gamma \sum_{s=1}^m (1 - \gamma \kappa)^{s-1} \right). \quad (6.9)$$

Remark that when $\kappa > 0$, $\gamma \sum_{s=1}^m (1 - \gamma \kappa)^{s-1} \leq 1/\kappa$ so that (6.8) and (6.9) yield uniform in time estimates. On the contrary, when $\kappa < 0$, the estimates are exponentially bad in $t = m\gamma$.

Proof. We start with the proof of (6.8), for $m \geq 1$ (the case $m = 0$ being trivial). From the triangular inequality, Proposition 6.2.3 and Lemma 6.2.1,

$$r_m := \mathcal{W}_{\rho_N}(\eta_0^{\otimes N} R^m, \eta_m^{\otimes N}) \leq \mathcal{W}_{\rho_N}(\eta_0^{\otimes N} R^m, \eta_{m-1}^{\otimes N} R) + \mathcal{W}_{\rho_N}(\eta_{m-1}^{\otimes N} R, \eta_{m-1}^{\otimes N} Q_{\eta_{m-1}}^{\otimes N})$$

$$\leq (1 - \kappa\gamma)r_{m-1} + \gamma NC_1 \int_{\mathbb{T}^{dN}} \mathcal{W}_\rho(\pi(x), \eta_{m-1}) \eta_{m-1}^{\otimes N}(dx).$$

Since $\mathcal{W}_\rho \leq \mathcal{W}_1$, estimating the last term is a classical question, that is to bound the expected Wasserstein distance between the empirical measure of a sample of N independent and identically distributed random variables and their common law. From [62, Theorem 1] (and since on the torus the moments of probability measures are uniformly bounded), there exists some $C' > 0$ independent from η_0 , m , N and γ such that

$$\int_{\mathbb{T}^{dN}} \mathcal{W}_1(\pi(x), \eta_{m-1}) \eta_{m-1}^{\otimes N}(dx) \leq C' \alpha(N).$$

Since $r_0 = 0$, a direct induction concludes the proof of (6.8).

To prove (6.9), let (\mathbf{X}, \mathbf{Y}) be an optimal coupling of $\eta_0^{\otimes N} R^m$ and $\eta_m^{\otimes N}$. Considering $J \sim \mathcal{U}(\llbracket 1, N \rrbracket)$ independent from (\mathbf{X}, \mathbf{Y}) then, conditionally to (\mathbf{X}, \mathbf{Y}) , (X_J, Y_J) is a coupling of $\pi(\mathbf{X})$ and $\pi(\mathbf{Y})$, so that

$$\mathcal{W}_\rho(\pi(\mathbf{X}), \pi(\mathbf{Y})) \leq \mathbb{E}(\rho(X_J, Y_J) \mid (\mathbf{X}, \mathbf{Y})) = \frac{1}{N} \rho_N(\mathbf{X}, \mathbf{Y}).$$

Taking the expectation in

$$\mathcal{W}_\rho(\pi(\mathbf{X}), \eta_m) \leq \mathcal{W}_\rho(\pi(\mathbf{X}), \pi(\mathbf{Y})) + \mathcal{W}_\rho(\pi(\mathbf{Y}), \eta_m),$$

we conclude with (6.8) and [62, Theorem 1] again. \square

Corollary 6.2.1. *With the notations of Proposition 6.2.4, for all $k \in \llbracket 1, N \rrbracket$,*

$$\mathcal{W}_{\rho_k}(\mathcal{L}aw(X_{1,m}, \dots, X_{k,m}), \eta_m^{\otimes k}) \leq C_2 k \alpha(N) \gamma \sum_{s=1}^m (1 - \gamma \kappa)^{s-1}.$$

Proof. Let (\mathbf{X}, \mathbf{Y}) be an optimal coupling of $\eta_0^{\otimes N} R^m$ and $\eta_m^{\otimes N}$, and let σ be uniformly distributed over the set of permutations of N elements, independent from (\mathbf{X}, \mathbf{Y}) . Since the laws of \mathbf{X} and \mathbf{Y} are exchangeable, $\mathbf{X}_\sigma = (X_{\sigma(1)}, \dots, X_{\sigma(N)})$ has the same law as \mathbf{X} , in particular $(\mathbf{X}_{\sigma(1)}, \dots, X_{\sigma(k)})$ has the same law as (X_1, \dots, X_k) . The same goes for \mathbf{Y}_σ , and

$$\begin{aligned} \mathbb{E} \left(\sum_{i=1}^k \rho(X_{\sigma(i)}, Y_{\sigma(i)}) \right) &= k \mathbb{E}(\rho(X_{\sigma(1)}, Y_{\sigma(1)})) = \frac{k}{N} \mathbb{E}(\rho_N(\mathbf{X}, \mathbf{Y})) \\ &= \frac{k}{N} \mathcal{W}_{\rho_N}(\eta_0^{\otimes N} R^m, \eta_m^{\otimes N}), \end{aligned}$$

and Proposition 6.2.4 concludes. \square

Corollary 6.2.1 means that, for any fixed $k \in \mathbb{N}_*$, as N goes to infinity, the k -marginals of the system of particles converge toward the law of k independent non-linear chains, which is the so-called propagation of chaos phenomenon.

6.2.4 Discrete to continuous time

We start by defining $(\bar{Y}_t)_{t \geq 0}$ and $(\bar{\mathbf{X}}_t)_{t \geq 0}$ the continuous-time analogous of the chains $(Y_k)_{k \in \mathbb{N}}$ on \mathbb{T}^d and $(\mathbf{X}_k)_{k \in \mathbb{N}}$ on \mathbb{T}^{dN} defined in Section 6.1.2. We start with the non-linear process. For

$t \geq 0$, let

$$\bar{\eta}_t = \mathcal{L}aw(Z_t \mid T > t)$$

where Z solves (6.1) with initial distribution η_0 and T is given by (6.2). We define $(\bar{Y}_t)_{t \geq 0}$ as follows. Set $\bar{Y}_0 = Z_0 \sim \eta_0$, $T_0 = 0$ and suppose that T_n and $(\bar{Y}_t)_{t \in [0, T_n]}$ have been defined for some $n \in \mathbb{N}$. Let $(B_t)_{t \geq 0}$ be a new Brownian motion on \mathbb{T}^d and $E \sim \mathcal{E}(1)$, independent one from the other. Let \tilde{Y} be the solution of

$$d\tilde{Y}_t = b(\tilde{Y}_t)dt + dB_t$$

for $t \geq T_n$ with $\tilde{Y}_{T_n} = \bar{Y}_{T_n}$ and let

$$T_{n+1} = \inf \left\{ t > T_n, E \leq \int_{T_n}^t \lambda(\tilde{Y}_s) ds \right\}.$$

For $t \in (T_n, T_{n+1})$, set $\bar{Y}_t = \tilde{Y}_t$. Finally, draw a new $\bar{Y}_{T_{n+1}}$ according to $\bar{\eta}_{T_{n+1}}$. By induction T_n and $(\bar{Y}_t)_{t \in [0, T_n]}$ are then defined for all $n \in \mathbb{N}$. Since λ is bounded, T_n almost surely goes to infinity when $n \rightarrow \infty$ so that $(\bar{Y}_t)_{t \geq 0}$ is defined for all $t \geq 0$. Similarly to Proposition 6.1.1, it can be established that $\mathcal{L}aw(\bar{Y}_t) = \bar{\eta}_t$ for all $t \geq 0$.

Now, as in Section 6.1.2, from the non-linear process $(\bar{Y}_t)_{t \geq 0}$, the interacting particles $(\bar{\mathbf{X}}_t)_{t \geq 0}$ are obtained by replacing $\bar{\eta}_t$ by the empirical distribution of the system when particles die and are resurrected.

More precisely, let $(E_{i,k}, B_{i,k}, J_{i,k})_{i \in \llbracket 1, N \rrbracket, k \in \mathbb{N}}$ be a family of independent triplet of independent random variables where, for all $i \in \llbracket 1, N \rrbracket$ and $k \in \mathbb{N}$, $E_{i,k} \sim \mathcal{E}(1)$, $J_{i,k} \sim \mathcal{U}(\llbracket 1, N \rrbracket)$ (except if $k = 0$, in which case $J_{i,k} = i$ almost surely) and $B_{i,k} = (B_{i,k,t})_{t \geq 0}$ is a d -dimensional Brownian motion. From these variables, we simultaneously define by induction the process and its death times $(T_{i,k})_{i \in \llbracket 1, N \rrbracket, k \in \mathbb{N}}$ as follows. First, set $\bar{\mathbf{X}}_0 = x$ and $T_{i,0} = 0$ for all $i \in \llbracket 1, N \rrbracket$. For all $i \in \llbracket 1, N \rrbracket$, set $\hat{X}_{i,0,0} = x_i$ and for $k \geq 1$, assuming that $\bar{\mathbf{X}}$ has been constructed up to time $T_{i,k}$, set

$$\hat{X}_{i,k,0} = \lim_{t \nearrow T_{i,k}} \bar{X}_{J_{i,k},t}. \quad (6.10)$$

For all $k \in \mathbb{N}$, for $t \geq T_{i,k}$, let $\hat{X}_{i,k}$ solve

$$d\hat{X}_{i,k,t} = b(\hat{X}_{i,k,t}) dt + dB_{i,k,t},$$

set

$$T_{i,k+1} = T_{i,k} + \inf \left\{ t \geq 0, E_{i,k} \leq \int_0^t \lambda(\hat{X}_{i,k,s}) ds \right\}$$

and for all $t \in [T_{i,k}, T_{i,k+1})$, set $\bar{X}_{i,t} = \hat{X}_{i,k,t-T_{i,k}}$.

Then $\bar{\mathbf{X}}_t = (\bar{X}_{1,t}, \dots, \bar{X}_{N,t})$ is well-defined for all $t \geq 0$. Indeed, it is well defined for all $t < S_1 := \min\{T_{i,1}, i \in \llbracket 1, N \rrbracket\}$ the first death time of some particle, and is equal on this interval to $(\hat{X}_{1,0,t}, \dots, \hat{X}_{N,0,t})$, which is continuous on $[0, S_1]$. Hence, the limits involved in (6.10) are well defined for $k = 1$ and all $i \in \llbracket 1, N \rrbracket$ such that $T_{i,1} = S_1$. Then the algorithm above similarly defines the process up to the second time some particles die, etc.

Remark that most of the times (6.10) simply reads $\hat{X}_{i,k,T_{i,k}} = \bar{X}_{J_{i,k},T_{i,k}}$ (at its k^{th} death time, the i^{th} particle is resurrected at the current position of the $J_{i,k}^{\text{th}}$ particle). Indeed, the only case when this is not true is when the $J_{i,k}^{\text{th}}$ particle dies at time $T_{i,k}$. Since the probability that

two or more particles die simultaneously is zero, this almost surely only occurs if $J_{i,k} = i$, i.e. if the particle is resurrected at its own position.

Denote $(P_t)_{t \geq 0}$ the Markov semi-group associated with $(\bar{\mathbf{X}}_t)_{t \geq 0}$, i.e. for all $t \geq 0$, P_t is the Markov kernel given by

$$P_t f(x) = \mathbb{E}(f(\mathbf{X}_t) \mid \mathbf{X}_0 = x).$$

We sometimes write $P_t = P_{N,t}$ to specify the number of particles.

Lemma 6.2.2. *There exist $C_4 > 0$ such that for all $N \in \mathbb{N}$, $\gamma \in (0, \gamma_0]$ and $\mu \in \mathcal{P}(\mathbb{T}^{dN})$,*

$$\mathcal{W}_{\rho_N}(\mu R_{N,\gamma}, \mu P_{N,\gamma}) \leq NC_4 \gamma^{3/2}.$$

Proof. As in the proof of Lemma 6.2.1, it is sufficient to treat the case $\mu = \delta_x$ with a fixed $x \in \mathbb{T}^{dN}$. Let $(\bar{\mathbf{X}}_t)_{t \geq 0}$ be defined as above from random variables $(E_{i,k}, B_{i,k}, J_{i,k})_{i \in \llbracket 1, N \rrbracket, k \in \mathbb{N}}$. In particular, $\bar{\mathbf{X}}_\gamma \sim \delta_x P_\gamma$.

To define $\mathbf{X}_1 \sim \delta_x R$, for all $i \in \llbracket 1, N \rrbracket$ and $k \in \mathbb{N}$, consider $(\tilde{X}_{i,k,t})_{t \geq 0}$ the solution to $\tilde{X}_{i,k,0} = x_{J_{i,k}}$ and

$$d\tilde{X}_{i,k,t} = b(\tilde{X}_{i,k,t}) dt + dB_{i,k,t}.$$

Denoting

$$H_i = \inf \left\{ k \in \mathbb{N}, E_{i,k} \geq \gamma \lambda \left(\tilde{X}_{i,k,\gamma} \right) \right\},$$

set $\mathbf{X}_1 := (\tilde{X}_{1,H_1,\gamma}, \dots, \tilde{X}_{N,H_N,\gamma})$.

Then $(\mathbf{X}_1, \bar{\mathbf{X}}_\gamma)$ is a coupling of $R(x, \cdot)$ and $P_\gamma(x, \cdot)$, so that

$$\mathcal{W}_{\rho_N}(R(x, \cdot), P_\gamma(x, \cdot)) \leq \mathbb{E}(\rho_N(\mathbf{X}_1, \bar{\mathbf{X}}_\gamma)) = \sum_{i=1}^N \mathbb{E}(\rho(X_{i,1}, \bar{X}_{i,\gamma})).$$

We now distinguish four cases, considering the events

$$\begin{aligned} B_{i,1} &= \{H_i = 0 \text{ and } T_{i,1} > \gamma\} \\ B_{i,2} &= \{H_i = 1 \text{ and } T_{i,1} \leq \gamma < T_{i,2} \wedge T_{J_{i,0},1}\} \\ B_{i,3} &= \{H_i = 1 \text{ and } T_{i,1} > \gamma\} \cup \{H_i = 0 \text{ and } T_{i,1} \leq \gamma\} \\ B_{i,4} &= \{H_i \geq 2\} \cup \{T_{i,2} \leq \gamma\} \cup \{T_{i,1} \vee T_{J_{i,1},1} \leq \gamma\}, \end{aligned}$$

that is, respectively: none of the two i^{th} particles dies; both the i^{th} particles die exactly once; one particle dies but not the other; at least two deaths are involved for one of the two particle. For all $i \in \llbracket 1, N \rrbracket$, $\Omega = \cup_{j=1}^4 B_{i,j}$, so that

$$\mathbb{E}(\rho(X_{i,1}, \bar{X}_{i,\gamma})) \leq \mathbb{E}(\rho(X_{i,1}, \bar{X}_{i,\gamma}) (\mathbb{1}_{B_{i,1}} + \mathbb{1}_{B_{i,2}} + \mathbb{1}_{B_{i,3}} + \mathbb{1}_{B_{i,4}})).$$

Conclusion follows by gathering the four cases.

Case 1. It reduces to the classical case of diffusions, since

$$\mathbb{E}(|X_{i,1} - \bar{X}_{i,\gamma}| \mathbb{1}_{B_{i,1}}) = \mathbb{E}(|\tilde{X}_{i,0,\gamma} - \hat{X}_{i,0,\gamma}| \mathbb{1}_{B_{i,1}}) \leq \mathbb{E}(|\tilde{X}_{i,0,\gamma} - \hat{X}_{i,0,\gamma}|).$$

Then

$$\begin{aligned} |\tilde{X}_{i,0,t} - \hat{X}_{i,0,t}| &= \left| \int_0^t (b(x_i) - b(\hat{X}_{i,0,s})) ds \right| \\ &\leq \|\nabla b\|_\infty \int_0^t (|\tilde{X}_{i,0,s} - \hat{X}_{i,0,s}| + |x_i - \tilde{X}_{i,0,s}|) ds \end{aligned}$$

By the Gronwall Lemma, for all $t \geq 0$, almost surely,

$$\sup_{s \in [0,t]} |\tilde{X}_{i,0,t} - \hat{X}_{i,0,t}| \leq \|\nabla b\|_\infty e^{t\|\nabla b\|_\infty} \int_0^t |x_i - \tilde{X}_{i,0,s}| ds. \quad (6.11)$$

Since $\tilde{X}_{i,0,s}$ is a Gaussian variable with mean $x_i + sb(x_i)$ and variance s ,

$$\mathbb{E}(|x_i - \tilde{X}_{i,0,s}|) \leq sb(x_i) + \mathbb{E}(|x_i + sb(x_i) - \tilde{X}_{i,0,s}|) \leq \|b\|_\infty s + \sqrt{s}. \quad (6.12)$$

As a consequence, for $\gamma \leq \gamma_0$,

$$\mathbb{E}(|\tilde{X}_{i,0,\gamma} - \hat{X}_{i,0,\gamma}|) \leq \|\nabla b\|_\infty e^{\gamma_0\|\nabla b\|_\infty} \int_0^\gamma \mathbb{E}(|x_i - \tilde{X}_{i,0,s}|) ds \leq c\gamma^{3/2}. \quad (6.13)$$

Case 2. We bound

$$\mathbb{E}(|X_{i,1} - \bar{X}_{i,\gamma}| \mathbb{1}_{B_{i,2}}) \leq \mathbb{E}(|\tilde{X}_{i,1,\gamma} - x_{J_{i,0}}| + |\hat{X}_{i,1,\gamma} - x_{J_{i,0}}|) \mathbb{1}_{B_{i,2}}.$$

Similarly to (6.12),

$$\mathbb{E}(|\tilde{X}_{i,1,\gamma} - x_{J_{i,0}}| \mathbb{1}_{B_{i,2}}) \leq \mathbb{E}(|\tilde{X}_{i,1,\gamma} - x_{J_{i,0}}| \mathbb{1}_{E_{i,0} \leq \gamma\|\lambda\|_\infty}) \leq c\gamma^{3/2},$$

where we used the independence of $E_{i,0}$ from $J_{i,1}$ and $(\tilde{X}_{i,1,t})_{t \geq 0}$. Denote $(X'_i)_{t \geq 0}$ the solution of

$$dX'_{i,t} = b(X'_{i,t}) dt + \begin{cases} dB_{J_{i,0},0,t} & \text{for } t < T_{i,0} \\ dB_{i,1,t} & \text{for } t \geq T_{i,0}. \end{cases}$$

with $X'_{i,0} = x_{J_{i,0}}$. Under the event $B_{i,2}$, $\hat{X}_{i,1,\gamma} = X'_{i,\gamma}$. Moreover, $J_{i,0}$, $B_{J_{i,0},0}$ and $B_{i,1}$ are independent from $T_{i,0}$ and thus, by the strong Markov property, $(X'_{i,t})_{t \geq 0}$ is independent from $T_{i,0}$ and conditionally to $J_{i,0}$ it has the same distribution as $\hat{X}_{J_{i,0},0,t}$ (namely it is a diffusion solving (6.1) with initial condition $x_{J_{i,0}}$). Hence,

$$\mathbb{E}(|\hat{X}_{i,1,\gamma} - x_{J_{i,0}}| \mathbb{1}_{B_{i,2}}) \leq \mathbb{E}(|X'_{i,\gamma} - y_{J_{i,0}}| \mathbb{1}_{E_{i,0} \leq \gamma\|\lambda\|_\infty}) \leq c'\gamma^{3/2}.$$

Case 3. We bound

$$\begin{aligned} \mathbb{E}(\rho(X_{i,1}, \bar{X}_{i,\gamma}) \mathbb{1}_{B_{i,3}}) &\leq \frac{1}{a} \mathbb{P}(B_{i,3}) \\ &\leq \frac{1}{a} \mathbb{P}\left(\int_0^\gamma \lambda(\hat{X}_{i,0,s}) ds \wedge (\gamma \lambda(\tilde{X}_{i,0,\gamma})) \leq E_{i,0} \leq \int_0^\gamma \lambda(\hat{X}_{i,0,s}) ds \vee (\gamma \lambda(\tilde{X}_{i,0,\gamma}))\right) \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{a} \mathbb{E} \left(\left| \exp \left(- \int_0^\gamma \lambda(\hat{X}_{i,0,s}) ds \right) - \exp \left(-\gamma \lambda(\tilde{X}_{i,0,\gamma}) \right) \right| \right) \\
&\leq \frac{1}{a} \mathbb{E} \left(\left| \int_0^\gamma \lambda(\hat{X}_{i,0,s}) ds - \gamma \lambda(\tilde{X}_{i,0,\gamma}) \right| \right).
\end{aligned}$$

Now,

$$\left| \int_0^\gamma \lambda(\hat{X}_{i,0,s}) ds - \gamma \lambda(\tilde{X}_{i,0,\gamma}) \right| \leq L_\lambda \left(\int_0^\gamma |\hat{X}_{i,0,s} - x_i| ds + \gamma |x_i - \tilde{X}_{i,0,\gamma}| \right).$$

Using (6.11) together with (6.12) yields

$$\mathbb{E} (\rho (X_{i,1}, \bar{X}_{i,\gamma}) \mathbb{1}_{B_{i,3}}) \leq c_3 \gamma^{3/2}.$$

Case 4. We bound

$$\begin{aligned}
\mathbb{E} (\rho (X_{i,1}, \bar{X}_{i,\gamma}) \mathbb{1}_{B_{i,4}}) &\leq \frac{1}{a} \mathbb{P} (B_{i,4}) \\
&\leq \mathbb{P} (E_{i,0} \vee E_{i,1} \leq \gamma \|\lambda\|_\infty) + \mathbb{P} (E_{i,0} \vee E_{J_{i,0},0} \leq \gamma \|\lambda\|_\infty) \\
&\leq 2 \left(1 - e^{-\gamma \|\lambda\|_\infty} \right)^2 \leq 2\gamma^2 \|\lambda\|_\infty^2.
\end{aligned}$$

□

Proposition 6.2.5. *There exist $C_5 > 0$ such that for all $N \in \mathbb{N}$, $\gamma \in (0, \gamma_0]$ and $\eta_0 \in \mathcal{P}(\mathbb{T}^d)$,*

$$\mathcal{W}_{\rho_N} (\mu R_{N,\gamma}^m, \mu P_{N,m\gamma}) \leq \sqrt{\gamma} N C_5 \gamma \sum_{s=1}^m (1 - \gamma \kappa)^{s-1}.$$

As for Proposition 6.2.4, when $\kappa > 0$, $\gamma \sum_{s=1}^m (1 - \gamma \kappa)^{s-1} \leq 1/\kappa$ so that (6.8) and (6.9) yield uniform in time estimates. On the contrary, when $\kappa < 0$, the estimates are exponentially bad in $t = m\gamma$.

Proof. The proof is similar to Proposition 6.2.4. Denoting $\mu_m = \mu R^m$ and $\nu_m = \mu P_{m\gamma}$, from the triangular inequality, Proposition 6.2.3 and Lemma 6.2.2,

$$\begin{aligned}
r_m := \mathcal{W}_{\rho_N} (\mu_m, \nu_m) &\leq \mathcal{W}_{\rho_N} (\mu_m, \nu_{m-1} R) + \mathcal{W}_{\rho_N} (\nu_{m-1} R, \nu_{m-1} P_\gamma) \\
&\leq (1 - \gamma \kappa) r_{m-1} + N C_4 \gamma^{3/2},
\end{aligned}$$

and an induction concludes. □

6.2.5 Conclusion

In this section we use the notations of the previous ones, in particular κ is given by (6.5) and the constants C_2 , C_3 and C_5 are those of Propositions 6.2.4 and 6.2.5. We can now gather all these previous results.

Letting either γ vanish or N go to infinity in Proposition 6.2.3, we obtain long-time convergence for, respectively, the non-homogeneous self-interacting Markov chain $(Y_k)_{k \in \mathbb{N}}$ introduced in Section 6.1.2 and the continuous-time Markov chain $(\bar{\mathbf{X}}_t)_{t \geq 0}$ defined in Section 6.2.4.

Corollary 6.2.2. *Let $(\eta_m)_{m \in \mathbb{N}}$ be such as defined in Section 6.1.2, and $(\tilde{\eta}_m)_{m \in \mathbb{N}}$ be similarly defined but with a different initial distribution $\tilde{\eta}_0 \in \mathcal{P}(\mathbb{T}^d)$. For all $m \in \mathbb{N}$ and all $\gamma \in (0, \gamma_0]$,*

$$\mathcal{W}_\rho(\eta_m, \tilde{\eta}_m) \leq (1 - \gamma\kappa)^m \mathcal{W}_\rho(\eta_0, \tilde{\eta}_0).$$

Corollary 6.2.3. *For all $N \in \mathbb{N}_*$, $t \geq 0$ and $\mu, \nu \in \mathcal{P}(\mathbb{T}^{dN})$,*

$$\mathcal{W}_{\rho_N}(\mu P_{N,t}, \nu P_{N,t}) \leq e^{-\kappa t} \mathcal{W}_{\rho_N}(\mu, \nu).$$

Proof of Corollary 6.2.2. The proof is based on the simple equality: For all $N \in \mathbb{N}$ and $\mu, \nu \in \mathcal{P}(\mathbb{T}^d)$,

$$\mathcal{W}_{\rho_N}(\mu^{\otimes N}, \nu^{\otimes N}) = N \mathcal{W}_\rho(\mu, \nu). \quad (6.14)$$

Indeed, by considering N independent couplings $(X_i, Y_i)_{i \in [1, N]}$,

$$\mathcal{W}_{\rho_N}(\mu^{\otimes N}, \nu^{\otimes N}) \leq \mathbb{E}(\rho_N(\mathbf{X}, \mathbf{Y})) = \sum_{i=1}^N \mathbb{E}(\rho(X_i, Y_i)) = N \mathcal{W}_\rho(\mu, \nu).$$

Conversely, if (\mathbf{X}, \mathbf{Y}) is an optimal coupling of $\mu^{\otimes N}$ and $\nu^{\otimes N}$, then

$$\mathcal{W}_\rho(\mu, \nu) \leq \mathbb{E}(\rho(X_1, Y_1)) = \frac{1}{N} \mathbb{E}(\rho_N(\mathbf{X}, \mathbf{Y})) = \frac{1}{N} \mathcal{W}_{\rho_N}(\mu^{\otimes N}, \nu^{\otimes N}).$$

By the triangular inequality,

$$\begin{aligned} \mathcal{W}_\rho(\eta_m^{\otimes N}, \tilde{\eta}_m^{\otimes N}) &\leq \mathcal{W}_\rho(\eta_m^{\otimes N}, \eta_0^{\otimes N} R^m) + \mathcal{W}_\rho(\eta_0^{\otimes N} R^m, \tilde{\eta}_0^{\otimes N} R^m) + \mathcal{W}_\rho(\tilde{\eta}_0^{\otimes N} R^m, \tilde{\eta}_m^{\otimes N}) \\ &\leq (1 - \gamma\kappa)^m \mathcal{W}_\rho(\eta_0^{\otimes N}, \tilde{\eta}_0^{\otimes N}) + 2C_2 N \alpha(N) \gamma \sum_{s=1}^m (1 - \gamma\kappa)^{s-1}. \end{aligned}$$

where we applied Propositions 6.2.3 and 6.2.4. Using the equality 6.14, dividing by N and letting N go to infinity concludes the proof of Corollary 6.2.2. \square

Remark that the beginning of the proof also applies for $\mu, \nu \in \mathcal{P}(\mathbb{T}^{dN})$ that are exchangeable (i.e. invariant by any permutation of the d -dimensional coordinates), in which case, denoting, $\mu^{(1)}$ and $\nu^{(1)}$ their d -dimensional marginals, we get that

$$\mathcal{W}_\rho(\mu^{(1)}, \nu^{(1)}) \leq \frac{1}{N} \mathcal{W}_{\rho_N}(\mu, \nu).$$

Proof of Corollary 6.2.3. Similarly to the previous proof, Corollary 6.2.3 is a direct consequence of Propositions 6.2.3 and 6.2.5, letting m go to infinity at a fixed t and N in

$$\begin{aligned} \mathcal{W}_{\rho_N}(\mu P_{N,t}, \nu P_{N,t}) &\leq \mathcal{W}_{\rho_N}(\mu P_{N,t}, \mu R_{N,t/m}^m) + \mathcal{W}_{\rho_N}(\mu R_{N,t/m}^m, \nu R_{N,t/m}^m) \\ &\quad + \mathcal{W}_{\rho_N}(\nu R_{N,t/m}^m, \nu P_{N,t}). \end{aligned}$$

\square

We now turn to the continuous-time limit of the non-linear chain $(Y_k)_{k \in \mathbb{N}}$.

Corollary 6.2.4. *There exists $C_6 > 0$ such that for all $\eta_0 \in \mathcal{P}(\mathbb{T}^d)$ and all $\gamma \in (0, \gamma_0]$, if $(\eta_m)_{m \in \mathbb{N}}$ is such as defined in Section 6.1.2, and $(\bar{\eta}_t)_{t \geq 0}$ is such as defined in Section 6.2.4 (with $\bar{\eta}_0 = \eta_0$),*

then

$$\mathcal{W}_1(\eta_1, \bar{\eta}_\gamma) \leq C_6 \gamma^{3/2},$$

and for all $m \geq 1$,

$$\mathcal{W}_\rho(\eta_m, \bar{\eta}_{m\gamma}) \leq \sqrt{\gamma} C_6 \gamma \sum_{s=1}^m (1 - \gamma\kappa)^{s-1}.$$

Proof. For the first inequality, we could follow the proof of Lemma 6.2.2, but, using the notations of the introduction, we will rather use the fact that

$$\eta_1 = \mathcal{L}aw(\tilde{Z}_1 \mid \tilde{T} > \gamma), \quad \bar{\eta}_\gamma = \mathcal{L}aw(Z_\gamma \mid T > \gamma),$$

where the gaussian variable G_0 in (6.3) is equal to $B_\gamma/\sqrt{\gamma}$ where $(B_t)_{t \geq 0}$ is the Brownian motion involved in (6.1), and T and \tilde{T} are defined with the same $E \sim \mathcal{E}(1)$. Recall the estimate (6.13) for the error from an Euler scheme to its initial diffusion. Then we bound

$$\begin{aligned} \mathbb{E}(|\tilde{Z}_1 - Z_\gamma| \mid T > \gamma, \tilde{T} > \gamma) &\leq \left(\mathbb{P}(T > \gamma, \tilde{T} > \gamma) \right)^{-1} \mathbb{E}(|\tilde{Z}_1 - Z_\gamma|) \\ &\leq \left(1 - e^{-\gamma_0 \|\lambda\|_\infty} \right)^{-1} c \gamma^{3/2}, \end{aligned}$$

which concludes the first part of the corollary.

For the second part, denoting $r_m = \mathcal{W}_\rho(\eta_m, \bar{\eta}_{m\gamma})$, we bound

$$\begin{aligned} r_m &\leq \mathcal{W}_\rho(\eta_m, \bar{\eta}_{m-1} Q_{\bar{\eta}_{\gamma(m-1)}}) + \mathcal{W}_\rho(\bar{\eta}_{m-1} Q_{\bar{\eta}_{m-1}}, \bar{\eta}_{m\gamma}) \\ &\leq (1 - \gamma\kappa) r_{m-1} + C_6 \gamma^{3/2}, \end{aligned}$$

where we used the first part of the corollary and Corollary 6.2.2. An induction concludes. \square

We can now prove propagation of chaos results for the continuous-time process:

Corollary 6.2.5. *For all $N \in \mathbb{N}$, $k \in \llbracket 1, N \rrbracket$ and all $t \geq 0$, if $(\bar{\mathbf{X}}_t)_{t \geq 0}$ is a Markov process with initial distribution $\eta_0^{\otimes N}$ associated to the semigroup $(P_{N,t})_{t \geq 0}$ then, first,*

$$\mathcal{W}_{\rho_k}(\mathcal{L}aw(\bar{X}_{1,t}, \dots, \bar{X}_{k,t}), \bar{\eta}_t^{\otimes k}) \leq C_2 k \alpha(N) \int_0^t e^{-\kappa s} ds,$$

and second,

$$\mathbb{E}(\mathcal{W}_\rho(\pi(\bar{\mathbf{X}}_t), \bar{\eta}_t)) \leq C_3 \alpha(N) \left(1 + \int_0^t e^{-\kappa s} ds \right).$$

Proof. As shown in the proof of Proposition 6.2.4, if (\mathbf{X}, \mathbf{Y}) is an optimal coupling of μ and ν ,

$$\mathbb{E}(\mathcal{W}_\rho(\pi(\mathbf{X}), \pi(\mathbf{Y}))) \leq \frac{1}{N} \mathcal{W}_{\rho_N}(\mu, \nu).$$

Thus, considering a time step $\gamma = t/m$, $m \in \mathbb{N}$, we decompose

$$\mathcal{W}_\rho(\pi(\bar{\mathbf{X}}_t), \bar{\eta}_t) \leq \mathcal{W}_\rho(\pi(\bar{\mathbf{X}}_t), \pi(\mathbf{X}_m)) + \mathcal{W}_\rho(\pi(\mathbf{X}_m), \eta_m) + \mathcal{W}_\rho(\eta_m, \bar{\eta}_t),$$

take the expectation, apply Propositions 6.2.4 and 6.2.5 and Corollary 6.2.4 and let m go to

infinity. This proves the second point, and the proof of the first one is similar, with Corollary 6.2.1. \square

Up to now, we have sent either N or γ to their limit. When $\kappa > 0$, if we let $t = m\gamma$ go to infinity at fixed N and γ , we recover results on the equilibria of the processes. Indeed, note that Corollary (6.2.2) together with the Banach fixed-point theorem imply that $n \mapsto \eta_n$ admits a limit which is independent from η_0 . Together with Proposition 6.1.1, this is the unique QSD of the Markov chain (6.3). Denote it ν_γ . Similarly, Proposition 6.2.3 implies that $R_{N,\gamma}$ admits a unique invariant measure. Denote it $\mu_{\infty,N,\gamma}$, and $\mu_{\infty,N,\gamma}^{(k)}$ its first kd -dimensional marginal for $k \in \llbracket 1, N \rrbracket$ (i.e. the law of (X_1, \dots, X_k) if $\mathbf{X} \sim \mu_{\infty,N,\gamma}$). Third, Corollary 6.2.3 implies that $(P_{N,t})_{t \geq 0}$ admits a unique invariant measure $\bar{\mu}_{\infty,N}$.

Corollary 6.2.6. *If $\kappa > 0$, then for all $N \in \mathbb{N}$ and $\gamma \in (0, \gamma_0]$*

$$\mathcal{W}_{\rho_N}(\mu_{\infty,N,\gamma}, \bar{\mu}_{\infty,N}) \leq \sqrt{\gamma} N \kappa^{-1} C_5,$$

Corollary 6.2.7. *If $\kappa > 0$, then for all $N \in \mathbb{N}$, $k \in \llbracket 1, N \rrbracket$ and $\gamma \in (0, \gamma_0]$, first,*

$$\mathcal{W}_{\rho_k}(\mu_{\infty,N,\gamma}^{(k)}, \nu_\gamma^{\otimes k}) \leq \kappa^{-1} C_2 k \alpha(N),$$

and second,

$$\mathbb{E}_{\mu_{\infty,N,\gamma}}(\mathcal{W}_\rho(\pi(\mathbf{X}), \nu_\gamma)) \leq \kappa^{-1} C_3 \alpha(N).$$

Proofs of Corollaries 6.2.6 and 6.2.7. Considering any $\eta_0 \in \mathcal{P}(\mathbb{T}^d)$ and $m \in \mathbb{N}$,

$$\begin{aligned} \mathcal{W}_{\rho_N}(\mu_{\infty,N,\gamma}, \bar{\mu}_{\infty,N}) &\leq \mathcal{W}_{\rho_N}(\mu_{\infty,N,\gamma}, \eta_0^{\otimes N} R^m) + \mathcal{W}_{\rho_N}(\eta_0^{\otimes N} R^m, \eta_0^{\otimes N} P_{\gamma m}) \\ &\quad + \mathcal{W}_{\rho_N}(\eta_0^{\otimes N} P_{\gamma m}, \bar{\mu}_{\infty,N}) \end{aligned}$$

Apply Proposition 6.2.3 with $\mu = \mu_{\infty,N,\gamma}$ and $\nu = \eta_0^{\otimes N}$, Corollary 6.2.3 with the same ν and with $\mu = \bar{\mu}_{\infty,N}$, and Proposition 6.2.5. Letting m go to infinity concludes the proof of Corollary 6.2.6. The proof of Corollary 6.2.7 is similar (based on Proposition 6.2.4 and Corollary 6.2.1, like Corollary 6.2.5). \square

Next, we can send two parameters to their limit. Sending N to infinity and γ to zero, we get the long time convergence of the non-linear process $(\bar{Y}_t)_{t \geq 0}$ introduced in Section 6.2.4 (or, equivalently, of the process Z solving (6.1) conditioned not to be dead):

Corollary 6.2.8. *Let $(\bar{\eta}_t)_{t \geq 0}$ be such as defined in Section 6.1.2, and $(\hat{\eta}_t)_{t \geq 0}$ be similarly defined but with a different initial distribution $\hat{\eta}_0 \in \mathcal{P}(\mathbb{T}^d)$. For all $t \geq 0$,*

$$\mathcal{W}_\rho(\bar{\eta}_t, \hat{\eta}_t) \leq e^{-\kappa t} \mathcal{W}_\rho(\bar{\eta}_0, \hat{\eta}_0).$$

Proof. Thanks to Corollary 6.2.4, let $\gamma = t/m$ vanish in Corollary 6.2.2. \square

In particular, if $\hat{\eta}_0$ is the QSD ν_* , by definition, $\hat{\eta}_t = \nu_*$ for all $t \geq 0$, so that Corollary 6.2.8 yields the uniqueness of the QSD and the exponential convergence of $\mathcal{L}aw(Z_t \mid T > t)$ toward ν_* (which is a result in the spirit of [32, 36, 47, 7]).

Now, at a fixed $\gamma > 0$, letting t and N go to infinity, we obtain an error bound between the QSD ν_* of the continus process (6.1) and the QSD ν_γ of the discrete scheme.

Corollary 6.2.9. *If $\kappa > 0$, then for all $\gamma \in (0, \gamma_0]$*

$$\mathcal{W}_\rho(\nu_\gamma, \nu_*) \leq \sqrt{\gamma} \kappa^{-1} C_6,$$

Proof. Thanks to Corollaries 6.2.2 and 6.2.8 (applied with one of the initial condition being the equilibrium), let m go to infinity in Corollary 6.2.4. \square

Finally, letting γ vanish and t go to infinity at a fixed $N \in \mathbb{N}$, we obtain a propagation of chaos result at stationarity (as established first in [5], and more recently with a CLT in [108] in the case of a finite state space) for the continuous time system of interacting particle $(\bar{\mathbf{X}}_t)_{t \geq 0}$ introduced in Section 6.2.4.

Corollary 6.2.10. *If $\kappa > 0$ and if $\bar{\mathbf{X}}$ is a random variable with law $\bar{\mu}_{\infty, N}$, then for all $N \in \mathbb{N}$ and $k \in \llbracket 1, N \rrbracket$,*

$$\mathcal{W}_{\rho_N}(\text{Law}(X_1, \dots, X_k), \nu_*^{\otimes k}) \leq \kappa^{-1} C_2 k \alpha(N),$$

and second,

$$\mathbb{E}(\mathcal{W}_\rho(\pi(\bar{\mathbf{X}}), \nu_*)) \leq C_3 \alpha(N) (1 + \kappa^{-1}).$$

Proof. The proof is similar to Corollary 6.2.5, letting t go to infinity in Corollary 6.2.5 thanks to Corollaries 6.2.3 and 6.2.8. \square

Remark that our results at stationarity (Corollaries 6.2.6, 6.2.7, 6.2.9 and 6.2.10) all require the perturbative condition $\kappa > 0$. Yet, propagation of chaos at stationarity for the continuous time process follows from the works [5, 108, 46, 44, 149] in a much broader (non-perturbative) framework (and, although it doesn't seem to have been studied yet, the situation should be similar for error bounds in γ rather than N). As previously discussed, error bounds on N (and possibly γ) that are uniform in time can be obtained thanks to the long-time convergence of the limit ($N = +\infty$) non-linear process. In our case, when $\kappa > 0$, this long-time convergence follows from the (uniform in N) long-time convergence of the particle system (whether it is possible to obtain the latter from the former is unclear), but it holds in more general cases (see [32, 36, 47, 7] and references within) and, in those cases, results similar to Corollaries 6.2.6, 6.2.7, 6.2.9 and 6.2.10 should hold. The question of establishing propagation of chaos or discretization error bounds at stationarity in a more general case (i.e. without the condition $\kappa > 0$) is out of the scope of the present work.

All our results are summarised in Figure 6.1.

Finally, we detail the proof of our main result.

Proof of Theorem 6.1.2. For $\eta_0 \in \mathcal{P}(\mathbb{T}^d)$, let (\mathbf{X}, \mathbf{Y}) be an optimal coupling of $\mu_0 R^{\lfloor t/\gamma \rfloor}$ and $\eta_0^{\otimes N} R^{\lfloor t/\gamma \rfloor}$. As in the proof of Proposition 6.2.4,

$$\mathbb{E}(\mathcal{W}_\rho(\pi(\mathbf{X}), \pi(\mathbf{Y}))) \leq \frac{1}{N} \mathcal{W}_{\rho_N}(\mu R^{\lfloor t/\gamma \rfloor}, \eta_0^{\otimes N} R^{\lfloor t/\gamma \rfloor}) \leq a e^{-\kappa(t-\gamma_0)},$$

where we used Proposition 6.2.3 and the fact that $\rho_N(x, y) \leq Na$ for all $x, y \in \mathbb{T}^{dN}$. Then, by the triangular inequality,

$$\mathcal{W}_\rho(\pi(\mathbf{Y}), \nu_*) \leq \mathcal{W}_\rho(\pi(\mathbf{Y}), \eta_{\lfloor t/\gamma \rfloor}) + \mathcal{W}_\rho(\eta_{\lfloor t/\gamma \rfloor}, \nu_\gamma) + \mathcal{W}_\rho(\nu_\gamma, \nu_*).$$

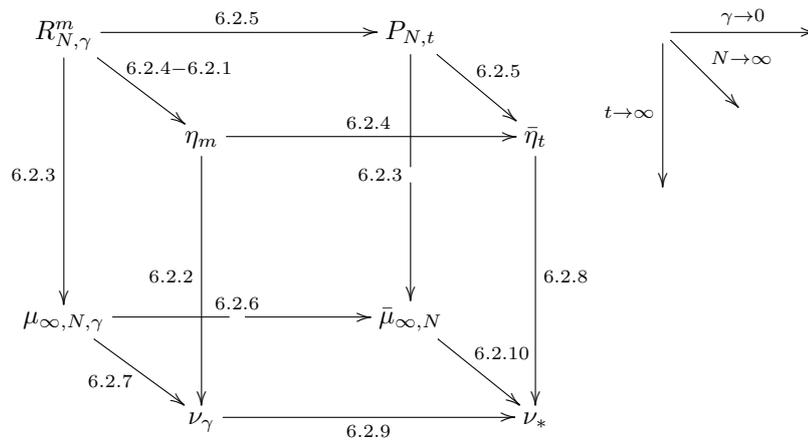


Figure 6.1: Summary of the different results. The label of each arrow indicates the corollary or proposition where the corresponding quantitative convergence is stated. Vertical, horizontal and diagonal arrows correspond respectively to t , γ and N going to their limit.

Taking the expectation, applying Proposition 6.2.4 and Corollaries 6.2.2 (applied with $\tilde{\eta}_0 = \nu_\gamma$) and 6.2.9, the boundedness of ρ and the equivalence of \mathcal{W}_ρ and \mathcal{W}_1 concludes. \square

Chapter 7

Uniform convergence of the Fleming-Viot process in a hard killing metastable case

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Abstract : We study the long-time convergence of a Fleming-Viot process, in the case where the underlying process is a metastable diffusion killed when it reaches some level set. Through a coupling argument, we establish the long-time convergence of the Fleming-Viot process toward some stationary measure at an exponential rate independent of N , the size of the system, as well as uniform in time propagation of chaos estimates.

7.1 Introduction

Given some open bounded domain $D \subset \mathbb{R}^d$, and some potential $U : \mathbb{R}^d \rightarrow \mathbb{R}_+$, we are interested in the process:

$$dX_t = -\nabla U(X_t)dt + \sqrt{2\varepsilon}dB_t \tag{7.1}$$

with small $\varepsilon > 0$, killed when it reaches ∂D the boundary of D . More precisely, write:

$$\tau_{\partial D} = \inf \{t \geq 0, X_t \notin D\}. \quad (7.2)$$

Denote by $\mathcal{M}^1(D)$ the set of probability measures on D , and \mathbb{P}_μ the law of the process (7.1), with initial condition $\mu \in \mathcal{M}^1(D)$. Then we say that $\nu \in \mathcal{M}^1(D)$ is a quasi-stationary distribution (QSD) of the process (7.1) if for all $t \geq 0$:

$$\mathbb{P}_\nu (X_t \in \cdot \mid \tau_{\partial D} > t) = \nu.$$

It is shown in [104] that, under some mild assumptions on U and D , the process (7.1) admits a unique QSD, that we will denote by ν_∞^ε . It is also proven that there is convergence for all initial condition of the law of the process conditioned on its survival toward this QSD, namely, for all $\mu \in \mathcal{M}^1(D)$,

$$\mathbb{P}_\mu (X_t \in \cdot \mid \tau_{\partial D} > t) \xrightarrow[t \rightarrow +\infty]{} \nu_\infty^\varepsilon.$$

The fact that the process is killed when it exits a domain is classically referred to as a *hard killing* case, by contrast with the *soft killing* case where the process is killed according to a inhomogeneous Poisson process as in [94].

The present work is concerned with the question of sampling the QSD ν_∞^ε . More precisely, in practice, the QSD is approximated by the empirical measure of a system of interacting particles, called a Fleming-Viot (FV) process, at stationarity. This FV process is defined informally as follows: for a given N , let X^1, \dots, X^N be N independent diffusions until one of them reaches ∂D . The diffusion that has been killed then branches onto one of the $N - 1$ remaining ones, chosen uniformly at random. In very general settings, it is known that if the initial condition consists in N independent random variables distributed according to a common law μ , then for any time $t \geq 0$, we have:

$$a.s. \quad \pi^N(X_t^1, \dots, X_t^N) \xrightarrow[N \rightarrow \infty]{weak} \mathbb{P}_\mu (X_t \in \cdot \mid \tau_{\partial D} > t), \quad (7.3)$$

(see Section 1.3.3) where

$$\pi^N(x) = \frac{1}{N} \sum_{i=1}^N \delta_{x_i} \quad (7.4)$$

stands for the empirical measure of a vector $(x_1, \dots, x_N) \in D^N$. This would simply be the law of large numbers if the particles were independent, which they are not due to the resurrection mechanism. For mean-field interacting particle systems as the FV process, such a convergence is known as a propagation of chaos phenomenon.

Two questions are addressed in this work. First, the long-time relaxation of the FV process toward its invariant measure: a quantitative convergence in the total variation distance sense at a rate independent from N is stated in Theorem 7.1.1. Second, the propagation of chaos: Theorem 7.1.2 gives a quantitative version of (7.3), with a bound uniform in time. Combining both results yields a quantitative estimate for the convergence of the empirical measure of the FV process toward the QSD as $N, t \rightarrow \infty$.

As detailed below, these results are established under the condition that D is a metastable state for the diffusion (7.1), in the sense that the mixing time of (7.1) within D is shorter than the typical exit time from D . Mathematically speaking, this is reflected by the fact that c^* , the critical height within D , is smaller than U_0 , the height of the boundary ∂D (see below for the definition of c^* and U_0), and the temperature ε is small enough. This metastable context is

typically the one where QSD are of interest, since in that case the (non-conditional) law of the process is close to the QSD for times in intermediary scales between the mixing time and the extinction time. Moreover, it is exactly the context of some algorithms in molecular dynamics, such as the parallel replica algorithm presented in [104], which involves the sampling of the QSD. In fact, for technical reasons, we will work under a stronger condition than simply $c_* < U_0$ (see Assumption 7.1.3 below), which is also related to the metastability of D . While we haven't succeeded in this endeavor, we think that the proof may possibly be modified to work only with the condition $c_* < U_0$, without the additional condition.

The paper is organized as follows. The remainder of this introduction is dedicated to the statement of the main results. Some preliminary properties of the FV process are studied in Section 7.2, and the main theorems are proven in Section 7.3. Finally, we prove in Section 7.4 the technical lemma which involves the additional condition.

7.1.1 Main Result

Define the critical height $c^* = c^*(U)$ of U as $c^* = \sup_{x_1, x_2 \in D} c(x_1, x_2)$ with

$$c(x_1, x_2) = \inf \left\{ \max_{0 \leq t \leq 1} U(\xi(t)) - U(x_1) - U(x_2) \right\},$$

where the infimum runs over $\{\xi \in \mathcal{C}([0, 1], D), \xi(0) = x_1, \xi(1) = x_2\}$. The critical height c^* represents the largest energy barrier the process has to cross in order to go from any local minimum to any global one (within D).

The following conditions are enforced throughout all this work.

Assumption 7.1.1. • $D \subset \mathbb{R}^d$ is open, bounded, connected and its boundary is \mathcal{C}^2 .

• $U : \mathbb{R}^d \rightarrow \mathbb{R}_+$ is smooth on some neighborhood of \overline{D} .

• $\min_D U = 0$.

• $U|_{\partial D}$ is constant, and

$$U_0 = U(\partial D) > c^*. \quad (7.5)$$

• For $x \in \partial D$, denote by $n(x)$ the outward normal to D . For all $x \in \partial D$,

$$n(x) \cdot \nabla U(x) > 0. \quad (7.6)$$

The condition $\min_D U = 0$ is just a choice of normalisation since the process is unchanged if a constant is added to U . Under Assumption 7.1.1, neglecting sub-exponential terms, for small ε , the mixing rate of the non-killed process (7.1) is known to be of order $e^{c_*/\varepsilon}$ (see [83]) while, according to the theory of Freidlin-Wentzell (see [65]), the exit time $\tau_{\partial D}$ is of order $e^{U_0/\varepsilon}$. As already mentioned, the condition $U_0 > c^*$ thus describes a difference of timescales between the mixing time and the death time. More precisely, it is known that for any neighborhood \mathfrak{B}_1 of ∂D and any $a < U_0$, $\sup_{x \in D \setminus \mathfrak{B}_1} \mathbb{P}_x(\tau_{\partial D} < e^{a/\varepsilon})$ vanishes with ε . The assumption that U is constant over ∂D , which is consistent with the idea that D is a local potential well, could possibly be relaxed, with the condition (7.5) being replaced by $\inf_{\partial D} U > c^*$, however this adjustment would introduce additional technical complexities to the construction of a Lyapunov function, see Lemma 7.2.3. We will need an even stronger uniformity in terms of the initial condition. For now, let us state it as an assumption:

Assumption 7.1.2. *There exist $a > c^*$ and a neighborhood \mathfrak{B}_1 of ∂D such that the following holds:*

- $\min_{\mathfrak{B}_1} U > a$,
- $\min_{x \in \mathfrak{B}_1} |\nabla U(x)| > 0$,
- for a fixed Brownian motion $(B_t)_{t \geq 0}$, denoting by $(X_t^x)_{t \geq 0}$ the solution of (7.1) with initial condition x for all $x \in D$ and by $\tau_{\partial D}(X^x)$ its first exit time from D , we have

$$\bar{p}_\varepsilon := \mathbb{P} \left(\exists x \in D \setminus \mathfrak{B}_1, \tau_{\partial D}(X^x) < e^{a/\varepsilon} \right) \xrightarrow{\varepsilon \rightarrow 0} 0. \quad (7.7)$$

We are able to prove that this is implied by the following condition, which in dimension $d > 1$ strengthens (7.5):

Assumption 7.1.3. *One of the following is satisfied:*

- $d = 1$.
- *There exist a neighborhood $\tilde{\mathfrak{B}}_1$ of ∂D such that $\inf_{\tilde{\mathfrak{B}}_1} |\nabla U| > 0$ and*

$$c^* < \frac{U_0 - U_1}{2}, \quad \text{where} \quad U_1 = \min_{\tilde{\mathfrak{B}}_1} U.$$

As stated in Lemma 7.4.1 below, Assumptions 7.1.1 and 7.1.3 together imply Assumption 7.1.2. However we don't think that Assumption 7.1.3 is sharp, and thus we state our main results in terms of Assumption 7.1.2. Notice that Assumption 7.1.3 is always implied by Assumption 7.1.1 when $c_* = 0$.

We define the semi-group $(P_t)_{t \geq 0}$ associated to a Markov process $(X_t)_{t \geq 0}$ in \mathbb{R}^d by:

$$P_t f(x) = \mathbb{E}_x(f(X_t))$$

for any bounded measurable function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and any $t \geq 0$, where \mathbb{E}_x stands for the expectation under $\mathbb{P}_x = \mathbb{P}_{\delta_x}$. We denote $\llbracket 1, N \rrbracket = \{1, \dots, N\}$.

Now, let us define rigorously the FV process, starting from some initial condition $\mu \in \mathcal{M}^1(D^N)$. Let $(I_n^i)_{i \in \llbracket 1, N \rrbracket, n \in \mathbb{N}}$ be a family of independent random variables, where for $i \in \llbracket 1, N \rrbracket$, I_n^i is uniform on $i \in \llbracket 1, N \rrbracket \setminus \{i\}$. Let $(B^i)_{i \in \llbracket 1, N \rrbracket}$ be N independent Brownian motions, and $\mathbf{X}_0 = (X_0^1, \dots, X_0^N)$ be distributed according to μ . Define \bar{X}^i as the solution to:

$$\bar{X}_t^i = X_0^i - \int_0^t \nabla U(\bar{X}_s^i) ds + \sqrt{2\varepsilon} B_t^i$$

and set

$$\tau_1 = \min_i \inf \{t \geq 0, \bar{X}_t^i \notin D\}.$$

Then, denote by i_1 the index of the particle which exits the domain at time τ_1 . It is uniquely defined almost surely because, since the hitting time of the boundary has a density on \mathbb{R}_+ , the probability that two particles hit the boundary at the same time is zero (this is true for the Brownian motion, and the general case follows from an application of the Girsanov theorem). For $i \neq i_1$, $0 \leq t \leq \tau_1$, or $i = i_1$ and $1 \leq t < \tau_1$, simply let:

$$X_t^i = \bar{X}_t^i \quad \text{and} \quad X_{\tau_1}^{i_1} = \bar{X}_{\tau_1}^{i_1}.$$

This defines the process between times 0 and τ_1 . The process is then defined on (τ_1, ∞) by induction: if the process is defined up to time τ_{n-1} , we define it between time τ_{n-1} and τ_n in the same way, with \mathbf{X}_0 replaced by $\mathbf{X}_{\tau_{n-1}}$, i_1 by i_n the index of the particle that hits ∂D at time τ_n , and $I_1^{i_0}$ by $I_n^{i_n}$. Thus, $(\tau_n)_n$ is the sequence of branching times of the process.

Under Assumption 7.1.1, the FV process $\mathbf{X} = (X^1, \dots, X^N)$ is well-defined and does not explode in finite time, meaning that $\sup_n \tau_n = \infty$ almost surely, see [166, Theorem 2.1]. This defines a Markov process, and we denote by $P^{N,\varepsilon} = (P_t^{N,\varepsilon})_{t \geq 0}$ the associated semi-group.

A law $\mu \in \mathcal{M}^1(D^N)$ is said to be exchangeable if it is invariant by any permutation of the particles, i.e. $(X^{\sigma(i)})_{i \in \llbracket 1, N \rrbracket} \sim \mu$ if $(X^i)_{i \in \llbracket 1, N \rrbracket} \sim \mu$ for all permutations σ of $\llbracket 1, N \rrbracket$. For $k \in \llbracket 1, N \rrbracket$, we denote by $\mu^k \in \mathcal{M}^1(D^k)$ the marginal law of the k first particles under μ (which, for exchangeable laws, is thus the marginal law of any subset of k particles).

Our first main result concerns the long time behavior of the FV process.

Theorem 7.1.1. *Under Assumptions 7.1.1 and 7.1.2, there exist $\varepsilon_0, c, C > 0$ such that, for all $\varepsilon \in (0, \varepsilon_0]$, $N \in \mathbb{N}$, $t \geq 0$, setting $t_\varepsilon = e^{\alpha/\varepsilon}$, the following holds.*

1. For all $\mu, \nu \in \mathcal{M}^1(D^N)$,

$$\|\mu P_t^{N,\varepsilon} - \nu P_t^{N,\varepsilon}\|_{TV} \leq CN(1 - c)^{t/t_\varepsilon}.$$

2. The semi-group $P^{N,\varepsilon}$ admits a unique invariant measure $\nu_\infty^{N,\varepsilon}$, which is exchangeable.

3. For all exchangeable $\mu, \nu \in \mathcal{M}^1(D^N)$, for all $k \in \llbracket 1, N \rrbracket$,

$$\|(\mu P_t^N)^k - (\nu P_t^N)^k\|_{TV} \leq Ck(1 - c)^{t/t_\varepsilon}.$$

Our second result is a uniform in time propagation of chaos estimate.

Theorem 7.1.2. *Under Assumptions 7.1.1 and 7.1.2, there exists $\varepsilon_0 > 0$ such that for all compact set $K \subset D$, all $\varepsilon \in (0, \varepsilon_0]$, there exist $C_\varepsilon, \eta_\varepsilon > 0$ such that for all $\mu_0 \in \mathcal{M}^1(D)$ satisfying $\mu_0(K) \geq 1/2$, all bounded $f : D \rightarrow \mathbb{R}_+$ and all $N \in \mathbb{N}$,*

$$\sup_{t \geq 0} \mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_t) - \mathbb{E}_{\pi^N(\mathbf{x}_0)}(f(X_t) | \tau_{\partial D} > t) \right| \right) \leq \frac{C_\varepsilon \|f\|_\infty}{N\eta_\varepsilon},$$

where X solves (7.1), $\tau_{\partial D}$ is defined in (7.2), π^N in (7.4), and \mathbf{X} is a FV-process with initial condition $\mu_0^{\otimes N}$.

In Theorem 7.1.1, the dependency in N of the speed of convergence is the same as for N independent diffusion processes. Moreover, the dependency in ε is also sharp. Indeed, in Assumption 7.1.2, we can take a arbitrarily close to c^* , which means that we get a mixing time smaller than $e^{(c^* + \delta)/\varepsilon}$ for any $\delta > 0$, which is the order of the mixing time for the non-killed process. However, as far as Theorem 7.1.2 is concerned, for independent processes, one would get from the Bienaymé-Chebyshev inequality the explicit rate $1/\sqrt{N}$. This is indeed what is proven in [165, Theorem 1] for the FV process, but with a bound that depends on time. In other words, we improve the result of [165] to a uniform in time bound, but at the cost of a loss in the rate in N . Notice that η_ε may be made explicit by carefully following the proofs.

7.2 Preliminary results

For any two probability measures μ, ν , we call (X, Y) a coupling of μ and ν if the law of X (resp. Y) is μ (resp. ν). For any distance \mathbf{d} on a set E (here $E = D$ or $E = D^N$), the associated Kantorovich distance on $\mathcal{M}^1(E)$, is defined by

$$W_{\mathbf{d}}(\mu, \nu) = \inf \{ \mathbb{E}(\mathbf{d}(X, Y)), (X, Y) \text{ coupling of } \mu \text{ and } \nu \}.$$

We say that (X, Y) is an optimal coupling if $W_{\mathbf{d}}(\mu, \nu) = \mathbb{E}(\mathbf{d}(X, Y))$. The existence of an optimal coupling results from [164, Theorem 4.1]. Given a Markov semi-group P , we call a coupling of $(\mu P_t)_{t \geq 0}$ and $(\nu P_t)_{t \geq 0}$ a stochastic process $(X_t, Y_t)_{t \geq 0}$ such that $(X_t)_{t \geq 0}$ and $(Y_t)_{t \geq 0}$ are Markov processes of semi-group $(P_t)_{t \geq 0}$ and initial condition μ for X and ν for Y . In particular, we have that for such a coupling and all $t \geq 0$,

$$W_{\mathbf{d}}(\mu P_t, \nu P_t) \leq \mathbb{E}(\mathbf{d}(X_t, Y_t)).$$

We also say that the processes X and Y have coupled at time $t \geq 0$ if $X_t = Y_t$. Finally, in the case where $\mathbf{d}(x, y) = 2\mathbb{1}_{x \neq y}$, we recover the total variation distance which we write $W_{\mathbf{d}}(\mu, \nu) = \|\mu - \nu\|_{TV}$.

The proof of our theorems relies on the construction of a coupling of $(\mu P_t^{N, \varepsilon})_{t \geq 0}$ and $(\nu P_t^{N, \varepsilon})_{t \geq 0}$. This coupling will yield that $P_t^{N, \varepsilon}$ is a contraction for some particular distance defined in Section 7.3.

In order to do this, we first need some preliminary results, which is the subject of this section. We start by studying the mixing properties of the non-killed process in Subsection 7.2.1 by embedding D into a torus. In Subsection 7.2.2, We construct a Lyapunov functional for each particle. In Subsection 7.2.3, using the Lyapunov functional, we study the number of particle that may stay near the boundary of the domain.

In the rest of the paper, we fix some $a \in (c^*, U_0)$ satisfying assumption 7.1.2 and set $t_\varepsilon = e^{a/\varepsilon}$. Furthermore, bold letters will always denote particle systems, in the sense that \mathbf{X} can always be written $\mathbf{X} = (X^1, \dots, X^N)$ where for all $1 \leq i \leq N$, $X^i \in D$.

7.2.1 Coupling of the non-killed diffusion

In this section, we show that we are able to couple two diffusions solution of (7.1) on a torus in total variation distance in a time t_ε with a probability that goes to 1 as ε goes to 0, uniformly on D . Since we are studying a process killed at the boundary of D , we are not interested in what the potential might look like outside of D . Consider some torus $\mathbb{T}^d = (\mathbb{R}/2L\mathbb{Z})^d$, with L big enough so that as a subset of \mathbb{R}^d (meaning seeing \mathbb{T}^d as $[-L, L]^d$), we have that $D \subset \mathbb{T}^d$. Then consider some periodic potential $\tilde{U} : \mathbb{R}^d \rightarrow \mathbb{R}_+$, equal to U on D as a periodic function, and such that $c^*(\tilde{U}) = c^*(U)$, where $c^*(\tilde{U})$ is defined as $c^*(U)$ with U replaced by \tilde{U} . Such a function exists, as shown in [64, Section 4]. We still denote by \tilde{U} the associated function on \mathbb{T}^d , and this potential defines a diffusion on \mathbb{T}^d as:

$$d\tilde{X}_t = -\nabla \tilde{U}(\tilde{X}_t) dt + \sqrt{2\varepsilon} dB_t. \quad (7.8)$$

We note \tilde{P} its semi-group. If we see \tilde{X} as a process in \mathbb{R}^d , then we have that $X_t = \tilde{X}_t$ for all $t \leq \tau_{\partial D}$, where $\tau_{\partial D}$ is the death time (7.2).

Now, we construct a coupling for the process \tilde{X} , for all initial condition $(x, y) \in (\mathbb{T}^d)^2$. To do this, we use Sobolev and Poincaré inequalities. The Sobolev inequality is used for ultracontractivity, whereas the Poincaré inequality is used to get an optimal convergence rate for the

process (7.8). Let μ_ε denote the probability measure on \mathbb{T}^d :

$$\mu_\varepsilon(dx) = \mathcal{Z} e^{-\tilde{U}(x)/\varepsilon} dx$$

where \mathcal{Z} is the normalization constant. Recall those inequalities:

Lemma 7.2.1. μ_ε satisfies a Poincaré and a Sobolev inequality: there exist $p > 2$, $C, \lambda_\varepsilon > 0$, such that

$$\varepsilon \ln(\lambda_\varepsilon) \rightarrow -c^*$$

as $\varepsilon \rightarrow 0$, and for all smooth $f : \mathbb{T}^d \mapsto \mathbb{R}$ with $\int_{\mathbb{T}^d} f d\mu_\varepsilon = 0$

$$\lambda_\varepsilon \int_{\mathbb{T}^d} f^2 d\mu_\varepsilon \leq \int_{\mathbb{T}^d} |\nabla f|^2 d\mu_\varepsilon \quad (PI),$$

$$\left(\int_{\mathbb{T}^d} f^p d\mu_\varepsilon \right)^{\frac{2}{p}} \leq C e^{\|\tilde{U}\|_\infty/\varepsilon} \left(\int_{\mathbb{T}^d} f^2 d\mu_\varepsilon + \int_{\mathbb{T}^d} |\nabla f|^2 d\mu_\varepsilon \right) \quad (SI).$$

Moreover, for all $t > 0$, the law of \tilde{X}_t with initial condition x has a density $h_t^\varepsilon(x, \cdot)$ with respect to μ_ε , and both inequalities together imply the existence of some constant $\tilde{C} > 0$ such that, for all $t \geq 1$ and $\varepsilon > 0$,

$$\|h_t^\varepsilon(\cdot, \cdot) - 1\|_\infty \leq \tilde{C} e^{\tilde{C}\varepsilon^{-1} - \lambda_\varepsilon t}. \quad (7.9)$$

Proof. The Poincaré inequality, as well as the asymptotic on λ_ε , have been proven in [83]. The uniform measure on \mathbb{T}^d satisfies a Sobolev inequality, see [6, section 6]. Then we can write:

$$\begin{aligned} \left(\int_{\mathbb{T}^d} f^p d\mu_\varepsilon \right)^{\frac{2}{p}} &\leq \mathcal{Z}^{-\frac{2}{p}} \left(\int_{\mathbb{T}^d} f^p \right)^{\frac{2}{p}} \\ &\leq C \mathcal{Z}^{-\frac{2}{p}} \left(\int_{\mathbb{T}^d} f^2 + \int_{\mathbb{T}^d} |\nabla f|^2 \right) \\ &\leq C \mathcal{Z}^{1-\frac{2}{p}} e^{\|\tilde{U}\|_\infty/\varepsilon} \left(\int_{\mathbb{T}^d} f^2 d\mu_\varepsilon + \int_{\mathbb{T}^d} |\nabla f|^2 d\mu_\varepsilon \right). \end{aligned}$$

\mathcal{Z} is bounded by the volume of \mathbb{T}^d , hence $\mathcal{Z}^{1-\frac{2}{p}}$ is bounded uniformly on ε because $p > 2$ (and thus $1 - \frac{2}{p} > 0$). Therefore, we have the Sobolev inequality with the said constant. The last two points are [6, Theorem 6.3.1 and Proposition 6.3.4].

□

Lemma 7.2.2. Recall that $t_\varepsilon = e^{a/\varepsilon}$ for some $a > c^*$. Under Assumption 7.1.1, there exists $\varepsilon_0 > 0$, such that for all $0 < \varepsilon < \varepsilon_0$, there exists $c_\varepsilon > 0$ such that for all $x, y \in D$, there exists a coupling $(\tilde{X}_t, \tilde{Y}_t)_{t \geq 0}$ of $(\delta_x \tilde{P}_t)_{t \geq 0}$ and $(\delta_y \tilde{P}_t)_{t \geq 0}$ such that:

$$\mathbb{P} \left(\tilde{X}_{t_\varepsilon} = \tilde{Y}_{t_\varepsilon} \right) \geq c_\varepsilon.$$

Moreover, as $\varepsilon \rightarrow 0$,

$$c_\varepsilon \rightarrow 1.$$

Proof. We start by bounding the total variation distance between the law of \tilde{X}_t and the equilibrium μ_ε . Recall that $h_t^\varepsilon(x, \cdot)$ denotes the density of the law of \tilde{X}_t with respect to μ_ε . For $x \in D$,

using (7.9), we have:

$$\|\delta_x \tilde{P}_t - \mu_\varepsilon\|_{TV} = \int_{\mathbb{R}^d} |h_t^\varepsilon - 1| d\mu_\varepsilon \leq \|h_t^\varepsilon(\cdot, \cdot) - 1\|_\infty \leq \tilde{C} e^{\tilde{C}\varepsilon^{-1} - \lambda_\varepsilon t}.$$

Since $t_\varepsilon = e^{a/\varepsilon}$, and $\varepsilon \ln(\lambda_\varepsilon) \rightarrow -c^*$ as $\varepsilon \rightarrow 0$, we have that $\lambda_\varepsilon t_\varepsilon \geq e^{b/\varepsilon}$, for ε small enough and all $b < a - c^*$. Then, we may fix some $b < a - c^*$ and let:

$$c_\varepsilon = 1 - 2\tilde{C} e^{\tilde{C}\varepsilon^{-1} - e^{b/\varepsilon}},$$

so that $\lim_{\varepsilon \rightarrow 0} c_\varepsilon = 1$ and for all $x, y \in D$,

$$\|\delta_x \tilde{P}_t - \delta_y \tilde{P}_t\|_{TV} \leq \|\delta_x \tilde{P}_t - \mu_\varepsilon\|_{TV} + \|\delta_y \tilde{P}_t - \mu_\varepsilon\|_{TV} \leq 1 - c_\varepsilon.$$

The existence of the coupling of the trajectories results from the total variation distance properties, see for example [133, Lemma 9]. \square

7.2.2 Lyapunov functional

In order to show the convergence of the particle system, we need first the construction of some Lyapunov function for each particle, that is to say some function of one particle that decreases in average over time, as long as it starts large enough. This is the part where we need U to be constant on the boundary of D . This part relies on a result first shown in [71], similar to Ito's formula. The process (7.1) has a generator \mathcal{L} defined for all smooth function $f : \mathbb{R}^d \rightarrow \mathbb{R}$ with compact support as:

$$\mathcal{L}f = \varepsilon \Delta f - \nabla U \cdot \nabla f. \quad (7.10)$$

For a smooth function $f : D^N \rightarrow \mathbb{R}_+$, and $1 \leq i \leq N$, write \mathcal{L}_{x_i} for the generator \mathcal{L} , acting only on the i -th variable:

$$\mathcal{L}_{x_i} f = \sum_{j=1}^d \varepsilon \partial_{(x_i)_j}^2 f - \partial_j U(x_i) \partial_{(x_i)_j} f.$$

Write as well $(\tau_n^i)_n$ for the sequence of death times of particle i :

$$\tau_0^i = 0, \quad \tau_{n+1}^i = \inf \{t > \tau_n^i, X_{t-}^i \in \partial D\}, \quad (7.11)$$

and R_i for the point process corresponding to the jumps of this particle:

$$R_i(t) = \sum_{n=1}^{\infty} \mathbb{1}_{\tau_n^i \leq t}.$$

For all $\mathbf{x} \in D^N$, $1 \leq i \neq j \leq N$, write:

$$x_k^{ij} = \begin{cases} x_k & \text{if } k \neq i \\ x_j & \text{else} \end{cases}.$$

Proposition 7.2.1 ([71], Proposition 1). *Let $N \in \mathbb{N}$, $f \in \mathcal{C}^0(\bar{D}^N) \cap \mathcal{C}^\infty(D^N)$. Denote by*

$$\mathbf{R}(f)(t) = \sum_{i=1}^N \frac{1}{N-1} \sum_{j \neq i} \int_0^t \left(f(\mathbf{X}_{s-}^{ij}) - f(\mathbf{X}_{s-}) \right) dR_i(s)$$

the finite variation process of the jump part, and

$$Q(f)(t) = \int_0^t \sum_{i=1}^N \mathcal{L}_{x_i} f(\mathbf{X}_s) ds$$

the finite variation process of the diffusion part. Then there exists a martingale $\mathcal{M}(f)$ such that almost surely for all $t \geq 0$:

$$f(\mathbf{X}_t) - f(\mathbf{X}_0) = \mathbf{R}(f)(t) + Q(f)(t) + \mathcal{M}(f)_t.$$

Moreover,

$$\mathbf{R}(f)(t) + \mathcal{M}(f)_t = \sum_{i=1}^N \int_0^t \nabla_{x_i} f(\mathbf{X}_s) \cdot dB_s^i + \sum_{n, \tau_n \leq t} f(\mathbf{X}_{\tau_n}) - f(\mathbf{X}_{\tau_n-}),$$

where the (B^i) 's are the Brownian motion used in the definition of the FV process, and the (τ_n) are the death times.

This decomposition will allow us to prove the existence of the Lyapunov functional. The idea is the following: the function V will be equal to U at the center of the domain, and near its boundary, V will be such that ∇V is proportional to ∇U , but with $|\nabla V|$ possibly greater than $|\nabla U|$. Since $n(x) \cdot \nabla U(x) > 0$ on the boundary, we will also have $n(x) \cdot \nabla V(x) > 0$, which means that, near the boundary, V tends to decrease along (7.1). If in addition V is maximal at the boundary, then it can only decrease at a jump time.

Lemma 7.2.3. *Under Assumption 7.1.1, there exists $C_1 > 0$ such that for all $V_0 > 0$ with*

$$V_0 \geq 4 \sup_D U + 1,$$

there exist $\varepsilon_0 > 0$ and a smooth function $V : \bar{D} \mapsto \mathbb{R}_+$ such that V is constant equal to V_0 on ∂D , $\sup_D V = V_0$, $4C_1 < V_0$, and for all $N \in \mathbb{N}$, $0 < \varepsilon < \varepsilon_0$, $\mathbf{x} \in D^N$, and $1 \leq i \leq N$, we have:

$$\mathbb{E}_{\mathbf{x}}(V(X_{t_\varepsilon}^i)) \leq \gamma_\varepsilon V(x_i) + C_1(1 - \gamma_\varepsilon) \quad (7.12)$$

where $\gamma_\varepsilon \in (0, 1)$ is independent from \mathbf{x} and vanishes as $\varepsilon \rightarrow 0$.

The value V_0 of V on the boundary is a fixed parameter that will be chosen in Section 7.3.

Proof. Fix some $V_0 \geq 4 \sup_D U + 1 =: 4\theta + 1$. Under Assumption 7.1.1, and in particular because of condition (7.6), there exists some set $F \subset D$ such that $\mathbb{R}^d \setminus F$ is a neighborhood of ∂D , there are no critical points of U on $\overline{D \setminus F}$ (the closure of $D \setminus F$), and

$$\sup_{D \setminus F} U \leq U_0.$$

Write

$$U_{min} = \min_{D \setminus F} U, \quad \zeta = \inf_{x \in D \setminus F} |\nabla U(x)|.$$

Notice that $\zeta > 0$ since $|\nabla U|$ is continuous and positive over the compact set $\overline{D \setminus F}$. Let $f : [0, U_0] \mapsto \mathbb{R}$ be some smooth function satisfying the following conditions:

- for all $u \leq U_{min}$, $f(u) = u$,

- $f(U_0) = V_0$,
- $\min_{U_{\min} \leq u \leq U_0} f'(u) > 0$.

Then, set $V(x) = U(x)$ for all $x \in F$, and $V(x) = f(U(x))$ for all $x \notin F$. The function V is smooth, constant equal to $V_0 = f(U_0)$ on ∂D , bounded above by V_0 , and we have for all $x \in D \setminus F$:

$$\mathcal{L}V = f'(U) (\varepsilon \Delta U - |\nabla U|^2) + \varepsilon f''(U) |\nabla U|^2.$$

Recall that $|\nabla U|$ is positive on $D \setminus F$. We consider ε_0 small enough so that on $D \setminus F$ we have, for all $\varepsilon < \varepsilon_0$:

$$\varepsilon f'(U) |\Delta U| + \varepsilon |f''(U)| |\nabla U| \leq 1/2 f'(U) |\nabla U|^2.$$

We then have for all $x \in D \setminus F$:

$$\mathcal{L}V(x) \leq -\omega V(x)$$

where

$$\omega = \frac{\zeta^2}{2V_0} \min_{U_1 \leq u \leq U_0} f'(u)$$

is independent of ε . Now, for $x \in F$:

$$\mathcal{L}V(x) \leq \varepsilon \sup_D |\Delta U| + \omega \theta - \omega V(x).$$

This inequality is thus true for all $x \in D$. Hence, we may plug it into the formula of Proposition 7.2.1 with $f(\mathbf{x}) = V(x_i)$. Recall the definition of $(\tau_n^i)_{n \in \mathbb{N}}$ from (7.11). For $n \in \mathbb{N}$, using the fact that V is maximal on the boundary of D , $\mathbf{R}(V) \leq 0$, and hence for all $0 \leq s \leq t$:

$$\mathbb{E} \left(V \left(X_{t \wedge \tau_n^i}^i \right) \right) - \mathbb{E} \left(V \left(X_{s \wedge \tau_n^i}^i \right) \right) \leq \int_s^t \left(-\omega \mathbb{E} \left(V \left(X_{u \wedge \tau_n^i}^i \right) \right) + \varepsilon \|\Delta U\|_\infty + \omega \theta \right) du.$$

Writing $g(t) = \mathbb{E} \left(V \left(X_{t \wedge \tau_n^i}^i \right) \right) - \theta - \varepsilon \|\Delta U\|_\infty / \omega$, we have for $t \geq 0$ and $h > 0$:

$$g(t+h) - g(t) \leq -\omega \int_t^{t+h} g(u) du.$$

We now suppose that g is continuous. Fix $\eta > 0$ and write:

$$T_\eta = \min \{ t \geq 0, g(t) \geq g(0)e^{\omega t} + \eta \}.$$

Suppose that $T_\eta < \infty$ and write:

$$s_\eta = \max \{ 0 \leq s \leq T_\eta, g(s) \leq g(0)e^{\omega s} \}.$$

Then by continuity we have:

$$\begin{aligned} g(0)e^{-\omega T_\eta} + \eta - g(0)e^{-\omega s_\eta} &= g(T_\eta) - g(s_\eta) \leq -\omega \int_{s_\eta}^{T_\eta} g(u) du \\ &< -\omega \int_{s_\eta}^{T_\eta} g(0)e^{-\omega u} du = g(0)e^{-\omega T_\eta} - g(0)e^{-\omega s_\eta}, \end{aligned}$$

hence necessarily $T_\eta = \infty$, for all $\eta > 0$, and thus for all $t \geq 0$,

$$g(t) \leq g(0)e^{-\omega t},$$

and

$$\mathbb{E} \left(V \left(X_{t_\varepsilon \wedge \tau_n^i}^i \right) \right) \leq \gamma_\varepsilon V(x_i) + \frac{\varepsilon \|\Delta U\|_\infty + \omega \theta}{\omega} (1 - \gamma_\varepsilon),$$

with $\gamma_\varepsilon = e^{-\omega t_\varepsilon}$. Because V is maximal at the boundary, $t \mapsto V(X_t^i)$ is lower-semicontinuous. Hence, since $V \geq 0$ and $\tau_n^i \rightarrow \infty$ as $n \rightarrow \infty$, using Fatou's lemma,

$$\begin{aligned} \mathbb{E} \left(V \left(X_{t_\varepsilon}^i \right) \right) &\leq \mathbb{E} \left(\liminf_{n \rightarrow \infty} V \left(X_{t_\varepsilon \wedge \tau_n^i}^i \right) \right) \\ &\leq \liminf_{n \rightarrow \infty} \mathbb{E} \left(V \left(X_{t_\varepsilon \wedge \tau_n^i}^i \right) \right) \leq \gamma_\varepsilon V(x_i) + \frac{\varepsilon \|\Delta U\|_\infty + \omega \theta}{\omega} (1 - \gamma_\varepsilon). \end{aligned}$$

Since $V_0 > 4\theta + 1$, we may take ε_0 small enough so that, for all $\varepsilon < \varepsilon_0$:

$$4 \frac{\varepsilon \|\Delta U\|_\infty + \omega \theta}{\omega} < 4 \sup_D U + 1 \leq V_0,$$

and hence the result with $C_1 = \sup_F U + 1/4$.

We are left to show that, for all $n \in \mathbb{N}$, $t \mapsto \mathbb{E}(V(X_{t \wedge \tau_n^i}^i))$ is continuous. Write $V^i(\mathbf{x}) = V(x_i)$. Then from Proposition 7.2.1, we get that:

$$\mathbb{E}(V(X_{t \wedge \tau_n^i}^i)) = \mathbb{E}(V(X_0^i)) + \mathbb{E}(Q(V^i)(t \wedge \tau_n^i)) + \mathbb{E}(\mathbf{R}(V^i)(t \wedge \tau_n^i)).$$

Since $\mathcal{L}_{x_i} V$ is bounded, $t \mapsto \mathbb{E}(Q(V^i)(t \wedge \tau_n^i))$ is continuous. For $0 \leq s \leq t$, we may write

$$\mathbb{E}(\mathbf{R}(V^i)(t \wedge \tau_n^i)) - \mathbb{E}(\mathbf{R}(V^i)(s \wedge \tau_n^i)) = \frac{1}{N-1} \sum_{k=1}^n \sum_{j \neq i} \mathbb{E} \left(\left(V(X_{\tau_k^j}^j) - V(X_{\tau_k^i}^i) \right) \mathbb{1}_{s \leq \tau_k^i \leq t} \right),$$

and hence

$$\left| \mathbb{E}(\mathbf{R}(V^i)(t \wedge \tau_n^i)) - \mathbb{E}(\mathbf{R}(V^i)(s \wedge \tau_n^i)) \right| \leq 2n \|V\|_\infty \mathbb{P}(X^i \text{ dies between time } s \text{ and } t).$$

The law of the death times have a density with respect to the Lebesgue measure. Hence we have that

$$\lim_{s \rightarrow t} \mathbb{P}(X^i \text{ dies between time } s \text{ and } t) = 0,$$

and this implies the continuity of $t \mapsto \mathbb{E}(\mathbf{R}(V^i)(t \wedge \tau_n^i))$, which concludes the proof. \square

Remark 7.2.1. When Assumption 7.1.2 also holds, we will additionally suppose that V is such that

$$\mathfrak{B}_1 \subset \{V > m\}$$

for some $m > 3C_1$, where \mathfrak{B}_1 is the set from Assumption 7.1.2. Indeed, in the proof of Lemma 7.2.3, we may choose F such that $U_{\min} < \min_{\mathfrak{B}_1} U$. In this case, since $V_0 > 4C_1$, we may impose on f that $f(\min_{\mathfrak{B}_1} U) > 3C_1$.

We are now interested in the death probability of a particle.

Proposition 7.2.2. *Under Assumption 7.1.1, denote by (X_t) the diffusion (7.1), and*

$$\tau_{\partial D} = \inf \{t \geq 0; X_t \notin D\}.$$

Consider any $C_2 \in (2C_1, 4C_1)$, where C_1 is given in Lemma 7.2.3. Then we have:

$$p_\varepsilon := \sup_{x \in \{V \leq C_2\}} \mathbb{P}_x(\tau_{\partial D} < t_\varepsilon) \rightarrow 0, \quad (7.13)$$

as $\varepsilon \rightarrow 0$.

Proof. Since $t_\varepsilon = e^{a/\varepsilon}$ with $a < U_0$, this is the theory of Freidlin-Wentzell, see [65, Chapter 6, Theorem 6.2]. Freidlin and Wentzell didn't state the uniformity, but it follows from their proof. \square

7.2.3 Particles near the boundary

We want to control the number of particles which are close to the boundary of D after a time t_ε . Consider the neighborhood

$$\mathfrak{B} = \{V > 3C_1\}$$

of ∂D , where C_1 is the constant from Lemma 7.2.3. For $\mathbf{x} = (x_1, \dots, x_N)$, write:

$$A(\mathbf{x}) = \# \{i \in \llbracket 1, N \rrbracket; x_i \in \mathfrak{B}\}, \quad (7.14)$$

where $\#$ stands for the cardinality of a set. We show that at time t_ε , the number of particles close to the boundary, $A(\mathbf{x})$, is a small fraction of N with high probability as N goes to infinity or as ε goes to 0.

Lemma 7.2.4. *For all $\alpha > 0$, there exists $\varepsilon_0 > 0$ such that for all $\varepsilon < \varepsilon_0$, there exists $q_\varepsilon > 0$ such that for all $N \in \mathbb{N}$ and $\mathbf{x} \in D^N$:*

$$\mathbb{P}_{\mathbf{x}}(A(\mathbf{X}_{t_\varepsilon}) > \alpha N) \leq q_\varepsilon^N \quad (7.15)$$

and $q_\varepsilon \rightarrow 0$ as $\varepsilon \rightarrow 0$.

Proof. The idea for the proof is the following: we want to compare the evolution of $V(X_t^i)$ and Ornstein-Uhlenbeck processes with small variance. If we had N independent diffusions, the result would derive from a simple enumeration. But then the interaction through jumps can only make the Lyapunov decrease. From Proposition 7.2.1 and the proof of Lemma 7.2.3, we have that almost surely for all $1 \leq i \leq N$ and $t \geq 0$:

$$V(X_t^i) \leq V(x_i) + \int_0^t (-\omega V(X_s^i) + \omega C_1) ds + \sqrt{2\varepsilon} \int_0^t \nabla V(X_s^i) \cdot dB_s^i.$$

for some $\omega > 0$ (independent from ε). Now introduce for $1 \leq i \leq N$ the process:

$$K_t^i = V(x_i)e^{-\omega t} + C_1(1 - e^{-\omega t}) + \sqrt{2\varepsilon} \int_0^t e^{\omega(s-t)} \nabla V(X_s^i) \cdot dB_s^i,$$

which solves

$$K_t^i = V(x_i) + \int_0^t (-\omega K_s^i + \omega C_1) ds + \sqrt{2\varepsilon} \int_0^t \nabla V(X_s^i) \cdot dB_s^i.$$

From proposition 7.2.1, we have that:

$$V(X_t^i) - K_t^i = \int_0^t (\mathcal{L}V(X_s^i) + \omega K_s^i - \omega C_1) ds + \sum_{n, \tau_n^i \leq t} V(X_{\tau_n^i}^i) - V(X_{\tau_n^i-}^i),$$

where (τ_n^i) are the death times of particle number i as defined in (7.11). Moreover, K^i is a continuous process, and $V(X^i)$ is continuous between death times. Hence, $V(X^i) - K^i$ is \mathcal{C}^1 between death times. Let $f(x, y) = ((x - y)_+)^2$, so that f is differentiable, and is non-decreasing in the variable x . By construction of V , for all $n \in \mathbb{N}$, $V(X_{\tau_n^i}^i) \leq V(X_{\tau_n^i-}^i)$, hence we have for all $t \geq 0$:

$$\left((V(X_t^i) - K_t^i)_+ \right)^2 \leq 2 \int_0^t \omega (K_s^i - V(X_s^i)) (V(X_s^i) - K_s^i)_+ ds \leq 0.$$

Thus, almost surely, $V(X_t^i)$ is bounded by K_t^i for all $t \geq 0$, and we are left to show that with high probability, there are only a few K^i 's which are greater than $3C_1$ at time t_ε . Write:

$$G_t^i = \sqrt{2\varepsilon} \int_0^t e^{\omega(s-t)} \nabla V(X_s^i) \cdot dB_s^i.$$

Fix some family of indexes $(i_1, \dots, i_k) \in \{1, \dots, N\}^k$. The G^{i_j} 's are L^2 -martingales, hence for any $\xi \in \mathbb{R}$, $\xi \sum_{j=1}^k G^{i_j}$ is a L^2 -martingale, and:

$$\exp \left(\xi \sum_{j=1}^k G^{i_j} - \xi^2 \left\langle \sum_{j=1}^k G^{i_j} \right\rangle \right)$$

is a local-martingale. We have that $\langle G^i, G^j \rangle = 0$ for all $i \neq j$ because the Brownian motions are independent, hence

$$\left\langle \sum_{j=1}^k G^{i_j} \right\rangle_t = \sum_{j=1}^k 2\varepsilon \int_0^t e^{2\omega(s-t)} |\nabla V(X_s^i)|^2 ds \leq \frac{\varepsilon k \|\nabla V\|_\infty}{\omega},$$

and using Fatou's Lemma:

$$\mathbb{E} \left(\exp \left(\xi \sum_{j=1}^k G_t^{i_j} \right) \right) \leq \exp \left(\frac{\varepsilon \xi^2 k \|\nabla V\|_\infty}{\omega} \right),$$

for all $t \geq 0$. Now we can write, using the Markov inequality:

$$\mathbb{P} (G_{t_\varepsilon}^{i_1} > C_1, \dots, G_{t_\varepsilon}^{i_k} > C_1) \leq \mathbb{P} \left(\exp \left(\xi \sum_{j=1}^k G^{i_j} \right) > e^{\xi k C_1} \right) \leq e^{-\xi k C_1} e^{\frac{\varepsilon \xi^2 k \|\nabla V\|_\infty}{\omega}}.$$

Taking $\xi = C_1 \omega / (2\varepsilon \|\nabla V\|_\infty)$, one gets:

$$\mathbb{P} (G_{t_\varepsilon}^{i_1} > C_1, \dots, G_{t_\varepsilon}^{i_k} > C_1) \leq \exp(-C_1^2 \omega / 2\varepsilon \|\nabla V\|_\infty)^k =: \tilde{q}_\varepsilon^k.$$

We chose ε_0 small enough so that:

$$V_0 e^{-\omega t_{\varepsilon_0}} + C_1(1 - e^{-\omega t_{\varepsilon_0}}) < 2C_1.$$

For all $1 \leq i \leq N$, we then have:

$$\{K_{t_\varepsilon}^i > 3C_1\} \subset \{G_{t_\varepsilon}^i > C_1\},$$

and we have for all family of indexes (i_1, \dots, i_k) :

$$\mathbb{P}(X_{t_\varepsilon}^{i_1} \in \mathfrak{B}, \dots, X_{t_\varepsilon}^{i_k} \in \mathfrak{B}) \leq \mathbb{P}(G_{t_\varepsilon}^{i_1} > C_1, \dots, G_{t_\varepsilon}^{i_k} > C_1) \leq \tilde{q}_\varepsilon^k.$$

Finally, we conclude with:

$$\begin{aligned} \mathbb{P}_x(A(\mathbf{X}_{t_\varepsilon}) > \alpha N) &\leq \mathbb{P}(\text{There exist at least } \alpha N \text{ indexes } i \text{ such that } X_{t_\varepsilon}^i \in \mathfrak{B}) \\ &\leq \sum_{\alpha N \leq k \leq N} \binom{n}{k} \tilde{q}_\varepsilon^k \\ &\leq (2(\tilde{q}_\varepsilon)^\alpha)^N =: q_\varepsilon^N. \end{aligned}$$

□

7.3 Proofs of the main theorems

Our goal is to construct a coupling of $\delta_{\mathbf{x}}P^{N,\varepsilon}$ and $\delta_{\mathbf{y}}P^{N,\varepsilon}$ for all $\mathbf{x}, \mathbf{y} \in D^N$ in such a way that some distance $\mathbf{d}(\mathbf{x}, \mathbf{y})$ is contracted on average by this coupling along time. The basic idea of the coupling is the following: particles are coupled by pair, namely we want the particle i of the system starting at \mathbf{x} to merge, after a time t_ε , with the particle i of the system starting at \mathbf{y} . However, contrary to the case of independent particles, here, even if two particles start at the same position (namely $x_i = y_i$), they have a positive probability to decouple before time t_ε . This can be particularly bad for some initial conditions: for instance if most of the pairs start merged but close to the boundary while a decoupled pair is in the middle of the domain, then this will typically lead to a lot of decoupling as coupled pairs rebirth on the uncoupled pair. This will be tackled through the definition of the distance \mathbf{d} .

7.3.1 Long time convergence

We now construct the coupling of $(\delta_{\mathbf{x}}P_t^{N,\varepsilon})_{t \geq 0}$ and $(\delta_{\mathbf{y}}P_t^{N,\varepsilon})_{t \geq 0}$ for all $\mathbf{x}, \mathbf{y} \in D^N$, that will yield a bound on the distance between $\delta_{\mathbf{x}}P_{t_\varepsilon}^{N,\varepsilon}$ and $\delta_{\mathbf{y}}P_{t_\varepsilon}^{N,\varepsilon}$. Fix $\mathbf{x}, \mathbf{y} \in D^N$, and a sequence (I_n^i) of independent random variable, where I_n^i is uniform on $\llbracket 1, N \rrbracket \setminus \{i\}$.

For all $1 \leq i \leq N$, consider a coupling $(\tilde{X}_t^i, \tilde{Y}_t^i)$ of the diffusion (7.8) starting from (x_i, y_i) such as the one constructed in Lemma 7.2.2 (with these processes being independent for two different values of the index i). Recall that $\mathbb{T}^d = (\mathbb{R}/2L\mathbb{Z})^d$, and L is great enough so that we may consider that $D \subset \mathbb{T}^d$. Hence we may write

$$\tilde{\tau}_1 = \inf \left\{ t \geq 0, \exists i \in \llbracket 1, N \rrbracket, \tilde{X}_t^i \notin D \text{ or } \tilde{Y}_t^i \notin D \right\}.$$

Denote by i_1 the index of the particles that exit the domain at time $\tilde{\tau}_1$. For all $i \neq i_1$ and

$0 \leq t \leq \tilde{\tau}_1$ or $i = i_1$ and $0 \leq t < \tilde{\tau}_1$, let:

$$X_t^i = \tilde{X}_t^i \quad \text{and} \quad Y_t^i = \tilde{Y}_t^i,$$

in the sense that X_t^i (resp. Y_t^i) is the only point of D whose projection is \tilde{X}_t^i (resp. \tilde{Y}_t^i). Finally, if $\tilde{X}_{\tilde{\tau}_1}^{i_1} \notin D$, then set $X_{\tilde{\tau}_1}^{i_1} = X_{\tilde{\tau}_1}^{I_1^{i_1}}$, else set $X_{\tilde{\tau}_1}^{i_1} = \tilde{X}_{\tilde{\tau}_1}^{i_1}$. The same goes for $Y_{\tilde{\tau}_1}^{i_1}$: if $\tilde{Y}_{\tilde{\tau}_1}^{i_1} \notin D$, then set $Y_{\tilde{\tau}_1}^{i_1} = Y_{\tilde{\tau}_1}^{I_1^{i_1}}$, else set $Y_{\tilde{\tau}_1}^{i_1} = \tilde{Y}_{\tilde{\tau}_1}^{i_1}$. The coupling can then be constructed by induction, just as for the construction of the FV processes in the introduction.

Basically, the coupling is as follow: two particles with same index will be an optimal coupling of the diffusion as long as they don't die as constructed in Lemma 7.2.2, and if they die while coupled, then they resurrect using the same index. By this we mean that the uniform variable I_n^i used in the construction of the process in Section 7.1.1 must be the same for both systems.

We will show that this coupling yields a contraction for the Wasserstein distance associated to a particular distance on D^N , namely:

$$\mathbf{d}(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^N \mathbb{1}_{x_i \neq y_i} (1 + \beta V(x_i) + \beta V(y_i)) + (1 + V_0) N (\mathbb{1}_{A(\mathbf{x}) > \alpha N} + \mathbb{1}_{A(\mathbf{y}) > \alpha N}) \mathbb{1}_{\mathbf{x} \neq \mathbf{y}}, \quad (7.16)$$

where $\beta, \alpha > 0$ are parameters that will be chosen small enough, and $A(\mathbf{x})$ has been defined in (7.14). We define as well:

$$d^1(x_i, y_i) = \mathbb{1}_{x_i \neq y_i} (1 + \beta V(x_i) + \beta V(y_i)).$$

The meaning of this distance, which follows the construction of Hairer and Mattingly in [79], is this: if $x_i \neq y_i$ and $V(x_i) + V(y_i) < C_2$, where C_2 is as in Proposition 7.2.2, then both particles of index i are in the center of the domain at initial time, and we are able to couple X^i and Y^i before time t_ε and before they die with high probability. If $x_i \neq y_i$ and $V(x_i) + V(y_i) \geq C_2$, then we may not be able to couple them, but the Lyapunov functional will decrease on average. In any case, if $x_i \neq y_i$, $\mathbb{E}(d^1(X_t^i, Y_t^i))$ will decrease between initial time and time t_ε . If $x_i = y_i$, then we cannot expect any contraction of $\mathbb{E}(d^1(X_t^i, Y_t^i))$, since it is equal to zero at initial time, and the probability that X^i and Y^i decouple is positive (if they die and resurrect on an uncoupled pair). In this case, if x_i is in the center of the domain, then, as we will see below, the probability of decoupling is very small and won't be an issue. But in the case where there are many particles coupled at $t = 0$ close to the boundary, many of them will get separated. This is why we added the additional term $N (\mathbb{1}_{A(\mathbf{x}) > \alpha N} + \mathbb{1}_{A(\mathbf{y}) > \alpha N}) \mathbb{1}_{\mathbf{x} \neq \mathbf{y}}$ in the definition of \mathbf{d} . If we are in this case, this term is initially not zero but, according to Lemma 7.2.4, it will probably be zero at time t_ε , which will compensate for the non-zero terms that will appear with other parts of the distance. In other words, this term plays the role of a global Lyapunov function, by contrast with the pairwise Lyapunov function $V(x_i) + V(y_i)$.

Let's start by bounding from above the probability to decouple. This is the part where we use Assumption 7.1.2.

Lemma 7.3.1. *Under Assumptions 7.1.1 and 7.1.2, there exists C_3 such that for all $0 < \alpha < 1/4$, there exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$, there exists $m_\varepsilon > 0$, such that for all $N \in \mathbb{N}$, $\mathbf{x}, \mathbf{y} \in D^N$ with $A(\mathbf{x}), A(\mathbf{y}) \leq \alpha N$, and all $i \in \llbracket 1, N \rrbracket$ such that $x_i = y_i$, we have:*

$$\mathbb{P}_{\mathbf{x}, \mathbf{y}}(X_{t_\varepsilon}^i \neq Y_{t_\varepsilon}^i) \leq \begin{cases} m_\varepsilon C_3 \bar{d}(\mathbf{x}, \mathbf{y}) / N & \text{if } x_i \notin \mathfrak{B} \\ C_3 d(\mathbf{x}, \mathbf{y}) / N & \text{if } x_i \in \mathfrak{B} \end{cases}$$

where $\bar{d}(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^N \mathbb{1}_{x_i \neq y_i}$, and $\lim_{\varepsilon \rightarrow 0} m_\varepsilon = 0$.

An intermediate lemma is needed. The goal of this lemma is to get bounds on the number of death events. This next lemma is where we use the neighborhood \mathfrak{B}_1 of ∂D from Assumption 7.1.2.

Lemma 7.3.2. *Under Assumptions 7.1.1 and 7.1.2, let \mathfrak{B}_1 be the neighborhood of ∂D from Assumption 7.1.2. Write the event:*

$$\mathcal{A} = \left\{ \# \{i \in \llbracket 1, N \rrbracket, \exists t \leq t_\varepsilon, X_t^i \in \mathfrak{B}_1\} \geq 2\alpha N \right\}.$$

1. There exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$, there exists $\tilde{p}_\varepsilon > 0$, such that for all $0 < \alpha < 1/4$, $N \in \mathbb{N}$, $\mathbf{x} \in D^N$ with $A(\mathbf{x}) \leq \alpha N$,

$$\mathbb{P}_{\mathbf{x}}(\mathcal{A}) \leq (2\tilde{p}_\varepsilon)^\alpha,$$

and $\lim_{\varepsilon \rightarrow 0} \tilde{p}_\varepsilon = 0$.

2. Moreover, if T denote the number of rebirth in the system before time t_ε , there exists $\varepsilon_0, \sigma > 0$, $0 < q < 1$, such that for all $0 < \varepsilon < \varepsilon_0$ and $0 < \alpha < 1/4$:

$$\mathbb{P}(T > \sigma N, \mathcal{A}^c) \leq q^N.$$

3. Write T^i the number of rebirth of particle i before time t_ε . We have as well that there exist $C, \varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$, for all $0 < \alpha < 1/4$, $\mathbf{x} \in D^N$ satisfying $A(\mathbf{x}) < \alpha N$:

$$\mathbb{E}_{\mathbf{x}}(T^i \mathbb{1}_{\mathcal{A}^c}) \leq \begin{cases} C\tilde{p}_\varepsilon & \text{if } x_i \notin \mathfrak{B} \\ C & \text{if } x_i \in \mathfrak{B}, \end{cases}$$

where \tilde{p}_ε is given in (7.7).

Proof. 1. At time $t = 0$, the condition on \mathbf{x} implies that there are less than αN particles in \mathfrak{B} . Under Assumption 7.1.2, we assumed in Remark 7.2.1 that

$$\min_{\mathfrak{B}_1} U > \max_{D \setminus \mathfrak{B}} U.$$

Hence $\mathfrak{B}_1 \subset \mathfrak{B}$, and this means that for \mathcal{A} to happen, namely for $2\alpha N$ particles to visit \mathfrak{B}_1 before time t_ε , at least αN particles that were initially in $D \setminus \mathfrak{B}$ must have reached \mathfrak{B}_1 before time t_ε . Write:

$$\tilde{p}_\varepsilon = \sup_{x \in D \setminus \mathfrak{B}} \mathbb{P}_x(\tau_{\mathfrak{B}_1} < t_\varepsilon),$$

where $\tau_{\mathfrak{B}_1}$ is the first hitting time of the set \mathfrak{B}_1 for the diffusion (7.1). Under Assumption 7.1.2, $a < \min_{\mathfrak{B}_1} U$. Together with the fact that $\min_{\mathfrak{B}_1} U > \max_{D \setminus \mathfrak{B}} U$ and [65, Chapter 6, Theorem 6.2] yields that $\tilde{p}_\varepsilon \rightarrow 0$ as $\varepsilon \rightarrow 0$. The fact that a particle reaches \mathfrak{B}_1 only depends on the Brownian motion driving it, hence we have:

$$\mathbb{P}(\mathcal{A}) \leq \sum_{k \geq \alpha N} \binom{(1-\alpha)N}{k} \tilde{p}_\varepsilon^k \leq (2\tilde{p}_\varepsilon)^\alpha.$$

2. In order to control the number of deaths of the i^{th} particle up to time t_ε , we are going to distinguish two types of rebirth events: either the particle is resurrected on a particle

which we know never reaches \mathfrak{B}_1 (i.e. stays away from the boundary), in which case we can bound the probability that the i^{th} particle dies again, or it is resurrected on a particle for which we have no information, in which case it can be arbitrarily close to the boundary and the time before the next death of the i^{th} particle can be arbitrarily small.

For convenience, we consider in the rest of the proof that the FV process has been defined thanks to a construction similar to the one presented in Section 7.1.1 except that the Brownian motions driving the SDEs are changed at each death event, namely along with the variables $(I_n^i)_{n \geq 0, i \in \llbracket 1, N \rrbracket}$, we consider a family of independent d -dimensional Brownian motions $((B_t^{n,i})_{t \geq 0})_{n \geq 0, i \in \llbracket 1, N \rrbracket}$, so that after its n^{th} death and up to its $(n+1)^{\text{th}}$ death the position of the particle i is given by $X_{\tau_n^i+t}^i = \bar{X}_t^i$ where \bar{X}^i is the solution of (7.1) driven by $B^{n,i}$ with initial condition $\bar{X}_0^i = X_{\tau_n^i}^i$ (recall the notation τ_n^i from (7.11)). Of course the law of the process is correct with this construction.

Denote:

$$\mathbf{S} = \{i \in \llbracket 1, N \rrbracket, \exists t < t_\varepsilon, X_t^i \in \mathfrak{B}_1\}.$$

Then the Markov inequality yields:

$$\mathbb{P}(T > \sigma N, \mathcal{A}^c) \leq e^{-\sigma N} \mathbb{E}(e^T \mathbb{1}_{\mathcal{A}^c}) = e^{-\sigma N} \sum_{\substack{S \in \mathcal{P}(\llbracket 1, N \rrbracket) \\ \#S \leq 2\alpha N}} \mathbb{E}\left(e^{\sum_{i=1}^N T_i} \mathbb{1}_{\mathbf{S}=S}\right).$$

Fix $S \in \mathcal{P}(\llbracket 1, N \rrbracket)$, such that $\#S < 2\alpha N$, and recall the definition of the variable I_n^i used in the construction of the FV process, which are independent uniform variables on $\llbracket 1, N \rrbracket \setminus \{i\}$. We define by induction $P_0^i = 0$ and :

$$P_k^i = \inf \{n > P_{k-1}^i, I_n^i \notin S\}.$$

Notice that, under the event $\{\mathbf{S} = S\}$, if $I_n^i \notin S$, it means that at its n^{th} rebirth the particle i is resurrected on a particle which never reaches \mathfrak{B}_1 before time t_ε .

Setting $k_0(i) = 1$ if $x_i \in \mathfrak{B}_1$ and $k_0(i) = 0$ otherwise, we define as well

$$P^i = \inf \left\{ k \geq k_0(i), \forall x \in D \setminus \mathfrak{B}_1, \tau_D(X^{x,i,P_k^i}) > t_\varepsilon \right\},$$

where for $n \in \mathbb{N}$ the family of processes $(X^{x,i,n})_{x \in D \setminus \mathfrak{B}_1}$ is as in Assumption 7.1.2 and are driven by the Brownian motion $B^{n,i}$. Since we have already observed that, for all $k > 0$, at its $(P_k^i)^{\text{th}}$ death, the particle i is resurrected at a position in $D \setminus \mathfrak{B}_1$, the event $\{\forall x \in D \setminus \mathfrak{B}_1, \tau_D(X^{x,i,P_k^i}) > t_\varepsilon\}$, which is measurable with respect to the Brownian motion $B^{P_k^i,i}$, implies that the particle does not die again before time t_ε . For $k = 0$, it depends whether initially $x_i \in \mathfrak{B}_1$: if $x_i \notin \mathfrak{B}_1$ (which is in particular the case if $x_i \notin \mathfrak{B}$) then, again, the event $\{\forall x \in D \setminus \mathfrak{B}_1, \tau_D(X^{x,i,0}) > t_\varepsilon\}$ implies that the particle doesn't die before time t_ε . This is not the case if $x_i \in \mathfrak{B}_1$. As a consequence, in any cases, under the event $\{\mathbf{S} = S\}$, we can bound the total number of death of the i^{th} particle by

$$T^i \leq \sum_{k=1}^{P^i} (P_k^i - P_{k-1}^i).$$

The variables $(P_k^i - P_{k-1}^i)_{k \geq 1, i}$ are independent geometric random variables of parameter

$1 - \#S > 1 - 2\alpha$. Under Assumption 7.1.2, if $x_i \in \mathfrak{B}_1$ (resp. if $x_i \notin \mathfrak{B}_1$) then P^i (resp. $P^i + 1$) is a geometric random variable of parameter $1 - \bar{p}_\varepsilon$. Moreover, $(P^i)_{1 \leq i \leq N}$ is a family of independent random variables, independent from $(P_k^i)_{k \geq 1, 1 \leq i \leq N}$. We have:

$$\mathbb{E} \left(e^{\sum_{i=1}^N T^i} \mathbb{1}_{\mathbf{S}=S} \right) \leq \mathbb{E} \left(e^{\sum_{i=1}^N \sum_{k=1}^{P^i} (P_k^i - P_{k-1}^i)} \right) = \left(\mathbb{E} \left(e^{\sum_{k=1}^{P^i} (P_k^i - P_{k-1}^i)} \right) \right)^N.$$

We are just left to show that $\mathbb{E} \left(\exp \sum_{k=1}^{P^i} (P_k^i - P_{k-1}^i) \right)$ is finite and bounded uniformly in $\varepsilon < \varepsilon_0$. Conditioning with respect to P^i we get :

$$\mathbb{E} \left(e^{\sum_{k=1}^{P^i} P_k^i - P_{k-1}^i} \right) = \mathbb{E} \left(\mathbb{E} \left(e^{P_0^i} \right)^{P^i} \right) \leq \mathbb{E} \left(\left(\frac{e}{1 - e\alpha} \right)^{P^i} \right),$$

hence the result if ε_0 satisfies $\bar{p}_{\varepsilon_0} < \frac{1 - e\alpha}{e}$, since we bound then

$$\mathbb{P}(T > \sigma N, \mathcal{A}^c) \leq \left(2e^{-\sigma} \mathbb{E} \left(\left(\frac{e}{1 - e\alpha} \right)^{P^i} \right) \right)^N.$$

3. In the same spirit, fix $i \in \llbracket 1, N \rrbracket$, and write now:

$$P_k^i = \inf \{ n > P_{k-1}^i, I_n^i \notin \mathbf{S}^i \},$$

where

$$\mathbf{S}^i = \left\{ j \in \llbracket 1, N \rrbracket \setminus \{i\}, \exists t < t_\varepsilon, X_t^j \in \mathfrak{B}_1 \right\},$$

and

$$\mathcal{A}^i = \left\{ \# \left\{ j \in \llbracket 1, N \rrbracket \setminus \{i\}, \exists t \leq t_\varepsilon, X_t^j \in \mathfrak{B}_1 \right\} \geq 2\alpha N \right\},$$

and the definition of P^i does not change. We have that $(P_k^i)_k$, and P^i are independent random variable, and P^i is independent of \mathcal{A}^i and \mathbf{S}^i . Indeed, \mathcal{A}^i and \mathbf{S}^i only depends on the Brownian motions that drive $(X^j)_{j \neq i}$. Under the event $(\mathcal{A}^i)^c$, the cardinality of \mathbf{S}^i is less than $2\alpha N$. Furthermore, we have that $\mathcal{A}^i \subset \mathcal{A}$, and hence, as in the previous step,

$$\mathbb{E} (T^i \mathbb{1}_{\mathcal{A}^c}) \leq \mathbb{E} \left(\sum_{k=1}^{P^i} (P_k^i - P_{k-1}^i) \mathbb{1}_{(\mathcal{A}^i)^c} \right) \leq \mathbb{E} (P^i \mathbb{E}(P_1^i | \mathbf{S}^i, \mathcal{A}^i, P^i)) \leq \frac{1}{1 - 2\alpha} \mathbb{E}(P^i),$$

and we conclude by bounding $\mathbb{E}(P^i) \leq \bar{p}_\varepsilon (1 - \bar{p}_\varepsilon)^{-1}$ if $x_i \notin \mathfrak{B}$ (since, then, $x_i \notin \mathfrak{B}_1$) and, otherwise, $\mathbb{E}(P^i) \leq (1 - \bar{p}_\varepsilon)^{-1}$. □

Proof of Lemma 7.3.1. Define the sets:

$$\begin{aligned} U_1(0) &= \{i \in \llbracket 1, N \rrbracket, x_i \neq y_i\}, \\ U_2(0) &= \{i \in \llbracket 1, N \rrbracket, x_i = y_i\}. \end{aligned}$$

Now, for $t \geq 0$, we want to define some sets $U_1(t)$, $U_2(t)$, such that if X^i and Y^i decouple at

some time $s \geq 0$, then for all $t \geq s$, $i \in U_1(t)$. For $i \in U_2(0)$, $n \in \mathbb{N}$, write:

$$\tau_n^i = \inf \{t > \tau_{n-1}^i, X_{t-}^i = Y_{t-}^i \in \partial D\},$$

as in(7.11), and

$$\bar{\tau}_d^i = \inf \{t \geq 0, X_t^i \neq Y_t^i\}.$$

Since the FV-process is well-defined, almost surely, there is only a finite number of such events before time t_ε , for all $1 \leq i \leq N$. Then define the set $U_1(t)$ and $U_2(t)$ for $t \in (\tau_{k-1}, \tau_k]$ by induction on $k \geq 1$. Assume that the sets have been defined up to the time τ_{k-1} for some $k \geq 1$. Set $U_j(t) = U_j(\tau_{k-1})$ for all $t \in (\tau_{k-1}, \tau_k)$. Let $i \in \llbracket 1, N \rrbracket$ be the index such that $\tau_k \in \cup_{n \in \mathbb{N}} \{\bar{\tau}_n^i\}$. Now we distinguish two cases. If $\tau_k \neq \bar{\tau}_d^i$, then $U_j(\tau_k) = U_j(\tau_{k-1})$ for $j = 1, 2$. Else set:

$$U_1(\tau_k) = U_1(\tau_{k-1}) \cup \{i\}, \quad U_2(\tau_k) = U_2(\tau_{k-1}) \cap \{i\}^c.$$

It is immediate to check that $U_1(t)$ and $U_2(t)$ form a partition of $\llbracket 1, N \rrbracket$ for all $t \geq 0$, and that $U_1(t)$ is non-decreasing with t and such that $\{i \in \llbracket 1, N \rrbracket, X_t^i \neq Y_t^i\} \subset U_1(t)$ for all $t \geq 0$. Recall from Lemma 7.3.2 the event:

$$\mathcal{A} = \{\#\{i \in \llbracket 1, N \rrbracket, \exists t \leq t_\varepsilon, X_t^i = Y_t^i \in \mathfrak{B}_1\} \geq 2\alpha N\}.$$

For $n \in \mathbb{N}$ and $j = 1, 2$, write $u_k^j = \#U_j(\tau_k)$. At each time τ_k , the probability that a particle goes from U_2 to U_1 is less than u_{k-1}^1/N . Hence, we have that for all $k \geq 1$:

$$\mathbb{E}(u_{k+1}^1 | \mathcal{F}_{\tau_k}) \leq u_k^1 \left(1 + \frac{1}{N}\right),$$

and thus

$$\mathbb{E}(u_k^1) \leq \bar{d}(x, y) \left(1 + \frac{1}{N}\right)^k.$$

Using the notations of Lemma 7.3.2, in particular T to denote the total number of death event before time t_ε , using that u_n^1 is non-decreasing, we bound

$$\begin{aligned} \mathbb{E}(u_T^1 \mathbb{1}_{\mathcal{A}^c}) &\leq \mathbb{E}(u_{\sigma N}^1) + N\mathbb{P}(T > \sigma N, \mathcal{A}^c) \\ &\leq e^\sigma \bar{d}(x, y) + Nq^N, \end{aligned}$$

which is bounded uniformly on $N \geq 1$ and ε small enough, by $\tilde{C}_3 \bar{d}(x, y)$, for some $\tilde{C}_3 > 0$, as soon as $\bar{d}(x, y) \geq 1$ (while, if $\bar{d}(x, y) = 0$ then the two processes remain equal for all times and thus the result is trivial). We get from all of this:

$$\mathbb{E}\left(\sup_{t \leq t_\varepsilon} \bar{d}(\mathbf{X}_t, \mathbf{Y}_t) \mathbb{1}_{\mathcal{A}^c}\right) \leq \mathbb{E}(u_T^1 \mathbb{1}_{\mathcal{A}^c}) \leq \tilde{C}_3 \bar{d}(x, y).$$

Now we can bound the probability to decouple starting from any $x_i = y_i \in D$, for a fixed i (recall the notation T^i from Lemma 7.3.2):

$$\begin{aligned} \mathbb{P}(\exists 0 < t < t_\varepsilon, X_t^i \neq Y_t^i) &\leq \sum_{n \geq 1} \mathbb{P}(\bar{\tau}_d^i = \bar{\tau}_n^i, \mathcal{A}^c, T_i > n) + \mathbb{P}(\mathcal{A}) \\ &= \sum_{n \geq 1} \mathbb{E}(\bar{d}(\mathbf{X}_{\tau_n}, \mathbf{Y}_{\tau_n})/N \mathbb{1}_{\mathcal{A}^c}) \mathbb{P}(T_i > n, \mathcal{A}^c) + (2\tilde{p}_\varepsilon^\alpha)^N \end{aligned}$$

$$\begin{aligned} &\leq \frac{1}{N} \sum_{n \geq 1} \mathbb{E} \left(\sup_{t \leq t_\varepsilon} \bar{d}(\mathbf{X}_t, \mathbf{Y}_t) \mathbb{1}_{\mathcal{A}^c} \right) \mathbb{P}(T_i > n, \mathcal{A}^c) + (2\tilde{p}_\varepsilon^\alpha)^N \\ &\leq \tilde{C}_3 \frac{\bar{d}(x, y)}{N} \mathbb{E}(T_i \mathbb{1}_{\mathcal{A}^c}) + (2\tilde{p}_\varepsilon^\alpha)^N. \end{aligned}$$

We conclude using Lemma 7.3.2. \square

We need to choose the parameters involved in the definition of the distance \mathbf{d} . There are three of them: α , β , and V_0 . We fix any $V_0 > 4C_1$ (which is required in Lemma 7.2.3), any $\beta < (2 \vee 4C_1)^{-1}$ and then α small enough so that

$$\frac{1 + 2\beta C_1}{1 + \beta C_2} \vee 4\beta C_1 + \alpha C_3(1 + 2\beta V_0) < 1, \quad (7.17)$$

and

$$\frac{1 + 2\beta V_0}{1 + V_0} < 1, \quad (7.18)$$

where we used in (7.17) that $C_2 > 2C_1$ from Proposition 7.2.2. This is possible by fixing first some small β , and then taking any $V_0 > 4C_1$, and finally α small enough.

Lemma 7.3.3. *Let $\mathbf{x}, \mathbf{y} \in D^N$ and $1 \leq i \leq N$ such that $x_i \neq y_i$ and $V(x_i) + V(y_i) \leq C_2$. Then with $\kappa_{1,\varepsilon} = \gamma_\varepsilon \vee (1 - c_\varepsilon + 2p_\varepsilon + 4\beta C_1(1 - \gamma_\varepsilon))$, where γ_ε has been defined in lemma 7.2.3, we have:*

$$\mathbb{E}(d^1(X_{t_\varepsilon}^i, Y_{t_\varepsilon}^i)) \leq \kappa_{1,\varepsilon} d^1(x_i, y_i).$$

Proof. Let $(\tilde{X}_t^i, \tilde{Y}_t^i)$ be the coupling of the diffusion (7.8) as in lemma 7.2.2, used in the construction of our coupling. Then, $(\tilde{X}_t^i, \tilde{Y}_t^i) = (X_t^i, Y_t^i)$ until X^i or Y^i reaches ∂D . We have :

$$\begin{aligned} \mathbb{P}(X_{t_\varepsilon}^i = Y_{t_\varepsilon}^i) &\geq \mathbb{P}(X_{t_\varepsilon}^i = Y_{t_\varepsilon}^i, \tau_{x_i} > t_\varepsilon, \tau_{y_i} > t_\varepsilon) \\ &= \mathbb{P}(\tilde{X}_{t_\varepsilon}^{x_i} = \tilde{Y}_{t_\varepsilon}^{y_i}, \tau_{x_i} > t_\varepsilon, \tau_{y_i} > t_\varepsilon) \\ &\geq \mathbb{P}(\tilde{X}_{t_\varepsilon}^{x_i} = \tilde{Y}_{t_\varepsilon}^{y_i}) - \mathbb{P}(\tau_{x_i} > t_\varepsilon) - \mathbb{P}(\tau_{y_i} > t_\varepsilon) \\ &\geq c_\varepsilon - 2p_\varepsilon. \end{aligned}$$

Using the property of the Lyapunov function described in (7.12), we then have:

$$\begin{aligned} \mathbb{E}(d^1(X_{t_\varepsilon}^i, Y_{t_\varepsilon}^i)) &\leq 1 - c_\varepsilon + 2p_\varepsilon + 2\beta C_1(1 - \gamma_\varepsilon) + \gamma_\varepsilon \beta (V(x_i) + V(y_i)) \\ &\leq \kappa_{1,\varepsilon} d^1(x_i, y_i). \end{aligned}$$

\square

Now we focus on the particles near the boundary that are not coupled:

Lemma 7.3.4. *Let $\mathbf{x}, \mathbf{y} \in D^N$ and $1 \leq i \leq N$ such that $V(x_i) + V(y_i) \geq C_2$ and $x_i \neq y_i$. Then with $\kappa_{2,\varepsilon} = \gamma_\varepsilon + (1 - \gamma_\varepsilon) \frac{1 + 2\beta C_1}{1 + \beta C_2}$, we have:*

$$\mathbb{E}(d^1(X_{t_\varepsilon}^i, Y_{t_\varepsilon}^i)) \leq \kappa_{2,\varepsilon} d^1(x_i, y_i).$$

Proof. Using the Lyapunov property and the fact that $\gamma_\varepsilon \leq \kappa_{2,\varepsilon}$, we have:

$$\begin{aligned} \mathbb{E} (d^1(X_{t_\varepsilon}^i, Y_{t_\varepsilon}^i)) &\leq 1 + 2\beta C_1(1 - \gamma_\varepsilon) + \beta\gamma_\varepsilon (V(x_i) + V(y_i)) \\ &\leq \kappa_{2,\varepsilon} d^1(x_i, y_i) + 1 + 2\beta C_1(1 - \gamma_\varepsilon) - \kappa_{2,\varepsilon} + \beta(\gamma_\varepsilon - \kappa_{2,\varepsilon}) (V(x_i) + V(y_i)). \end{aligned}$$

The fact that $V(x_i) + V(y_i) \geq C_2$ implies that

$$1 + 2\beta C_1(1 - \gamma_\varepsilon) - \kappa_{2,\varepsilon} + \beta(\gamma_\varepsilon - \kappa_{2,\varepsilon}) (V(x_i) + V(y_i)) \leq 0,$$

and thus the result. \square

Proof of Theorem 7.1.1. Let $\mathbf{x}, \mathbf{y} \in D^N$, $\kappa_\varepsilon = \kappa_{1,\varepsilon} \vee \kappa_{2,\varepsilon}$. First suppose that $\mathbb{1}_{A(\mathbf{x}) > \alpha N} = \mathbb{1}_{A(\mathbf{y}) > \alpha N} = 0$. We decompose:

$$\begin{aligned} \mathbb{E}(\mathbf{d}(\mathbf{X}_{t_\varepsilon}, \mathbf{Y}_{t_\varepsilon})) &= \sum_{i/x_i \neq y_i} \mathbb{E}(d^1(X_{t_\varepsilon}^i, Y_{t_\varepsilon}^i)) + \sum_{i/x_i=y_i \notin \mathfrak{B}} \mathbb{E}(d^1(X_{t_\varepsilon}^i, Y_{t_\varepsilon}^i)) + \sum_{i/x_i=y_i \in \mathfrak{B}} \mathbb{E}(d^1(X_{t_\varepsilon}^i, Y_{t_\varepsilon}^i)) \\ &\quad + N(1 + V_0) (\mathbb{P}(A(\mathbf{X}_{t_\varepsilon}) > \alpha N) + \mathbb{P}(A(\mathbf{Y}_{t_\varepsilon}) > \alpha N)). \quad (7.19) \end{aligned}$$

Thanks to Lemmas 7.3.3 and 7.3.4, we have that the first sum is less than $\kappa_\varepsilon d(\mathbf{x}, \mathbf{y})$. From Lemma 7.3.1, the second term is less than:

$$C_3 m_\varepsilon (1 + 2\beta V_0) \mathbf{d}(\mathbf{x}, \mathbf{y}),$$

and the third term is less than:

$$\alpha C_3 (1 + 2\beta V_0) \mathbf{d}(\mathbf{x}, \mathbf{y}).$$

Finally, thanks to Lemma 7.2.4, the last term is less than:

$$2N(1 + V_0) q_\varepsilon^N \mathbf{d}(\mathbf{x}, \mathbf{y}) \leq \frac{-2(1 + V_0)}{e \ln(q_\varepsilon)} \mathbf{d}(\mathbf{x}, \mathbf{y}).$$

Putting all of this together we get:

$$\mathbb{E}(\mathbf{d}(\mathbf{X}_{t_\varepsilon}, \mathbf{Y}_{t_\varepsilon})) \leq s_\varepsilon \mathbf{d}(\mathbf{x}, \mathbf{y})$$

where

$$s_\varepsilon = \kappa_\varepsilon + C_3(1 + 2\beta V_0) m_\varepsilon + \alpha C_3(1 + 2\beta V_0) + \frac{-2(1 + V_0)}{e \ln(q_\varepsilon)}.$$

As ε goes to 0, s_ε goes to $\frac{1+2\beta C_1}{1+\beta C_2} \wedge 4\beta C_1 + \alpha C_3(1 + 2\beta V_0) < 1$ because of our choice of constants (7.17).

Now, consider the case where $\mathbb{1}_{A(\mathbf{x}) > \alpha N} + \mathbb{1}_{A(\mathbf{y}) > \alpha N} > 0$. Assume that $\mathbf{x} \neq \mathbf{y}$, the result being trivial otherwise since the processes stay equal for all times. In that case, $\mathbf{d}(\mathbf{x}, \mathbf{y}) \geq N(1 + V_0)$ and we simply bound

$$\mathbb{E}(d(\mathbf{X}_{t_\varepsilon}, \mathbf{Y}_{t_\varepsilon})) \leq N(1 + 2\beta V_0 + (1 + V_0)q_\varepsilon) \leq \left(\frac{1 + 2\beta V_0}{1 + V_0} + q_\varepsilon \right) \mathbf{d}(\mathbf{x}, \mathbf{y}),$$

for ε small enough. Since $r_\varepsilon := \frac{1+2\beta V_0}{1+V_0} + q_\varepsilon$ is strictly less than 1 with our choice of constants (7.18) for ε small enough, we conclude that, with $c = 1 - \sup_{\varepsilon < \varepsilon_0} s_\varepsilon \wedge r_\varepsilon > 0$ where ε_0 is small

enough, we have for all $\mathbf{x}, \mathbf{y} \in D^N$:

$$\mathbb{E}_{\mathbf{x}, \mathbf{y}}(\mathbf{d}(\mathbf{X}_{t_\varepsilon}, \mathbf{Y}_{t_\varepsilon})) \leq (1-c)\mathbf{d}(\mathbf{x}, \mathbf{y}).$$

By conditioning with respect to the initial condition we get that:

$$W_{\mathbf{d}}(\mu P_{t_\varepsilon}^N, \nu P_{t_\varepsilon}^N) \leq (1-c)W_{\mathbf{d}}(\mu, \nu),$$

for all probability measures μ, ν in $\mathcal{M}^1(D^N)$, and by iteration:

$$\begin{aligned} W_{\mathbf{d}}(\mu P_t^N, \nu P_t^N) &\leq (1-c)^{\lfloor t/t_\varepsilon \rfloor} W_{\mathbf{d}}(\mu P_{t-\lfloor t/t_\varepsilon \rfloor t_\varepsilon}^N, \nu P_{t-\lfloor t/t_\varepsilon \rfloor t_\varepsilon}^N) \\ &\leq (1+2(\beta+1)V_0)N(1-c)^{\lfloor t/t_\varepsilon \rfloor}. \end{aligned}$$

We conclude the first point of the theorem using $\mathbb{1}_{\mathbf{x} \neq \mathbf{y}} \leq \mathbf{d}(\mathbf{x}, \mathbf{y})$.

Let's now prove the second point of Theorem 7.1.1. $\mathcal{M}^1(D^N)$ endowed with the distance \mathbf{d} is a complete space. The contraction of $P_{t_\varepsilon}^N$ yield the existence and uniqueness of the stationary measure $\nu_\infty^{N,\varepsilon}$, as well as the exponential convergence of $\mu P_t^{N,\varepsilon}$ towards $\nu_\infty^{N,\varepsilon}$. If μ is exchangeable, then $\mu P_t^{N,\varepsilon}$ is exchangeable for all $t \geq 0$. The convergence of $\mu P_t^{N,\varepsilon}$ toward $\nu_\infty^{N,\varepsilon}$ implies that $\nu_\infty^{N,\varepsilon}$ is exchangeable. Now consider an optimal coupling for the distance d of $\mu P_t^{N,\varepsilon}$ and $\nu_\infty^{N,\varepsilon} P_t^{N,\varepsilon}$. Using the exchangeability property we have:

$$\begin{aligned} \|\mu P_t^{N,k} - \nu_\infty^{N,\varepsilon,k}\|_{TV} &\leq \mathbb{E}\left(\mathbb{1}_{(X_t^1, \dots, X_t^k) \neq (Y_t^1, \dots, Y_t^k)}\right) \\ &\leq \sum_{i=1}^k \mathbb{E}\left(\mathbb{1}_{X_t^i \neq Y_t^i}\right) \\ &= k\mathbb{E}\left(\mathbb{1}_{X_t^1 \neq Y_t^1}\right) \\ &\leq \frac{k}{N} \sum_{i=1}^N \mathbb{E}\left(\mathbb{1}_{X_t^i \neq Y_t^i}\right), \end{aligned}$$

and we conclude with the first point of the theorem. \square

7.3.2 Propagation of chaos

Recall the definition of the empirical measure π^N in (7.4). As said in the introduction, the goal is to get a uniform in time propagation of chaos result. We start from a propagation of chaos result, with a time dependency, from [165]. Their result reads as follows:

Proposition 7.3.1 ([165], Theorem 1). *For all $\mu_0 \in \mathcal{M}^1(D^N)$, considering $(X_t^i)_{t \geq 0}$ the FV process with initial condition (X_0^i) which is a random variable of law μ_0 , and (X_t) the diffusion (7.1), then, for all bounded $f : D \rightarrow \mathbb{R}_+$, all $\varepsilon > 0$ and all $t \geq 0$:*

$$\mathbb{E}\left(\left|\int_D f d\pi^N(\mathbf{X}_t) - \mathbb{E}_{\pi^N(\mathbf{x}_0)}(f(X_t)|\tau_{\partial D} > t)\right|\right) \leq \frac{2(1+\sqrt{2})\|f\|_\infty}{\sqrt{N}} \sqrt{\mathbb{E}\left(\frac{1}{\mathbb{P}_{\pi^N(\mathbf{x}_0)}(\tau_{\partial D} > t)^2}\right)},$$

where $\tau_{\partial D}$ is defined in (7.2).

We also need a result on the convergence of the law of the diffusion (7.1), conditioned on survival, towards the QSD ν_∞^ε . This is from [35], although the statement is slightly modified to fit our setting.

Proposition 7.3.2. *Under Assumption 7.1.1, there exists $\varepsilon_0 > 0$ such that for all compact $K \subset D$, and all $0 < \varepsilon < \varepsilon_0$, there exists $C_\varepsilon, \tilde{C}_\varepsilon, \lambda_\varepsilon, \chi_\varepsilon > 0$ such that for all $\mu_0 \in \mathcal{M}^1(D)$ satisfying $\mu_0(K) \geq 1/4$:*

$$\|\mathbb{P}_{\mu_0}(X_t \in \cdot | \tau_{\partial D} > t) - \nu_\infty^\varepsilon\|_{TV} \leq C_\varepsilon e^{-\chi_\varepsilon t},$$

and

$$\mathbb{P}_{\mu_0}(\tau_{\partial D} > t) \geq \tilde{C}_\varepsilon e^{-\lambda_\varepsilon t}.$$

Proof. The process (7.1) satisfies equation (4.7) of [35], with $D_0 = F$, where F was defined in the proof of Lemma 7.2.3, some λ_1 independent from ε , and $\varphi = V$. The constant λ_0 defined in equation (4.4) of [35] goes to zero as ε goes to zero, hence we may choose ε_0 such that for all $\varepsilon < \varepsilon_0$, $\lambda_1 > \lambda_0$, and assumption of [35, Corollary 4.3] hold true. From [35, Theorem 4.1], this yields the existence of the QSD ν_∞^ε and of some function $\phi : D \rightarrow \mathbb{R}_+$, uniformly bounded away from 0 on all compact subsets of \bar{D} such that for all $\mu_0 \in \mathcal{M}^1(D)$:

$$\|\mathbb{P}_{\mu_0}(X_t \in \cdot | \tau_{\partial D} > t) - \nu_\infty^\varepsilon\|_{TV} \leq C_\varepsilon e^{-\chi_\varepsilon t} \mu_0(V) / \mu_0(\phi).$$

Since V is bounded, if $\mu_0(K) \geq 1/4$, then $\mu_0(\phi) \geq 1/4 \min_K \phi$, and we get that

$$\|\mathbb{P}_{\mu_0}(X_t \in \cdot | \tau_{\partial D} > t) - \nu_\infty^\varepsilon\|_{TV} \leq C_\varepsilon e^{-\chi_\varepsilon t} \frac{4\|V\|_\infty}{\inf_K \phi}.$$

For the second point, write:

$$\mathbb{P}_{\mu_0}(\tau_{\partial D} > t) \geq \frac{1}{4} \inf_{x \in K} \mathbb{P}_x(\tau_{\partial D} > t).$$

Now fix $0 < \tilde{U}_1 < \tilde{U}_0$ such that $K \subset F \cup \{U \leq \tilde{U}_0\} =: \tilde{F}$, and

$$\tilde{\omega} := \inf_{(F \cup \{U \leq \tilde{U}_1\})^c} |\nabla U| > 0$$

. Fix $T > 0$ such that $\tilde{U}_0 - \tilde{\omega}^2 T < \tilde{U}_1$, and some $\delta > 0$ such that:

$$\delta < \min \left(\text{dist} \left(F \cup \{U \leq \tilde{U}_1\}, (F \cup \{U \leq \tilde{U}_0\})^c \right), \text{dist} \left(F \cup \{U \leq \tilde{U}_0\}, \mathbb{R}^d \setminus D \right) \right).$$

Write:

$$\mathcal{E} = \left\{ \tau_{\partial D} > T, X_T \in \tilde{F} \right\},$$

as well as $\varphi_t(x)$ for the flow

$$\begin{cases} \varphi'_t = -\nabla U(\varphi_t) \\ \varphi_0(x) = x \end{cases}.$$

With our choice of T , \tilde{U}_0 and \tilde{U}_1 , we have that $\varphi_T \in F \cup \{U \leq \tilde{U}_1\}$ for all $x \in \tilde{F}$. We get using Gronwall's Lemma:

$$\sup_{0 \leq t \leq T} |X_t - \varphi_t| \leq e^{\|\nabla^2 U\|_\infty T} \sqrt{2\varepsilon} \sup_{0 \leq t \leq T} |B_t|.$$

If W is a one-dimensional Brownian motion, $\sup_{0 \leq t \leq T} W_t$ has the law of $|G|$ where G is a standard Normal random variable. Hence:

$$\mathbb{P} \left(\sup_{0 \leq t \leq T} |X_t - \varphi_t| \geq \delta \right) \leq 4d \mathbb{P} \left(G \geq \frac{\delta e^{-\|\nabla^2 U\|_\infty T}}{T\sqrt{2\varepsilon}} \right) \leq 4de^{-\frac{b}{\varepsilon}},$$

where $b = \frac{\delta e^{-\|\nabla^2 U\|_\infty T}}{2\sqrt{2}T}$.

Now write

$$\mathcal{E}_i = \left\{ \tau_{\partial D} > (i+1)T \text{ and } X_{(i+1)T} \in \tilde{F} \right\}.$$

We showed that for ε small enough, $\mathbb{P}(\mathcal{E}_{i+1}|\mathcal{E}_i) \geq 1 - e^{-b/\varepsilon}$. We also have for our choice of δ :

$$\{\tau_{\partial D} < t_\varepsilon\} \subset \mathcal{E}_{\lceil t/T \rceil}^c.$$

Hence for all $x \in \tilde{F}$:

$$\mathbb{P}_x(\tau_{\partial D} > t) \geq \left(1 - e^{-b/\varepsilon}\right)^{t/T},$$

and thus the result. \square

In our metastable setting, this already yields propagation of chaos at equilibrium. Indeed, if the FV process starts from its stationary measure, its law won't change. But then from Proposition 7.3.1, the empirical measure of this process is close to the law of the process (7.1) conditioned on survival at time $t \geq 0$ starting from $\nu_\infty^{N,\varepsilon}$, which is itself close to the QSD if t is large enough.

Lemma 7.3.5. *Under Assumption 7.1.1 and 7.1.2, there exists $\varepsilon_0 > 0$ such that for all $0 < \varepsilon < \varepsilon_0$, there exists $C_\varepsilon, \eta_{\varepsilon,1} > 0$ such that if \mathbf{X}_∞ is a random vector of law $\nu_\infty^{N,\varepsilon}$ on D^N , then for all bounded function $f : D \rightarrow \mathbb{R}_+$:*

$$\mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_\infty) - \int_D f d\nu_\infty^\varepsilon \right| \right) \leq \frac{C_\varepsilon \|f\|_\infty}{N^{\eta_{\varepsilon,1}}}.$$

Proof. Assumptions 7.1.1 and 7.1.2 yield the existence of $\nu_\infty^{N,\varepsilon}$. Introduce the FV process $(\mathbf{X}_t)_{t \geq 0}$ with initial condition \mathbf{X}_∞ . By definition, the law of \mathbf{X}_t is $\nu_\infty^{N,\varepsilon}$ for all $t \geq 0$. Recall the definition of \mathfrak{B} and A from (7.14), and set $K = D \setminus \mathfrak{B}$. Since $\nu_\infty^{N,\varepsilon}$ is the stationary measure of the FV process, we get from Lemma 7.2.4 applied with $\alpha = 1/2$ that for all $t \geq 0$:

$$\mathbb{P}(A(\mathbf{X}_t) > N/2) \leq q_\varepsilon^N,$$

where $q_\varepsilon > 0$ goes to zero as ε goes to zero. Recall the definition of λ_ε from Proposition 7.3.2, let $t = b \ln(N)$ for some $0 < b < 1/(2\lambda_\varepsilon)$, and write $\mathcal{A} = \{G_1(\mathbf{X}_t) > N/2\}$. We have that:

$$\mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_\infty) - \int_D f d\nu_\infty^\varepsilon \right| \right) = \mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_t) - \int_D f d\nu_\infty^\varepsilon \right| \right),$$

and

$$\begin{aligned} \mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_\infty) - \int_D f d\nu_\infty^\varepsilon \right| \right) &= \mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_t) - \int_D f d\nu_\infty^\varepsilon \right| \right) \\ &\leq \mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_t) - \mathbb{E}_{\pi^N(\mathbf{x}_\infty)}(f(X_t) | \tau_{\partial D} > t) \right| \right) \end{aligned}$$

$$+ \mathbb{E} \left(\left| \mathbb{E}_{\pi^N(\mathbf{X}_\infty)}(f(X_t)|\tau_{\partial D} > t) - \int_D f d\nu_\infty^\varepsilon \right| \right).$$

On \mathcal{G}_1^c , we have that $\pi^N(\mathbf{X}_\infty)(K) \geq 1/2$. Hence, from Proposition 7.3.1 and 7.3.2, there exists $C > 0$ such that:

$$\mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_t) - \mathbb{E}_{\pi^N(\mathbf{X}_\infty)}(f(X_t)|\tau_{\partial D} > t) \right| \right) \leq \frac{C\|f\|_\infty}{\sqrt{N}} \frac{1}{N^{-b\lambda_\varepsilon} - q_\varepsilon^N} = \frac{C\|f\|_\infty}{N^{1/2-b\lambda_\varepsilon}}.$$

From Proposition 7.3.2, we get that:

$$\mathbb{E} \left(\left| \mathbb{E}_{\pi^N(\mathbf{X}_\infty)}(f(X_t)|\tau_{\partial D} > t) - \int_D f d\nu_\infty^\varepsilon \right| \right) \leq (Ce^{-\lambda_\varepsilon t} + q_\varepsilon^N) \|f\|_\infty = \frac{C\|f\|_\infty}{N^{b\lambda_\varepsilon}}.$$

The fact that we chose $b < 1/2\lambda_\varepsilon$ concludes, as soon as ε is small enough so that $q_\varepsilon < 1$. \square

Proof of Theorem 7.1.2. Fix some $\varepsilon > 0$, some compact $K \subset D$, $\mu_0 \in \mathcal{M}^1(D)$ such that $\mu_0(K) \geq 1/2$, and a random variable \mathbf{X}_0 of law $\mu_0^{\otimes N}$. Write:

$$\mathcal{G}_2 = \{ \pi^N(\mathbf{X}_0)(K) \geq 1/4 \}.$$

We have that $\mathbb{E}(\pi^N(\mathbf{X}_0)(K)) = \mu_0(K)$, and $\text{Var}(\pi^N(\mathbf{X}_0)(K)) = \mu_0(K)(1 - \mu_0(K))/N$. Hence we have:

$$\mathbb{P}(\mathcal{G}_2^c) \leq 4/N.$$

We now fix $0 < b < 1/(2\lambda_\varepsilon)$. For all $t \leq b \ln(N)$, from Propositions 7.3.1 and 7.3.2, we get that there exists $C > 0$ such that:

$$\mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_t) - \mathbb{E}_{\pi^N(\mathbf{X}_0)}(f(X_t)|\tau_{\partial D} > t) \right| \right) \leq \frac{C\|f\|_\infty}{\sqrt{N}} \sqrt{\frac{1}{N^{-b\lambda_\varepsilon} - CN^{-1}}} \leq \frac{C\|f\|_\infty}{N^{1/2-b\lambda_\varepsilon/2}}.$$

If $t \geq b \ln(N)$, we consider a random variable $(\mathbf{X}_t, \mathbf{X}_\infty)$ which is an optimal coupling of $\mu_0^{\otimes N} P_t^{N,\varepsilon}$ and $\nu_\infty^{N,\varepsilon}$ for the distance \mathbf{d} defined in (7.16). We then bound as follow:

$$\begin{aligned} \mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_t) - \mathbb{E}_{\pi^N(\mathbf{X}_0)}(f(X_t)|\tau_{\partial D} > t) \right| \right) &\leq \mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_t) - \int_D f d\pi^N(\mathbf{X}_\infty) \right| \right) \\ &\quad + \mathbb{E} \left(\left| \int_D f d\pi^N(\mathbf{X}_\infty) - \int_D f d\nu_\infty \right| \right) \\ &\quad + \mathbb{E} \left(\left| \int_D f d\nu_\infty^\varepsilon - \mathbb{E}_{\pi^N(\mathbf{X}_0)}(f(X_t)|\tau_{\partial D} > t) \right| \right). \end{aligned}$$

From the proof of Theorem 7.1.1, the first term is bounded by:

$$\frac{\mathbb{E}(d(\mathbf{X}_t, \mathbf{X}_\infty))}{N} \|f\|_\infty \leq C(1-c)^{t/t_\varepsilon} \|f\|_\infty \leq CN^{\ln(1-c)/t_\varepsilon} \|f\|_\infty.$$

From Lemma 7.3.5, the second term is bounded by:

$$\frac{C}{N^{\eta_{\varepsilon,1}}} \|f\|_\infty.$$

Finally, by Proposition 7.3.2, the third term is bounded by:

$$(Ce^{-\chi_\varepsilon t} + 2\mathbb{P}(\mathcal{G}_2)) \|f\|_\infty \leq CN^{-\chi_\varepsilon b} \|f\|_\infty,$$

and thus the result. \square

7.4 Establishing Assumption 7.1.2

This section is devoted to the proof of the following:

Lemma 7.4.1. *Under Assumptions 7.1.1 and 7.1.3, Assumption 7.1.2 holds.*

Proof. 1. Suppose first that $d = 1$. Under Assumption 7.1.1, $D = (x_1, x_2)$ for some $x_1 < x_2$. Set $\mathfrak{B}_1 = (x_1, x_1 + \theta) \cup (x_2 - \theta, x_2)$ with $\theta > 0$ sufficiently small so that $U' \neq 0$ on \mathfrak{B}_1 (as a consequence of Assumption 7.1.1, U is thus decreasing (resp. increasing) on $(x_1, x_1 + \theta)$ (resp. $(x_2 - \theta, x_2)$)) and so that $\min(U(x_1 + \theta), U(x_2 - \theta)) > c_*$ (which is possible since $U(x_1) = U(x_2) = U_0 > c_*$). Take any $a \in (c^*, \min(U(x_1 + \theta), U(x_2 - \theta)))$. Using the uniqueness of the solution to equation (7.1) we have:

$$\{\exists x \in D \setminus \mathfrak{B}_1, \tau_{\partial D}(X^x) < t_\varepsilon\} = \{\tau_{\partial D}(X^{x_1 + \theta}) < t_\varepsilon\} \cup \{\tau_{\partial D}(X^{x_2 - \theta}) < t_\varepsilon\}.$$

We can conclude with [65, Chapter 6, Theorem 6.2].

2. We now suppose the second condition of Assumption 7.1.3. We set

$$\mathfrak{B}_1 = \{U > (U_0 + U_1)/2\} \cap \tilde{\mathfrak{B}}_1,$$

where $\tilde{\mathfrak{B}}_1$ is the set from Assumption 7.1.3, and we may choose any $a \in (c^*, (U_0 - U_1)/2)$. Fix some

$$\begin{aligned} U_2 &\in (a + (U_0 + U_1)/2, U_0), \\ U_3 &\in (U_1 + a, (U_0 + U_1)/2), \\ 0 &< \gamma < \min(U_3 - U_1 - a, U_2 - (U_0 + U_1)/2 - a), \end{aligned}$$

see Figure 7.1.

Fix as well some $T > 0$ (to be chosen large enough below, independently from ε) and for all $x \in D \setminus \mathfrak{B}_1$ write the event:

$$\mathcal{E}^x = \{U(X_T^x) < U_3 \text{ and } \forall 0 < t < T, U(X_t^x) < U_2\}.$$

Let's first show that there exists $C > 0$ such that $\mathbb{P}((\mathcal{E}^x)^c) \leq Ce^{-(a+\gamma)/\varepsilon}$ for ε small enough and T great enough, using Large Deviation results. In other words, in a fixed time interval, with high probability, starting from a medium energy level at most $(U_1 + U_0)/2$, the process will stay below the high energy level U_2 and will end below the medium energy level U_3 . According to [65, Chapter 4, Theorem 1.1], the action function of the process (7.1) is:

$$\begin{aligned} I(\varphi) &= \frac{1}{4\varepsilon} \int_0^T |\varphi'_s + \nabla U(\varphi_s)|^2 ds \\ &= \frac{1}{4\varepsilon} \int_0^T (|\varphi'_s|^2 + |\nabla U(\varphi_s)|^2) ds + \frac{U(\varphi_T) - U(\varphi_0)}{2\varepsilon} \end{aligned} \quad (7.20)$$

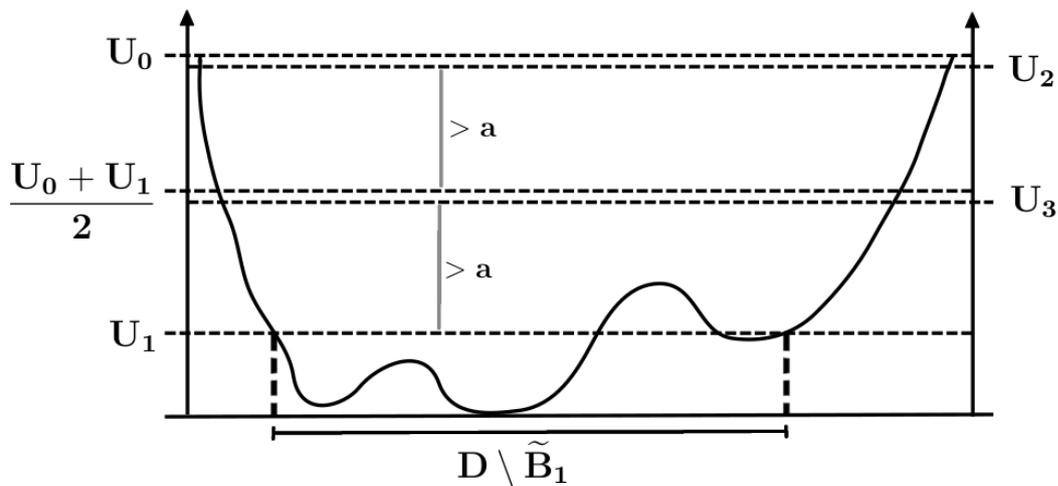


Figure 7.1: First, U_0 is the energy level on the boundary of \mathcal{D} . Then U_1 is taken as low as possible with the constraint that Assumption 7.1.3 holds, namely it is such that there exist a neighborhood $\tilde{\mathfrak{B}}_1$ of $\partial\mathcal{D}$ over which $U \geq U_1$ and $|\nabla U|$ is lower bounded by a positive constant. Then U_2 (resp. U_3) is taken slightly below U_0 (resp. $(U_1 + U_0)/2$) so that the length of the two grey lines in the figure is larger than a , which is itself a constant larger than the critical depth c_* . The condition that $c_* < (U_0 - U_1)/2$ means that it is possible to find U_2, U_3 and a to fulfill these constraints.

$$= \frac{1}{4\varepsilon} \int_0^T |\varphi'_s - \nabla U(\varphi_s)|^2 ds + \frac{U(\varphi_T) - U(\varphi_0)}{\varepsilon}. \quad (7.21)$$

For all function $\varphi : [0, T] \rightarrow D$ such that $\varphi_0 \notin \mathfrak{B}_1$ and there exists $t \in (0, T)$ such that $U(\varphi_t) \geq U_2$, using (7.21), we have:

$$\varepsilon I(\varphi) \geq \frac{1}{4} \int_0^t |\varphi'_s + \nabla U(\varphi_s)|^2 ds \geq U(\varphi_t) - U(\varphi_0) \geq U_2 - (U_0 + U_1)/2 > a + \gamma.$$

From this we deduce that for ε small enough, for all $x \notin \mathfrak{B}_1$:

$$\mathbb{P}(\exists t \in [0, T], U(X_t^x) \geq U_2) \leq e^{-(a+\gamma)/\varepsilon}.$$

Second, to bound the probability that $U(X_T^x) \geq U_3$, we consider two possible events: either the process stays during the whole interval $[0, T]$ above the energy level U_1 (which is unlikely because it would mean it stays in an unstable region where ∇U is non-zero) or the process goes down to U_1 but then climbs back in a time less than T to the level U_3 (which is also unlikely). More precisely, for all functions $\varphi : [0, T] \rightarrow D$ such that $\varphi_t \notin D \setminus \tilde{\mathfrak{B}}_1$ for all $t \in [0, T]$, using (7.20), we have that

$$\varepsilon I(\varphi) \geq T \inf_{\tilde{\mathfrak{B}}_1} |\nabla U|^2 / 4 - U_3 / 2.$$

We chose T great enough so that for all such functions, $\varepsilon I(\varphi) > a + \gamma$. Then for ε small enough we have that for all $x \notin \mathfrak{B}_1$,

$$\mathbb{P}(\exists t \in [0, T], X_t^x \notin \tilde{\mathfrak{B}}_1) \geq 1 - e^{-(a+\gamma)/\varepsilon}.$$

Next, for all functions $\varphi : [0, T] \rightarrow D$ such that $\varphi_0 \notin \tilde{\mathfrak{B}}_1$ and $U(\varphi_T) > U_3$,

$$\varepsilon I(\varphi) > U_3 - U_1.$$

Hence, for all x such that $x \notin \tilde{\mathfrak{B}}_1$ and ε small enough :

$$\mathbb{P}(\exists t \in [0, T], U(X_t^x) > U_3) \leq e^{-(a+\gamma)/\varepsilon}.$$

From those last two bounds we get for all $x \notin \mathfrak{B}_1$:

$$\begin{aligned} & \mathbb{P}(U(X_T^x) > U_3) \\ & \leq \mathbb{P}(\forall t < T, X_t^x \in \tilde{\mathfrak{B}}_1) + \mathbb{P}(\exists T > s > t > 0, X_t^x \notin \tilde{\mathfrak{B}}_1, U(X_s^x) > U_3) \\ & \leq 2e^{-(a+\gamma)/\varepsilon}. \end{aligned}$$

Finally we get for all $x \notin \mathfrak{B}_1$:

$$\mathbb{P}((\mathcal{E}^x)^c) \leq 3e^{-(a+\gamma)/\varepsilon}.$$

Up to now, we only have a control for a fixed initial condition x . To tackle simultaneously all initial conditions in $D \setminus \mathfrak{B}_1$, we use that, in a time T , two processes which start close

stays close (deterministically). More precisely, fix

$$\delta < \min \left(\text{dist}(\{U \leq U_2\}, \mathbb{R}^d \setminus D), \text{dist}(\{U \leq U_3\}, \mathfrak{B}_1) \right),$$

and $\delta' > 0$ such that $\delta' e^{\|\nabla^2 U\|_\infty T} < \delta$. Fix a family of point $z_1, \dots, z_k \notin \mathfrak{B}_1$ such that $D \setminus \mathfrak{B}_1 \subset \cup_{i=1}^k B(z_i, \delta')$, where $B(z, r)$ is the ball of center z and radius r . Write the event:

$$\mathcal{E} = \{\forall x \notin \mathfrak{B}_1, \tau_{\partial D}(X^x) > T \text{ and } X_T^x \notin \mathfrak{B}_1\}.$$

If $x \notin \mathfrak{B}_1$, there exists i such that $|x - z_i| < \delta'$. Gronwall's lemma then classically yields that

$$\sup_{0 \leq t \leq T} |X_t^x - X_t^{z_i}| \leq \delta' e^{\|\nabla^2 U\|_\infty T} < \delta.$$

In particular, $\tau_{\partial D}(X^x) < T$ implies that $U(X_t^{z_i}) \geq U_2$ for some $t \in [0, T]$. Hence we have that:

$$\bigcap_{i=1}^k \mathcal{E}^{z_i} \subset \mathcal{E},$$

and for ε small enough

$$\mathbb{P}(\mathcal{E}^c) \leq 3ke^{-(a+\gamma)/\varepsilon}.$$

Now write

$$\mathcal{E}_i = \left\{ \forall x \notin \mathfrak{B}_1, \tau_{\partial D}(X^x) > (i+1)T \text{ and } X_{(i+1)T}^x \notin \mathfrak{B}_1 \right\}.$$

We showed that for ε small enough, $\mathbb{P}(\mathcal{E}_{i+1} | \mathcal{E}_i) \geq 1 - 3ke^{-(a+\gamma)/\varepsilon}$. We also have that

$$\{\exists x \in D \setminus \mathfrak{B}_1, \tau_{\partial D}(X^x) < t_\varepsilon\} \subset \mathcal{E}_{[t_\varepsilon/T]}^c.$$

Hence:

$$\mathbb{P}(\forall x \in D \setminus \mathfrak{B}_1, \tau_{\partial D}(X^x) > t_\varepsilon) \geq \left(1 - e^{-(a+\gamma)/\varepsilon}\right)^{e^{a/\varepsilon}/T},$$

and thus this probability goes to 1 as ε goes to 0.

□

Chapter 8

The Fleming-Viot process in a high-killing regime: the soft killing case.

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Abstract : We study the Fleming-Viot particle system in the limit where the selection (or killing) rate tends to infinity. In this regime, and under two different sets of assumptions, we show that the empirical measure of this particle system converges towards a Dirac distribution with a moving mass. This stands in contrast to the mean-field limit, where the empirical measure exhibits a deterministic limit.

8.1 Introduction

8.1.1 Motivation

Fleming–Viot particle systems refer to population dynamics models in which n individuals are subjected to two mechanisms:

- individuals evolve in some state space as independent copies of a given continuous-time stochastic process (called the *mutation* process);
- they are killed at random times with a rate which depends on their current position, and are then instantaneously duplicated at the position of a uniformly chosen individual among the $n - 1$ remaining ones (this is the *selection* mechanism).

When the mutation process is a random walk on \mathbb{Z}^d and the killing rate $\lambda > 0$ is uniform on this space, the empirical measure of this particle system is known to converge, in the $n \rightarrow \infty$ limit and under a diffusive space-time rescaling for the mutation process, to the *Fleming–Viot superprocess* [61], which is a measure-valued process on \mathbb{R}^d introduced to describe the distribution of alleles in a population with a large number of possible genetic states [57]. In particular, in this regime, the selection mechanism is sped up by a factor n with respect to the mutation process.

The asymptotic behaviour of the system is also of interest without space-time rescaling. Indeed, denoting by $(X_t)_{t \geq 0}$ the mutation process and τ the killing time, it is known that the empirical measure of the system generally converges, when $n \rightarrow \infty$, to the deterministic quantity $\mathbb{P}(X_t \in \cdot | \tau > t)$, which is the law of X_t conditioned on survival up to time t . This observation, which also holds true for *hard* killing mechanism, that is to say instantaneous killing when the process reaches some subset of the state space, has motivated numerous developments on the study of propagation of chaos and hydrodynamic limit [25, 71, 119, 5, 165, 142, 94] as well as fluctuations [48, 108], for both soft and hard killing mechanisms, in both discrete and continuous spaces.

From a numerical point of view, Fleming–Viot particle systems can be seen as Interacting Particle Systems [46, 42, 149] allowing to approximate the conditional distribution $\mathbb{P}(X_t \in \cdot | \tau > t)$, whose evolution is given by a nonlinear Fokker–Planck equation and is therefore nontrivial to study. The $t \rightarrow \infty$ limit of this conditional distribution is called a *quasistationary distribution* (QSD) for the process $(X_t)_{t \geq 0}$ [39], and plays a prominent role in population dynamics [124], molecular dynamics [104, 49] or Monte Carlo methods [147]. For recent works on the existence and uniqueness of QSDs, as well as convergence of the conditional distribution $\mathbb{P}(X_t \in \cdot | \tau > t)$ towards the QSD, we refer to [35, 36, 8].

While the numerical interest of Fleming–Viot particle systems lies in the consistency of their $n \rightarrow \infty$ limit, in practice they can only be implemented with finitely many particles. In this context, one may expect their efficiency to depend on the intensity of the killing rate. More precisely, to approximate the QSD of the mutation process by the stationary distribution of the Fleming–Viot particle process, one needs the latter to reach stationarity on a shorter time scale than the typical killing time. This time scale separation is referred to as the *metastability* of the system [143]; in this situation, quantitative estimates for Fleming–Viot particle systems associated with diffusions with hard killing were recently obtained in [97]. The first motivation of the present article is to study the behaviour of Fleming–Viot particle systems in *non-metastable* systems, namely for which killing occurs on a faster time scale than convergence to stationarity for the mutation process.

We shall therefore consider the Fleming–Viot particle system for a mutation process $(X_t)_{t \geq 0}$ on a countably infinite space D , subjected to killing with a rate $\lambda : D \rightarrow [0, +\infty)$ which may

depend on the current position of the process, but which grows to $+\infty$ uniformly in the position. Before describing our results, let us mention that such a situation may also be relevant from the population dynamics point of view: for instance, the recent work [91] introduced a coupled PDE/ODE model for collective motion of cells driven by nutrient consumption and showed that in the limit where nutrient consumption is infinitely faster than the motion of cells, the cell distribution forms a Dirac mass whose motion is then determined by the nutrient distribution. The situation may also be compared with the well-known *condensation* phenomenon of zero-range processes with decreasing jump rates [74], although the interaction mechanism between particles is different and, in the present situation, leads to a cluster which concentrates *all* the system's mass, and not only a macroscopic fraction.

While our model is mathematically different, our main results show that in the high-killing regime, the Fleming–Viot particle system exhibits a similar behaviour: all particles concentrate in a single cluster whose evolution remains random and generally depends on both the mutation dynamics and the asymptotic ratio of the killing rates between neighbouring sites. This type of results for Fleming–Viot particle system and related models already appears in [33] (see also reference therein). In this work, it was proved that in the small mutation limit, after a time re-scaling, the empirical measure of a Fleming–Viot particle process on \mathbb{R} converges to a Dirac mass, concentrated on the solution to some ODE. Their proof follows an averaging method developed by Kurtz in [103], different from the one used in our present work, see Section 8.2.

8.1.2 Mathematical setting and notation

8.1.3 Mathematical setting and notation

Let D be a finite or countable set, $q : D \times D \rightarrow \mathbb{R}_+$ and $\lambda : D \rightarrow \mathbb{R}_+$. We suppose that

$$Q := \sup_{x \in D} \sum_{y \in D} q(x, y) < \infty, \quad \sup_{x \in D} \lambda(x) < \infty.$$

We consider the Fleming–Viot n -particle process $\mathbf{X} = (\mathbf{X}_t)_{t \geq 0}$ in D^n for a mutation mechanism with jump rates $q(x, y)$, and a selection mechanism with killing rates $\lambda(x)$. We are interested in the evolution of the empirical measure $\pi(\mathbf{X}_t)$ of the system, where π is defined by:

$$\pi(\mathbf{x}) = \frac{1}{n} \sum_{i=1}^n \delta_{x_i}. \quad (8.1)$$

We write $\mathcal{M}^1(D)$ for the set of probability measures on D and by $\mathcal{M}_n^1(D) \subset \mathcal{M}^1(D)$ the set of empirical measures of n particles in D :

$$\mathcal{M}_n^1(D) = \left\{ \left(\frac{k_x}{n} \right)_{x \in D} \left| \forall x \in D, k_x \in \mathbb{N} \text{ and } \sum_{x \in D} k_x = n \right. \right\}.$$

Let us also introduce the spaces:

$$\ell^1(\mathcal{M}_n^1(D)) = \{u : \mathcal{M}_n^1(D) \rightarrow \mathbb{R}, \|u\|_1 < \infty\}, \quad \|u\|_1 = \sum_{\xi \in \mathcal{M}_n^1(D)} |u(\xi)|,$$

and

$$\ell^\infty(\mathcal{M}_n^1(D)) = \{u : \mathcal{M}_n^1(D) \rightarrow \mathbb{R}, \|u\|_\infty < \infty\}, \quad \|u\|_\infty = \sup_{\xi \in \mathcal{M}_n^1(D)} |u(\xi)|.$$

The empirical measure $(\pi(\mathbf{X}_t))_{t \geq 0}$ of the Fleming-Viot process is a Markov process on the set $\mathcal{M}_n^1(D)$, whose infinitesimal generator L acts on $\ell^\infty(\mathcal{M}_n^1(D))$ and reads

$$L = L_m + L_s,$$

where L_m corresponds to the mutation process: for all $f \in \ell^\infty(\mathcal{M}_n^1(D))$, for all $\xi \in \mathcal{M}_n^1(D)$,

$$L_m f(\xi) = \sum_{x, y \in D} n \xi(x) q(x, y) \left(f \left(\xi + \frac{\delta_y - \delta_x}{n} \right) - f(\xi) \right), \quad (8.2)$$

and L_s corresponds to the selection mechanism: for all $f \in \ell^\infty(\mathcal{M}_n^1(D))$, for all $\xi \in \mathcal{M}_n^1(D)$,

$$L_s f(\xi) = \sum_{x, y \in D} \frac{n^2}{n-1} \xi(x) \lambda(x) \xi(y) \left(f \left(\xi + \frac{\delta_y - \delta_x}{n} \right) - f(\xi) \right).$$

For $u \in \ell^1(\mathcal{M}_n^1(D))$ and $v \in \ell^\infty(\mathcal{M}_n^1(D))$, we define the duality bracket by:

$$\langle u, v \rangle = \sum_{\xi \in \mathcal{M}_n^1(D)} u(\xi) v(\xi).$$

The adjoint operators L^* , L_m^* and L_s^* are defined through this duality bracket and therefore act on $\ell^1(\mathcal{M}_n^1(D))$.

As explained in Section 8.1.1, we are interested here in the high killing regime, namely

$$\inf_D \lambda \rightarrow \infty. \quad (8.3)$$

If the death rates are large with respect to the jump rates and the number of particles, the dynamics of the empirical measure will be dominated by the selection mechanism. If there was only this part, then the empirical measure would become a Dirac measure in finite time. In presence of mutation, and in the limit (8.3), the empirical measure of the Fleming-Viot system will still form a Dirac mass, but this Dirac mass will exhibit some dynamics, in the space

$$\Delta = \{\delta_x, x \in D\} \quad (8.4)$$

of Dirac masses on D .

We present in the next two subsections two results which confirm this intuition, respectively when the number of particles n is fixed, and when the number of particles also tends to infinity together with λ .

8.1.4 Fixed number of particles

In this section, the number of particles n is fixed, and we show that, in the limit (8.3), the trajectories of the empirical process $(\pi(\mathbf{X}_t))_{t \geq 0}$ converge towards trajectories in the set of Dirac measure. This limiting dynamics can be precisely described in terms of a Markov kernel on D .

In order to make precise the limiting regime (8.3), let us consider a family $(\lambda_r)_{r \in \mathbb{N}}$ of functions $D \rightarrow \mathbb{R}_+$, and introduce the notation

$$\underline{\lambda}_r = \inf_{x \in D} \lambda_r(x). \quad (8.5)$$

We set

$$\alpha_{x,y,r} = \frac{\lambda_r(y)}{\lambda_r(x)}, \quad (8.6)$$

and we denote by $\mathbf{X}^r = (\mathbf{X}_t^r)_{t \geq 0}$ the underlying Fleming-Viot n -particle processes. We work in this section in the following setting:

Assumption 8.1.1. *The number n of particles is fixed, $\lim_{r \rightarrow \infty} \underline{\lambda}_r = +\infty$, and for all $x, y \in D$, there exists $\alpha_{x,y,\infty} \in [0, \infty]$ such that:*

$$\lim_{r \rightarrow \infty} \alpha_{x,y,r} = \alpha_{x,y,\infty}. \quad (8.7)$$

As explained in Section 8.1.1, it is expected that $(\pi(\mathbf{X}_t^r))_{t \geq 0}$ converges to a process $(\delta_{Y_t})_{t \geq 0}$ where $(Y_t)_{t \geq 0}$ is a continuous-time Markov chain on D with a jump rate function which is a perturbation of q . Intuitively, the evolution of $(Y_t)_{t \geq 0}$ is driven by the following mechanism. If all the particles are in $x \in D$ at a given time t (i.e. $\bar{Y}_t = x$), then the rate at which one particle goes from x to y is given by $nq(x, y)$. After such a move of one particle from x to y , since the selection mechanism occurs on a much faster time scale than the mutation mechanism, all the particles will concentrate on one of the two states x or y before any other jumps occurs. The probability that a new Dirac mass at y is observed is given by a Gambler's ruin problem, and is equal to $(\alpha_{x,y,r} - 1)/(\alpha_{x,y,r}^n - 1)$ (this is a consequence of Lemma 8.2.6 below). This justifies the introduction of the new jump rates:

$$\tilde{q}_r(x, y) = \begin{cases} nq(x, y) \frac{\alpha_{x,y,r} - 1}{\alpha_{x,y,r}^n - 1} & \text{if } \alpha_{x,y,r} \neq 1, \\ q(x, y) & \text{otherwise,} \end{cases} \quad (8.8)$$

as well as their $r \rightarrow \infty$ limit:

$$\tilde{q}_\infty(x, y) = \begin{cases} nq(x, y) \frac{\alpha_{x,y,\infty} - 1}{\alpha_{x,y,\infty}^n - 1} & \text{if } \alpha_{x,y,\infty} \neq 1, \\ q(x, y) & \text{otherwise.} \end{cases} \quad (8.9)$$

In the above, $\tilde{q}_\infty(x, y) = 0$ in the case $\alpha_{x,y,\infty} = \infty$.

The first theorem concerns the limit of the time-marginal distribution of the empirical measure process under Assumption 8.1.1. For any random variable π in $\mathcal{M}_n^1(D)$, we identify the probability measure $\mathcal{L}aw(\pi)$ as an element of $\ell^1(\mathcal{M}_n^1(D))$ and therefore use the ℓ^1 norm to measure distances between such probability measures.

Theorem 8.1.1. *Under Assumption 8.1.1, for all $\eta \in \mathcal{M}_n^1(D)$, there exists a (deterministic) probability measure $\eta_\infty \in \mathcal{M}^1(D)$ described in Lemma 8.2.3, a random variable Y_0 of law η_∞ , such that if $(Y_t)_{t \geq 0}$ is a Markov process on D with jump rate $(\tilde{q}_\infty(x, y))_{(x,y) \in D}$ and initial condition Y_0 , then: for all $t > 0$,*

$$\lim_{r \rightarrow \infty} \|\mathcal{L}aw(\pi(\mathbf{X}_t^r)) - \mathcal{L}aw(\delta_{Y_t})\|_1 = 0.$$

Moreover, if $\pi(\mathbf{X}_0) = \delta_z$ for some $z \in D$, then for all $T > 0$, there exists $C > 0$ such that if $(Y_t^r)_{t \geq 0}$ is a Markov process on D with jump rate $(\tilde{q}_r(x, y))_{(x,y) \in D}$ and initial condition $Y_0^r = z$, then:

$$\sup_{t \in [0, T]} \|\mathcal{L}aw(\pi(\mathbf{X}_t^r)) - \mathcal{L}aw(\delta_{Y_t^r})\|_1 \leq \frac{C}{\underline{\lambda}_r}.$$

In the first statement of the theorem, the marginal distribution is taken at time $t > 0$. Indeed, if the Fleming-Viot particle system is initialized with a distribution which is not a Dirac distribution, namely with particles spread among several sites, then on the short time scale $1/\lambda_r$, the selection mechanism makes all particles condensate in a single site, whose distribution is precisely the probability measure η_∞ . This shows that, in general, the convergence of $\mathcal{L}aw(\pi(\mathbf{X}_t^r))$ to $\mathcal{L}aw(\delta_{Y_t})$ cannot hold uniformly on $[0, T]$. However, if the initial distribution of the Fleming-Viot particle system is already condensed on a single site, then the second statement of the theorem shows that the distance between $\mathcal{L}aw(\pi(\mathbf{X}_t^r))$ and $\mathcal{L}aw(\delta_{Y_t^r})$ may be controlled uniformly on $[0, T]$, with a quantitative bound which is obtained by using averaging methods, as presented in [144, Chapter 16]. The remaining distance, between $\mathcal{L}aw(\delta_{Y_t^r})$ and $\mathcal{L}aw(\delta_{Y_t})$, also vanishes (see Lemma 8.2.7), with a rate which depends on the convergence of $(\alpha_{x,y,r})_{x,y \in D}$ toward $(\alpha_{x,y,\infty})_{x,y \in D}$. The proof of Theorem 8.1.1 is given in Section 8.2.

We now state a convergence result for the Fleming-Viot particle system towards the Δ -valued dynamics $(\delta_{Y_t})_{t \geq 0}$ in the space of sample paths. For reasons which are detailed below, the Skorohod topologies for cadlag processes is not adapted to this system, and therefore we need to introduce another topology on the space of sample paths. To proceed, we first introduce the total variation norm $\|\cdot\|_{TV}$, and defined by: for $\nu, \mu \in \mathcal{M}^1(D)$,

$$\|\mu - \nu\|_{TV} = \sum_{x \in D} |\mu(x) - \nu(x)|.$$

Note that, since D is a finite or countably infinite set, the weak topology on $\mathcal{M}^1(D)$ is metrized by the total variation norm. Next, for any $T > 0$, let $\mathcal{D}([0, T], \mathcal{M}^1(D))$ be the set of *cadlag* functions from $[0, T]$ to $\mathcal{M}^1(D)$. For $\pi, \tilde{\pi} \in \mathcal{D}([0, T], \mathcal{M}^1(D))$, we define the L_{TV}^1 distance by:

$$\|\pi - \tilde{\pi}\|_{L_{TV}^1} = \int_0^T \|\pi_t(x) - \tilde{\pi}_t(x)\|_{TV} dt = \int_0^T \sum_{x \in D} |\pi_t(x) - \tilde{\pi}_t(x)| dt. \quad (8.10)$$

This defines a distance on $\mathcal{D}([0, T], \mathcal{M}^1(D))$, and the associated topology coincides in our case with the so-called Meyer-Zheng topology [127]. We then have:

Theorem 8.1.2. *Under Assumption 8.1.1, for all $T > 0$, the process $(\pi(\mathbf{X}_t^r))_{t \in [0, T]}$ converges in distribution, in L_{TV}^1 , to the process $(\delta_{Y_t})_{t \in [0, T]}$.*

The proof of this theorem is given in Section 8.3. Let us conclude this section with two remarks. First, due to the nature of the process, the convergence in Theorem 8.1.2 does not hold in the Skorohod topology based on ℓ^∞ norms, but in the L_{TV}^1 topology which is a weaker topology. Indeed, when a particle jumps from x to y , one observes motions from x to y and then back to x due to the selection mechanism, over a time-scale of order $1/\lambda_r$. This implies jumps of non vanishing heights (multiple of $1/n$) in the process $\pi(\mathbf{X}_t^r)$, and therefore, one cannot expect convergence to hold in the Skorohod topology. Second, since the mapping $\pi \in \mathcal{D}([0, T], \mathcal{M}^1(D)) \mapsto \pi_t \in \mathcal{M}^1(D)$ is not continuous with respect to the L_{TV}^1 distance, the convergence in Theorem 8.1.2 does not imply the convergence of the time-marginal distribution from Theorem 8.1.1.

8.1.5 Increasing number of particles

In this section, we are interested in a mean-field limit, namely an asymptotic regime where both the number of particles and the killing rates go to infinity. Therefore, in addition to the r -indexed family $(\lambda_r)_{r \in \mathbb{N}}$ of death rates, we introduce $(n_r)_{r \in \mathbb{N}} \subset \mathbb{N}^{\mathbb{N}}$ a sequence of numbers of particles,

and $(\mathbf{X}_0^r)_{r \in \mathbb{N}}$ a sequence of initial conditions, such that $\mathbf{X}_0^r \in D^{n_r}$. We will again denote by $\mathbf{X}^r = (\mathbf{X}_t^r)_{t \geq 0}$ the associated Fleming-Viot particle processes.

Compared to the previous setting, we restrict ourselves to a situation where $\lambda_r(x)$ is a bounded perturbation of $\underline{\lambda}_r$. In this regime, the quantities $\alpha_{x,y,\infty}$ defined in the previous section are all equal to 1, and therefore the jump rates $\tilde{q}_\infty(x,y)$ in (8.9) are equal to $q(x,y)$ whatever the value of n . As a consequence, letting $n \rightarrow \infty$, one may expect the limiting jump rates to be simply $q(x,y)$, and this will indeed be the case as stated in Theorem 8.1.3 below. Moreover, in order to keep a moving Dirac mass as a limiting process, we impose the rates to go to infinity much faster than the number of particles. Here is the precise setting of this section:

Assumption 8.1.2.

$$\sup_{r \in \mathbb{N}} \sup_{x,y \in D} |\lambda_r(x) - \lambda_r(y)| < \infty, \quad \lim_{r \rightarrow \infty} \frac{\lambda_r}{n_r} = \infty, \quad \text{and} \quad \exists \eta \in \mathcal{M}^1(D), \pi(\mathbf{X}_0^r) \xrightarrow{r \rightarrow \infty} \eta \text{ weakly.}$$

Theorem 8.1.3. *Let us assume that Assumption 8.1.2 holds. Let $(Y_t)_{t \geq 0}$ be a Markov process on D with jump rate $(q(x,y))_{(x,y) \in D}$ and initial condition η . Then, the following convergence in law holds: for all $t > 0$,*

$$\pi(\mathbf{X}_t^r) \xrightarrow{r \rightarrow \infty} \delta_{Y_t},$$

where the convergence in law is considered with respect to the topology defined by the total variation distance on $\mathcal{M}^1(D)$. Moreover, if $\pi(\mathbf{X}_0^r) = \delta_z$ for some $z \in D$ and for all $r \in \mathbb{N}$, then for all $T > 0$, there exists $C > 0$ such that for all $F : \mathcal{M}^1(D) \rightarrow \mathbb{R}$ bounded, and for all $t \in [0, T]$:

$$|\mathbb{E}(F(\pi(\mathbf{X}_t^r))) - \mathbb{E}(F(\delta_{Y_t}))| \leq C \|F\|_\infty \sqrt{\frac{n_r}{\lambda_r}}.$$

The proof is completely different in nature from the one of Theorem 8.1.1, and relies on the Kolmogorov equation associated with the dynamics on $(\pi(\mathbf{X}_t^r))_{t \geq 0}$, see Section 8.4.

Let us conclude this section with a few remarks. First, let us emphasize that if the killing rate is not large enough with respect to the number of particles, then there might not be creation of a Dirac mass. For instance, as already mentioned in Section 8.1.1, in the case $\underline{\lambda}_r = cn_r$, $\pi(\mathbf{X}_t^r)$ converges under a proper rescaling to the Fleming-Viot super-process, see [57]. Second, it is not difficult to check that if D is finite and the initial condition is a Dirac mass, then under Assumption 8.1.2, the convergence is uniform in time. Third, the speed of convergence in Theorem 8.1.3 is not optimal. Indeed, choosing $n_r = n$ constant (which is allowed in Assumption 8.1.2), Theorem 8.1.3 yields a rate of convergence of order $1/\sqrt{\lambda_r}$ whereas we know from Theorem 8.1.1 that it is of order $1/\underline{\lambda}_r$. Fourth, it would be interesting to generalize the results to the more general situation of arbitrary values of $\alpha_{x,y,\infty}$ in (8.7), and also to prove in the setting of this section a convergence result in path space similar to Theorem 8.1.2 (these are left for future work).

8.2 Proof of Theorem 8.1.1

We assume that Assumption 8.1.1 holds in all this section. For all $x \in D$, write:

$$\alpha_r(x) = \frac{\lambda_r(x)}{\underline{\lambda}_r}. \tag{8.11}$$

For all $x \in D$, $\alpha_r(x) \geq 1$, and we write:

$$L = L_m + \underline{\lambda}_r L_0^r, \tag{8.12}$$

where for $f \in \ell^\infty(\mathcal{M}_n^1(D))$ we denoted:

$$L_0^r f(\xi) = \sum_{x,y \in D} \frac{n^2}{n-1} \xi(x) \alpha_r(x) \xi(y) \left(f \left(\xi + \frac{\delta_y - \delta_x}{n} \right) - f(\xi) \right) = \frac{1}{\underline{\lambda}_r} L_s f(\xi).$$

For simplicity, we drop the dependence in r of L_0^r and we simply write L_0 .

The proof of Proposition 8.1.1 uses averaging methods [144, Chapter 16]. Let us first present the overall idea. Recall the notation (8.1) for the empirical measure. Denote for all $t \geq 0$ and $z \in D$

$$\pi_t(z) = \pi(\mathbf{X}_t^r)(z), \quad (8.13)$$

and let u be the law of the empirical measure process $(\pi_t)_{t \geq 0}$:

$$u(t, \xi) = \mathbb{P}(\pi_t = \xi), \quad \forall \xi \in \mathcal{M}_n^1(D).$$

For all $t \geq 0$, $u(t, \cdot) \in \ell^1(\mathcal{M}_n^1(D))$, and we have the Kolmogorov equation:

$$\partial_t u = L^* u,$$

where L^* denotes the adjoint of the generator L , and acts on $\ell^1(\mathcal{M}_n^1(D))$.

Let us present a formal argument in order to identify the limiting dynamics. If we assume an expansion of the form

$$u = u_0 + \frac{1}{\underline{\lambda}_r} u_1 + o\left(\frac{1}{\underline{\lambda}_r}\right),$$

with $\|u_0\|_1$ and $\|u_1\|_1$ bounded uniformly in $r \in \mathbb{N}$ and $t \geq 0$, then, using (8.12), a formal identification at order $(\underline{\lambda}_r)^{-1}$ yields that u_0 satisfies

$$L_0^* u_0 = 0,$$

which shows that one expects the limiting dynamics to only take Dirac mass values. Indeed, for all $r \in \mathbb{N}$, L_0 is the generator of a Markov process that corresponds to a Fleming-Viot process with no mutation mechanism and only selection dynamics. We will refer in the sequel to this dynamics as the selection dynamics. Under this dynamics, each particle of the Fleming-Viot process is killed at rate α_r , and then branches uniformly at random over the surviving particles. Let $(\pi_t^0)_{t \geq 0}$ be a Markov process with this generator L_0 . Every Dirac measure is an absorbing point of such dynamics, and thus $\text{Span}(\{\mathbb{1}_x, x \in D\}) \subset \text{Ker} L_0^*$, where

$$\mathbb{1}_x = \delta_{\delta_x} \quad (8.14)$$

is a probability measure on $\mathcal{M}_n^1(D)$, and can also be seen as an element of $\ell^1(\mathcal{M}_n^1(D))$. Actually, writing (remember the notation (8.4))

$$\tau = \inf \{t \geq 0, \pi_t^0 \in \Delta\}, \quad (8.15)$$

we will show that $\tau < \infty$ almost surely (as an application of Lemma 8.2.1 below), and this will allow us to prove that, as a bounded operator from $\ell^1(\mathcal{M}_n^1(D))$ to itself, L_0^* satisfies

$$\overline{\text{Span}(\{\mathbb{1}_x, x \in D\})} = \text{Ker} L_0^*,$$

see Lemma 8.2.4.

We will then postulate the limiting dynamics on u_0 using our intuition on how Dirac masses

evolve. Let us recall the intuition to derive these limiting dynamics: if the Dirac mass is at $x \in D$, at rate $nq(x, y)$ one particle will go from x to y . Since the selection dynamics is on a much faster time scale, we only have to consider this part of the dynamics, and the probability that the Dirac mass goes from x to y is given by the probability $p_{x,y}$ of a Gambler's ruin, see Lemma 8.2.6. Therefore, the rates at which the Dirac mass will move from x to y is simply $nq(x, y)p_{x,y}$.

To formalize this reasoning, after having introduced u_0 following the expected limiting dynamics described above, we will define u_1 as a solution to the Poisson equation

$$\partial_t u_0 - L_m^* u_0 = L_0^* u_1 \quad (8.16)$$

which is the equation formally obtained at order $(\lambda_r)^0$. The proof will then consist in proving that

$$u - u_0 - \frac{1}{\lambda_r} u_1$$

goes to 0 as $r \rightarrow \infty$.

8.2.1 A time-scale separation result

In the selection/mutation mechanism, there exists a cascade of time-scales. The largest time scale is the mutation one, which is independent of $r \in \mathbb{N}$. Besides, we may define an equivalence relation on D by $x \sim y$ if and only if $0 < \alpha_{x,y,\infty} < \infty$. Then, each equivalence class associated with this equivalence relation gives a different time scale, as, if $\alpha_{x,y,\infty} = \infty$, then all particles in y will jump away from y to go to a site with a lower death rate before any particle in x have time to jump or move, with probability going to 1 as r goes to infinity. Lemma 8.2.1 below describes this phenomenon, and is a cornerstone in the proofs of the results under Assumption 8.1.1. In particular, if at a given time, the empirical process is not a Dirac mass, it will give us information on the time taken by the process to reach the set of Dirac measures and on how the particles will be redistributed to form a Dirac mass.

Lemma 8.2.1. *Let $L_r = a_r L_r^1 + b_r L_r^2$ be a jump Markov process generator on the state space $\mathcal{M}_n^1(D)$, such that L_r^1 is a selection dynamics with partial rates:*

$$\forall f \in l^\infty(\mathcal{M}_n^1(D)), L_r^1 f(\eta) = \sum_{x \in \Theta, y \in D} \frac{n^2}{n-1} \eta(x) \gamma_r(x) \eta(y) \left(f \left(\eta + \frac{\delta_y - \delta_x}{n} \right) - f(\eta) \right),$$

for some $\Theta \subset D$ and $\gamma_r \geq 1$, and such that the coefficient of L_r^2 are bounded from above in r :

$$\forall f \in l^\infty(\mathcal{M}_n^1(D)), L_r^2 f(\eta) = \sum_{\xi \in \mathcal{M}_n^1(D)} \beta_r^2(\eta, \xi) (f(\xi) - f(\eta)), \quad \sum_{\xi \in \mathcal{M}_n^1(D)} \beta_r^2(\eta, \xi) \leq \bar{\mu},$$

for some $\bar{\mu} > 0$ and all $\eta \in \mathcal{M}_n^1(D)$. Let us assume that

$$\lim_{r \rightarrow \infty} \frac{b_r}{a_r} = 0,$$

and let us introduce $c_r > 0$ such that

$$\lim_{r \rightarrow \infty} \frac{c_r}{a_r} = \lim_{r \rightarrow \infty} \frac{b_r}{c_r} = 0.$$

Write

$$\mathbb{M}^1 = \{ \xi \in \mathcal{M}_n^1(D), L_r^1 f(\xi) = 0, \forall f \in l^\infty(\mathcal{M}_n^1(D)), \forall r \in \mathbb{N} \},$$

and

$$\tau_1^r = \inf \{ t \geq 0, \tilde{\pi}_t^r \in \mathbb{M}^1 \},$$

where $\tilde{\pi}^r$ is a Markov process with generator L_r . Denote by S_1 the first jump of the process coming from the $b_r L_r^2$ part of the generator. Then the following holds:

$$\lim_{r \rightarrow \infty} \inf_{\xi \in \mathcal{M}_n^1(D)} \mathbb{P}_\xi (\tau_1^r < c_r^{-1} < S_1) = 1. \quad (8.17)$$

Moreover, if $L_r^2 = 0$, then there exist $C, c > 0$ such that

$$\sup_{r \in \mathbb{N}} \sup_{\xi \in \mathcal{M}_n^1(D)} \mathbb{P}_\xi (\tau_1^r \geq t) \leq C e^{-c a_r t}. \quad (8.18)$$

This lemma will be applied to the Fleming-Viot generator (8.12), either with $\Theta = D$ or with Θ a subset of D such that the killing rates on Θ are much greater than the ones on $D \setminus \Theta$, in the sense that for all $x \in \Theta, y \notin \Theta, \alpha_{x,y,\infty} = 0$. In the latter case, the set \mathbb{M}^1 contains the Dirac measures, as well as the empirical measures of n particles with support in $D \setminus \Theta$.

Proof. Let $\bar{\pi}$ be a Markov process with generator L_r^1 , defined using the same jump events as $\tilde{\pi}$, and

$$\bar{\tau}_1^r = \inf \{ t \geq 0, \bar{\pi}_t^r \in \mathbb{M}^1 \}.$$

On the event $\tau_1^r < S_1$, we have $\tau_1^r = a_r^{-1} \bar{\tau}_1^r$. Let us show that there exist $C, c > 0$ such that

$$\sup_{r \in \mathbb{N}} \sup_{\xi \in \mathcal{M}_n^1(D)} \mathbb{P}_\xi (\bar{\tau}_1^r \geq t) \leq C e^{-c t}. \quad (8.19)$$

Fix $\xi \in \mathcal{M}_n^1(D)$, write $D_0 = \text{supp}(\xi)$ and

$$\underline{\gamma}_r = \min \{ \gamma_r(x), x \in D_0 \cap \Theta \}.$$

Since $\gamma_r(x) \geq 1$ for all $x \in D$, $\underline{\gamma}_r \geq 1$ for all $r \in \mathbb{N}$. Let $\underline{x}_r \in D$ be such that $\underline{\gamma}_r = \gamma_r(\underline{x}_r)$ if $D_0 \subset \Theta$, and let $\underline{x}_r \in D_0 \setminus \Theta$ otherwise. Let \mathbf{X} be a process whose empirical measure is given by $\bar{\pi}$, and let $i_0 \in \llbracket 1, n \rrbracket$ be such that $X_0^{i_0} = \underline{x}_r$. Denote

$$I = \{ i, X_0^i \in D_0 \setminus \Theta \} \cup \{ i_0 \}, \quad n_0 = |I \setminus \{ i_0 \}|,$$

and write:

$$\mathcal{A}_r = \left\{ \text{On } [0, 1/\underline{\gamma}_r], X^i, i \in I, \text{ do not die, and all other die once and branch on } X^{i_0} \right\}.$$

We have that $\mathcal{A}_r \subset \{ \bar{\tau}_1^r < 1 \}$. Since the number of death events for $(X_s^i)_{0 \leq s \leq 1/\underline{\gamma}_r}$ is upper (resp. lower) bounded by a Poisson random variable with parameter $\underline{\gamma}_r$ if $i \in I$ (resp. $i \notin I$), we have that:

$$\mathbb{P}_\xi (\mathcal{A}_r) \geq \frac{e^{-n} (1 - e^{-1})^{n-n_0}}{n^{n-n_0}},$$

and hence, we get that

$$\inf_{r \in \mathbb{N}} \inf_{\xi \in \mathcal{M}_n^1(D)} \mathbb{P}_\xi (\bar{\tau}_1^r < 1) \geq 1 - \omega,$$

for some $\omega \in [0, 1)$. Using the Markov property at time $t - 1$, this implies that for all $r \in \mathbb{N}$, $\xi \in \mathcal{M}_n^1(D)$, and $t \geq 1$:

$$\mathbb{P}_\xi(\bar{\tau}_1^r \geq t) \leq \omega \mathbb{P}_\xi(\bar{\tau}_1^r \geq t - 1),$$

and this implies

$$\sup_{r \in \mathbb{N}} \sup_{\xi \in \mathcal{M}_n^1(D)} \mathbb{P}_\xi(\bar{\tau}_1^r > t) \leq \omega^{\lfloor t \rfloor} \leq C e^{-ct},$$

with $c = -\ln(\omega) > 0$ and $C = \omega^{-1}$.

Writing $\beta_r^2(\eta) = \sum_{\xi \in \mathcal{M}_n^1(D)} \beta_r^2(\eta, \xi)$, S_1 is defined as:

$$S_1 = \inf \left\{ t \geq 0, E_1 \leq \int_0^t b_r \beta_r^2(\bar{\pi}_s^r) ds \right\} \geq \inf \{ t \geq 0, E_1 \leq b_r \bar{\mu} t \} = b_r^{-1} \tilde{S}_1,$$

where E_1 is an exponential random variable with parameter 1. Hence, S_1 is bounded from below by $b_r^{-1} \tilde{S}_1$, where \tilde{S}_1 is an exponential random variable with parameter $\bar{\mu}$. Finally, using the bound (8.19) we have:

$$\begin{aligned} \mathbb{P}(\tau_1^r < c_r^{-1} < S_1) &= \mathbb{P}(a_r^{-1} \bar{\tau}_1^r < c_r^{-1} < S_1) \\ &\geq 1 - \mathbb{P}\left(\bar{\tau}_1^r \geq \frac{a_r}{c_r}\right) - \mathbb{P}(S_1 < c_r^{-1}) \\ &\geq 1 - \mathbb{P}\left(\bar{\tau}_1^r \geq \frac{a_r}{c_r}\right) - \mathbb{P}\left(\tilde{S}_1 < \frac{b_r}{c_r}\right) \xrightarrow{r \rightarrow \infty} 1, \end{aligned}$$

and hence the limit (8.17). In the case where $L_r^2 = 0$, Equation (8.19) yields:

$$\mathbb{P}_\xi(\tau_1^r \geq t) = \mathbb{P}_\xi(\bar{\tau}_1^r \geq a_r t) \leq C e^{-ca_r t},$$

which concludes the proof. \square

8.2.2 The initial condition

Now, we aim to address the issue of the initial condition. Given some initial condition $\eta \in \mathcal{M}_n^1(D)$, write $D_0 = \text{supp}(\eta)$, where

$$\text{supp}(\eta) = \{x \in D, \eta(x) > 0\},$$

and

$$\Lambda = \left\{ x \in D_0, \min_{y \in D_0} \alpha_{x,y,\infty} > 0 \right\}. \quad (8.20)$$

This set Λ correspond to the subset of D_0 where, asymptotically in r , the order of magnitude of the killing rate is minimal. Thanks to Lemma 8.2.1, we will be able to show that in the limit (8.3), all particles from $D_0 \setminus \Lambda$ will be redistributed instantaneously (ie on a time scale faster than $1/\inf_{D_0} \lambda_r$) in Λ , with no movement from the particles in Λ . Moreover, the law of the configuration obtained in Λ after this instantaneous redistribution is given by a Polya's urn problem, with $|\Lambda|$ possible colors and initial condition $n\eta|_\Lambda$, after $n\eta(D_0 \setminus \Lambda)$ draws. On the time scale $1/\inf_{D_0} \lambda_r$, this measure will then form a Dirac mass according to the probability given by commitor functions, that we are now going to define.

Recall that π^0 denotes a Markov process with generator L_0 , and the definition (8.15) of τ . Let us apply Lemma 8.2.1, with $L_r^2 = 0$, $a_r = 1$, $\Theta = \text{supp}(\pi_0^0)$, $\gamma_r = \alpha_r$, so that $L_r^1 = L_0$ and

$\tau_r^1 = \tau$. Equation (8.18) then yields that $\tau < \infty$ almost surely. Denote for $\eta \in \mathcal{M}_n^1(D)$:

$$\psi_x^r(\eta) = \mathbb{P}_\eta(\pi_\tau^0 = \delta_x). \quad (8.21)$$

The functions ψ_x^r are the so called committor functions, and [140, Theorem 3.3.1.] yields that they satisfy:

$$\psi_x^r(\delta_x) = 1, \psi_x^r(\delta_y) = 0 \forall y \neq x, L_0 \psi_x^r(\xi) = 0, \forall \xi \in \mathcal{M}_n^1(D) \setminus \Delta. \quad (8.22)$$

Remark that for all $\xi \in \Delta$, $f \in \ell^\infty(\mathcal{M}_n^1(D))$, $L_0 f(\xi) = 0$, so that we actually have $L_0 \psi_x^r(\xi) = 0$, for all $\xi \in \mathcal{M}_n^1(D)$. The next lemma proves that the committor functions are the unique solution to (8.22) in $\ell^\infty(\mathcal{M}_n^1(D))$.

Lemma 8.2.2. *Let $\Theta \subset D$ and $\gamma : \Theta \rightarrow [1, +\infty)$. Let L^1 be defined by: $\forall f \in \ell^\infty(\mathcal{M}_n^1(\Theta))$,*

$$L^1 f(\eta) = \sum_{x, y \in \Theta} \frac{n^2}{n-1} \eta(x) \gamma(x) \eta(y) \left(f\left(\eta + \frac{\delta_y - \delta_x}{n}\right) - f(\eta) \right).$$

For all $x \in \Theta$, if $f \in \ell^\infty(\mathcal{M}_n^1(\Theta))$ satisfies

$$f(\delta_x) = 1, f(\delta_y) = 0 \forall y \neq x, L^1 f(\xi) = 0, \forall \xi \in \mathcal{M}_n^1(\Theta) \setminus \Delta, \quad (8.23)$$

then for all $\xi \in \mathcal{M}_n^1(\Theta)$

$$f(\xi) = \mathbb{P}_\xi(\pi_{\tau_1}^1 = \delta_x),$$

where $\tau_1 = \inf\{t \geq 0, \pi_t^1 \in \Delta\}$ and π^1 is a Markov process with generator L^1 and values in $\mathcal{M}_n^1(\Theta)$.

In particular, ψ_x^r defined by (8.21) are the unique solution to (8.22) in $\ell^\infty(\mathcal{M}_n^1(D))$.

Proof. Let f be a solution to Equation (8.23). Let $\xi \in \mathcal{M}_n^1(\Theta)$ and π^1 be a Markov process with generator L^1 and initial condition ξ . The map $t \mapsto f(\pi_{\tau_1 \wedge t}^1)$ is a martingale, and hence for all $t \geq 0$,

$$\mathbb{E}_\xi(f(\pi_{\tau_1 \wedge t}^1)) = f(\xi). \quad (8.24)$$

Equation (8.18) from Lemma 8.2.1 yields that $\tau_1 < \infty$ almost surely, and since f is bounded, letting t go to infinity in (8.24) yields that $f(\xi) = \mathbb{P}_\xi(\pi_{\tau_1}^1 = \delta_x)$. \square

We are now able to prove

Lemma 8.2.3. *For all $\eta \in \mathcal{M}_n^1(D)$, there exists $\eta_\infty \in \mathcal{M}^1(D)$ such that if π^0 is a Markov process with generator L^0 and initial condition η , and Y_0 is a random variable with law η_∞ , then*

$$\lim_{r \rightarrow \infty} \|\mathcal{L}aw(\pi_\tau^0) - \mathcal{L}aw(\delta_{Y_0})\|_{TV} = 0.$$

In the statement of Theorem 8.1.1, η_∞ is the law of the initial condition Y_0 .

Proof. Fix $\eta \in \mathcal{M}_n^1(D)$ and write $\bar{\eta}_r = \mathcal{L}aw(\pi_\tau^0) \in \mathcal{M}^1(\Delta)$. Denote $D_0(\eta) = \text{supp}(\eta)$ and

$$\underline{\alpha}_r = \inf_{x \in D_0} \alpha_r(x),$$

where $\alpha_r(x)$ is defined in (8.11). Recall the definition of Λ from (8.20). We distinguish two cases: if $\Lambda = D_0$, then we can find the limit of $\bar{\eta}_r$ when $r \rightarrow \infty$ using the fact that $\bar{\eta}_r(\delta_x) = \psi_x^r(\eta)$ and

that $(\psi_x^r(\eta))_{\eta \in \mathcal{M}_n^1(\Lambda)}$ is the unique solution to a Dirichlet equation on a finite set. If $\Lambda \neq D_0$, then using Lemma 8.2.1, we show that all particles from $D_0 \setminus \Lambda$ will first be distributed on Λ , without any particles from Λ moving, and then we can apply the argument from the case $D_0 = \Lambda$.

Let us suppose that $\Lambda = D_0$. Write $L_0^{D_0, r}$ the re-normalised generator of the selection dynamics

$$L_0^{D_0, r} f(\xi) = \sum_{x, y \in D_0} \frac{\alpha_r(x)}{\alpha_r} \xi(x) \xi(y) \left(f \left(\xi + \frac{\delta_y - \delta_x}{n} \right) - f(\xi) \right),$$

defined for $f : \mathcal{M}_n^1(D_0) \rightarrow \mathbb{R}$. Denote also

$$\alpha_{D_0, \infty}(x) = \lim_{r \rightarrow \infty} \alpha_r(x) / \alpha_r = \frac{1}{\min_{y \in D_0} \alpha_{x, y, \infty}},$$

which is well defined and lies in $[1, \infty)$ in the case $D_0 = \Lambda$, as well as

$$L_0^{D_0, \infty} f(\xi) = \sum_{x, y \in D_0} \alpha_{D_0, \infty}(x) \xi(x) \xi(y) \left(f \left(\xi + \frac{\delta_y - \delta_x}{n} \right) - f(\xi) \right).$$

$L_0^{D_0, \infty}$ is the generator of a selection dynamics with death rates α_{∞, D_0} . We have that

$$\bar{\eta}_r(\delta_x) = \psi_x^r(\eta),$$

and for all $x \in D_0$ and $\xi \in \mathcal{M}_n^1(D_0)$,

$$L_0^{D_0, r} \psi_x^r(\xi) = 0. \tag{8.25}$$

Since $D_0 \times \mathcal{M}_n^1(D_0)$ is a finite set, we may consider $(\psi_x^\infty(\xi))_{x \in D_0, \xi \in \mathcal{M}_n^1(D_0)}$ a sub-sequential limit of $(\psi_x^r(\xi))_{x \in D_0, \xi \in \mathcal{M}_n^1(D_0)}$. Passing to the limit in equation (8.25), we get that for all $x \in D_0$ and $\xi \in \mathcal{M}_n^1(D_0)$:

$$L_0^{D_0, \infty} \psi_x^\infty(\xi) = 0,$$

as well as $\psi_x^\infty(\delta_y) = \mathbb{1}_{x \neq y}$. Lemma 8.2.2 then implies that

$$\psi_x^\infty(\xi) = \mathbb{P}_\xi (\pi_\tau^{0, \infty} = \delta_x),$$

where $\pi^{0, \infty}$ is a Markov process with generator $L_0^{D_0, \infty}$. Hence there is a unique sub-sequential limit, and $\psi_x^r(\xi)$ converge for all $\xi \in \mathcal{M}_n^1(D_0)$ and $x \in D_0$, and this is particularly true for $\xi = \eta$.

We now suppose that $\Lambda \neq D_0$. In this case, for all $x \in D_0 \setminus \Lambda$, $\alpha_{D_0, \infty} = \infty$ and $L_0^{D_0, \infty}$ is ill-defined. To resort to the previous case, write

$$S_1^\Lambda = \inf \{t \geq 0, \text{ one particle starting from } \Lambda \text{ dies}\},$$

and

$$\tau_{\mathcal{M}_n^1(\Lambda)} = \inf \{t \geq 0, \pi_t^0 \in \mathcal{M}_n^1(\Lambda)\}.$$

Using the notation of Lemma 8.2.1, write

$$\Theta = D_0 \setminus \Lambda, \quad a_r = \inf \{\alpha_r(x) / \alpha_r, x \in D_0 \setminus \Lambda\}, \quad b_r = 1, \quad L_r^2 = L_0^{D_0, r}.$$

In this case, we have $\mathbb{M}^1 = \Delta \cup \mathcal{M}_n^1(\Lambda)$, and because $\Lambda \neq D_0$, $a_r \xrightarrow{r \rightarrow \infty} \infty$, and Lemma 8.2.1

(with $c_r = \sqrt{a_r}$) yields that:

$$\lim_{r \rightarrow \infty} \mathbb{P}_\eta (S_1^\Lambda \leq \tau_{\mathcal{M}_n^1(\Lambda)}) = 0.$$

Now, using the strong Markov property at time $\tau_{\mathcal{M}_n^1(\Lambda)}$, write:

$$\mathbb{P}_\eta (\pi_\tau^0 = \delta_x) = \sum_{\xi \in \mathcal{M}_n^1(\Lambda)} \mathbb{P}_\eta (S_1^\Lambda > \tau_{\mathcal{M}_n^1(\Lambda)}) \mathbb{P}_\eta \left(\pi_{\tau_{\mathcal{M}_n^1(\Lambda)}}^0 = \xi \mid S_1^\Lambda > \tau_{\mathcal{M}_n^1(\Lambda)} \right) \mathbb{P}_\xi (\pi_\tau^0 = \delta_x) + R_r,$$

where a rest satisfying

$$R_r \leq \mathbb{P}_\eta (S_1^\Lambda \leq \tau_{\mathcal{M}_n^1(\Lambda)}) \xrightarrow{r \rightarrow \infty} 0.$$

From the case $D_0 = \Lambda$ we get that for all $\xi \in \mathcal{M}_n^1(\Lambda)$, $\mathbb{P}_\xi (\pi_\tau^0 = \delta_x)$ admits a limit as r goes to infinity. In addition,

$$\mathbb{P}_\eta \left(\pi_{\tau_{\mathcal{M}_n^1(\Lambda)}}^0 = \pi \mid S_1^\Lambda > \tau_{\mathcal{M}_n^1(\Lambda)} \right)$$

corresponds to the law of a Polya urn Markov chain with with color indexed by Λ , initial condition $n\eta|_\Lambda$, after $|D_0 \setminus \Lambda|$ draws, and is hence independent of r . This concludes the convergence of $\mathbb{P}_\eta (\pi_\tau^0 = \delta_x)$ towards some $\bar{\eta}_\infty \in \mathcal{M}^1(\Delta)$. If $Y_0 \in D$ is such that $\mathcal{L}aw(\delta_{Y_0}) = \bar{\eta}_\infty$, η_∞ is then the law of Y_0 . \square

8.2.3 The Poisson equation

Let us now consider the Poisson equation (8.16). Before showing existence and uniqueness of a solution to this equation, let us describe the kernel of L_0^* and L_0 . Although this is not strictly necessary for the proof of Theorem 8.1.1, this makes the functional setting clearer. To proceed, let us recall that L_0 is defined as an operator of $\ell^\infty(\mathcal{M}_n^1(D))$, and L_0^* as an operator of $l^1(\mathcal{M}_n^1(D))$. Define the weak-* topology on $\ell^\infty(\mathcal{M}_n^1(D))$ by the fact that a sequence of elements $(w_k)_{k \geq 1}$ weak-* converges to w if $\langle v, w_k \rangle \rightarrow \langle v, w \rangle$ for any $v \in l^1(\mathcal{M}_n^1(D))$. Then $l^1(\mathcal{M}_n^1(D))$ equipped with the (strong) topology induced by the norm $\|\cdot\|_1$, and $\ell^\infty(\mathcal{M}_n^1(D))$ equipped with the weak-* topology, are each other's topological dual. Let us now write

$$(\text{Ker}L_0)^\perp = \{v \in l^1(\mathcal{M}_n^1(D)), \langle v, w \rangle = 0, \forall w \in \text{Ker}L_0\},$$

recall the definition of the commitor functions from (8.21), and denote by \bar{A} the closure of a set A for the topology at hand.

Lemma 8.2.4. *We have*

$$(\text{Ker}L_0)^\perp = \{v \in l^1(\mathcal{M}_n^1(D)), \langle v, \psi_x^r \rangle = 0, \forall x \in D\},$$

as well as

$$\overline{\text{Span}(\mathbb{1}_x, x \in D)} = \text{Ker}L_0^*.$$

However, the inclusion

$$\text{Span}(\psi_x, x \in D) \subset \text{Ker}L_0$$

is strict if D is infinite, and the kernel of L_0 is given by

$$\overline{\text{Span}(\psi_x, x \in D)}^{w*} = \text{Ker}L_0,$$

where \bar{A}^{w*} denotes the closure for the weak-* topology of a set $A \subset \ell^\infty(\mathcal{M}_n^1(D))$.

Proof. For all $x \in D$, Lemma 8.2.2 yields that $\psi_x^r \in \text{Ker}L_0$, so that:

$$(\text{Ker}L_0)^\perp \subset \{v \in \ell^1(\mathcal{M}_n^1(D)), \langle v, \psi_x^r \rangle = 0, \forall x \in D\}.$$

Let $v \in \ell^1(\mathcal{M}_n^1(D))$ such that $\langle v, \psi_x^r \rangle = 0$ for all $x \in D$, and $w \in \text{Ker}L_0$ (and thus $w \in \ell^\infty(\mathcal{M}_n^1(D))$). The map $t \mapsto w(\pi_{t \wedge \tau}^0)$ is a martingale, and hence for all $t \geq 0$,

$$w(\xi) = \mathbb{E}_\xi(w(\pi_{\tau \wedge t}^0)).$$

Since w is bounded, and $\tau < \infty$ almost surely, letting t go to infinity and the dominated convergence theorem yields that for all $\xi \in \mathcal{M}_n^1(D)$:

$$w(\xi) = \sum_{x \in D} w(\delta_x) \psi_x(\xi), \quad (8.26)$$

and the sum is actually finite because $\psi_x(\xi) = 0$ if $x \notin \text{supp}(\xi)$. We have:

$$\sum_{\xi \in \mathcal{M}_n^1(D)} \sum_{x \in D} |w(\delta_x) v(\xi) \psi_x(\xi)| = \sum_{\xi \in \mathcal{M}_n^1(D)} |v(\xi)| \sum_{x \in D} |w(\delta_x) \psi_x^r(\xi)| \leq \|v\|_1 \|w\|_\infty < \infty.$$

Hence, the following computation holds:

$$\langle v, w \rangle = \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \sum_{x \in D} w(\delta_x) \psi_x(\xi) = \sum_{x \in D} w(\delta_x) \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \psi_x(\xi) = \sum_{x \in D} w(\delta_x) \langle v, \psi_x^r \rangle = 0,$$

which yields that $v \in (\text{Ker}L_0)^\perp$, and concludes the first point.

We already saw in the introduction of Section 8.2 that $\text{Span}(\mathbb{1}_x, x \in D) \subset \text{Ker}L_0^*$. Since L_0^* is a bounded operator, $\text{Ker}L_0^*$ is closed and

$$\overline{\text{Span}(\mathbb{1}_x, x \in D)} \subset \text{Ker}L_0^*.$$

For $v \in \text{Ker}L_0^*$, the map

$$t \mapsto \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \mathbb{P}_\xi(\pi_t^0 = \eta)$$

is constant for all $\eta \in \mathcal{M}_n^1(D)$. Write for all $\eta \in \mathcal{M}_n^1(D)$:

$$\begin{aligned} \mathbb{P}_\xi(\pi_s^0 = \eta) - \mathbb{P}_\xi(\pi_\tau^0 = \eta) &= \mathbb{P}_\xi(\pi_s^0 = \eta, \tau > s) + \mathbb{P}_\xi(\pi_s^0 = \eta, \tau < s) - \mathbb{P}_\xi(\pi_\tau^0 = \eta) \\ &= \mathbb{P}_\xi(\pi_s^0 = \eta, \tau > s) - \mathbb{P}_\xi(\pi_\tau^0 = \eta, \tau > s), \end{aligned}$$

which yields

$$\sum_{\eta \in \mathcal{M}_n^1(D)} |\mathbb{P}_\xi(\pi_s^0 = \eta) - \mathbb{P}_\xi(\pi_\tau^0 = \eta)| \leq 2\mathbb{P}_\xi(\tau > s). \quad (8.27)$$

Using the notations of Lemma 8.2.1, write:

$$\Theta = D, \quad a_r = 1, \quad \gamma_r = \alpha_r, \quad L_r^2 = 0.$$

Lemma 8.2.1 then yields that there exist $C, c > 0$ such that for all $s \geq 0$

$$\sup_{r \in \mathbb{N}} \sup_{\xi \in \mathcal{M}_n^1(D)} \mathbb{P}_\xi(\tau > s) \leq C e^{-cs}. \quad (8.28)$$

The bound (8.27) and (8.28) yields that we may let t go to infinity and get:

$$v = \sum_{x \in D} v(\delta_x) \mathbb{1}_x.$$

Since this sum converges in $l^1(\mathcal{M}_n^1(D))$ as soon as $v \in l^1(\mathcal{M}_n^1(D))$, $v \in \overline{\text{Span}(\mathbb{1}_x, x \in D)}$, which concludes the second point.

Define for all $\xi \in \mathcal{M}_n^1(D)$,

$$f(\xi) = \sum_{x \in D} \psi_x(\xi).$$

In this sum, there are at most n non-vanishing terms, and thus $f \in \ell^\infty(\mathcal{M}_n^1(D))$. It is easily seen that $L_0 f = 0$. If $g = \sum_{x \in D_0} a_x \psi_x(\xi)$ for some finite subset $D_0 \subset D$ and $a_x \in \mathbb{R}$, we have that $\|f - g\|_\infty \geq 1$, yielding that

$$f \in \text{Ker} L_0 \setminus \overline{\text{Span}(\mathbb{1}_x, x \in D)}.$$

However, for all $w \in \text{Ker} L_0$, the sum (8.26) converges for the weak-* topology, which proves the last point. \square

We are now ready to solve the Poisson equation (8.16), which relies on the next statement. For any $v \in \ell^1(\mathcal{M}_n^1(D))$ and $s \geq 0$, let us introduce the notation

$$ve^{sL_0}(\eta) = \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \mathbb{P}_\xi(\pi_s^0 = \eta), \quad (8.29)$$

which defines an element of $\ell^1(\mathcal{M}_n^1(D))$.

Lemma 8.2.5. *For all $v \in (\text{Ker} L_0)^\perp (\subset \ell^1(\mathcal{M}_n^1(D)))$, there exists a unique $w \in (\text{Ker} L_0)^\perp$ such that*

$$L_0^* w = v, \quad (8.30)$$

given by:

$$w = - \int_0^\infty ve^{sL_0} ds.$$

Moreover, there exists $C > 0$ independent of r and v such that

$$\|w\|_1 \leq C \|v\|_1.$$

Proof. Let us start with the existence. Write, for $\eta \in \mathcal{M}_n^1(D)$

$$w(\eta) = - \left(\int_0^\infty ve^{sL_0} ds \right) (\eta) = - \int_0^\infty \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \mathbb{P}_\xi(\pi_s^0 = \eta) ds.$$

We first show that w is well-defined. Recall the stopping time τ defined in (8.15). Since $v \in (\text{Ker} L_0)^\perp$, Lemma 8.2.4 yields that $\langle v, \psi_x^r \rangle = 0$ for all $x \in D$, and we have

$$\sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \mathbb{P}_\xi(\pi_\tau^0 = \delta_x) = \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \psi_x^r(\xi) = 0.$$

Since, if $\eta \notin \Delta$, $\mathbb{P}_\xi(\pi_\tau^0 = \eta) = 0$, we have that

$$\sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \mathbb{P}_\xi(\pi_s^0 = \eta) = \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) (\mathbb{P}_\xi(\pi_s^0 = \eta) - \mathbb{P}_\xi(\pi_\tau^0 = \eta)).$$

The bounds (8.27) and (8.28) imply that w is well-defined, because $v \in \ell^1(\mathcal{M}_n^1(D))$, and we have

$$\|w\|_1 \leq 2C \int_0^\infty e^{-cs} ds \|v\|_1 = \frac{2C}{c} \|v\|_1.$$

The Kolmogorov equations yield that $L_0^* \mathbb{P}_\xi(\pi_s^0 = \cdot) = \partial_s \mathbb{P}_\xi(\pi_s^0 = \cdot)$, and hence for all $\eta \in \mathcal{M}_n^1(D)$:

$$\begin{aligned} L_0^* w(\eta) &= - \int_0^\infty \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) L_0^* \mathbb{P}_\xi(\pi_s^0 = \cdot)(\eta) ds \\ &= - \int_0^\infty \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \partial_s \mathbb{P}_\xi(\pi_s^0 = \eta) ds \\ &= - \int_0^\infty \partial_s \left(\sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \mathbb{P}_\xi(\pi_s^0 = \eta) \right) ds. \end{aligned}$$

We already saw that

$$\lim_{s \rightarrow \infty} \sum_{\xi \in \mathcal{M}_n^1(D)} v(\xi) \mathbb{P}_\xi(\pi_s^0 = \eta) = 0,$$

and hence $L_0^* w(\eta) = v(\eta)$, which concludes the existence.

To prove uniqueness, fix $w \in \text{Ker} L_0^* \cap (\text{Ker} L_0)^\perp$. The fact that $L_0^* w = 0$ yields that for all $\eta \in \mathcal{M}_n^1(D)$, $t \geq 0$:

$$w(\eta) = \sum_{\xi \in \mathcal{M}_n^1(D)} w(\xi) \mathbb{P}_\xi(\pi_t^0 = \eta).$$

Letting $t \rightarrow \infty$, because $w \in \ell^1(\mathcal{M}_n^1(D))$, Inequalities (8.27), and (8.28) then imply that

$$w(\eta) = \sum_{\xi \in \mathcal{M}_n^1(D)} w(\xi) \mathbb{P}_\xi(\pi_\tau^0 = \eta) \quad \forall \eta \in \mathcal{M}_n^1(D),$$

and thus we may write $w = \sum_{x \in D} w(\delta_x) \mathbb{1}_x$, where $\mathbb{1}_x$ was defined in (8.14), and where the equality holds in $\mathcal{M}_n^1(D)$. In particular, $w(\eta) = 0$ for all $\eta \in \mathcal{M}_n^1(D) \setminus \Delta$. We have for all $x \in D$:

$$\sum_{\eta \in \mathcal{M}_n^1(D)} \sum_{y \in D} |w(\delta_y) \mathbb{1}_{\eta=\delta_y} \psi_x^r(\eta)| = \sum_{y \in D} |w(\delta_y) \psi_x^r(\delta_y)| \leq \|w\|_1 < \infty,$$

and hence the following computation holds:

$$\begin{aligned} 0 = \langle w, \psi_x^r \rangle &= \sum_{\eta \in \mathcal{M}_n^1(D)} w(\eta) \psi_x^r(\eta) \\ &= \sum_{\eta \in \mathcal{M}_n^1(D)} \left(\sum_{y \in D} w(\delta_y) \mathbb{1}_{\eta=\delta_y} \right) \psi_x^r(\eta) = \sum_{y \in D} w(\delta_y) \psi_x^r(\delta_y) = w(\delta_x). \end{aligned}$$

Thus, $w = 0$, which concludes for the uniqueness. \square

In the proof of Theorem 8.1.1, in order to apply Lemma 8.2.5, we need to show that for all $x \in D$,

$$\langle \partial_t u_0 - L_n^* u_0, \psi_x^r \rangle = 0.$$

To this end, let us introduce

$$\delta_{x;y} = \frac{n-1}{n} \delta_x + \frac{1}{n} \delta_y \in \mathcal{M}_n^1(D).$$

The next lemma provides an explicit formula for $\psi_x^r(\delta_{x;y})$. The fact that we only need the values of the committor functions on the set $\Delta \cup \{\delta_{x;y}; x, y \in D\}$ is a consequence of the fact that, as explained above, in the limiting regime, the selection dynamics is much faster than the mutation dynamics, so that the support of π_t is concentrated on $\{x, y\}$ in the transition from δ_x to δ_y .

Lemma 8.2.6. *For all $x, y \in D$, $x \neq y$, the committor functions ψ_x^r satisfy:*

$$\psi_x^r(\delta_{x;y}) = \alpha_{x,y,r} \frac{\alpha_{x,y,r}^{n-1} - 1}{\alpha_{x,y,r}^n - 1}, \quad \psi_x^r(\delta_{y;x}) = \alpha_{x,y,r}^{n-1} \frac{\alpha_{x,y,r} - 1}{\alpha_{x,y,r}^n - 1},$$

where $\alpha_{x,y,r}$ is defined in (8.6).

Proof. The selection dynamics cannot extend the support of a measure, hence if $\text{supp } \pi_0^0 = \{x, y\}$, then $\text{supp } \pi_t^0 \subset \{x, y\}$ for all $t \geq 0$ and $Z_t = \pi_t^0(x)$ completely determines π_t^0 . The process Z corresponds to a Gambler's ruin problem, namely a Markov process on $\{0, \dots, n\}$ with jump rates

$$p(k, k+1) = \alpha_r(y) \frac{k(n-k)}{n-1}, \quad p(k, k-1) = \alpha_r(x) \frac{k(n-k)}{n-1},$$

where α_r is given by (8.11). Denote by R its generator,

$$\tau_i(Z) = \inf \{t \geq 0, Z_t = i\}, \quad g(k) = \mathbb{P}_k(\tau_n(Z) < \tau_0(Z)).$$

Then, g is solution to the problem:

$$Rg = 0, \quad g(0) = 0, \quad g(n) = 1.$$

We have:

$$Rg(k) = \alpha_r(y) \frac{k(n-k)}{n-1} (g(k+1) - g(k)) + \alpha_r(x) \frac{k(n-k)}{n-1} (g(k-1) - g(k)).$$

Hence:

$$g(k+1) - g(k) = \alpha_{x,y,r}^{-1} (g(k) - g(k-1)),$$

\Leftrightarrow

$$g(k) - g(k-1) = \alpha_{x,y,r}^{-(k-1)} (g(1) - g(0)) = \alpha_{x,y,r}^{-(k-1)} g(1),$$

\Leftrightarrow

$$g(k) = \frac{\alpha_{x,y,r}^{-k} - 1}{\alpha_{x,y,r}^{-1} - 1} g(1).$$

The condition $g(n) = 1$ yields:

$$g(1) = \frac{\alpha_{x,y,r}^{-1} - 1}{\alpha_{x,y,r}^{-n} - 1},$$

and finally:

$$\psi_x^r(\delta_{x;y}) = g(n-1) = \frac{\alpha_{x,y,r}^{-(n-1)} - 1}{\alpha_{x,y,r}^{-n} - 1}, \quad \psi_x^r(\delta_{y;x}) = g(1) = \frac{\alpha_{x,y,r}^{-1} - 1}{\alpha_{x,y,r}^{-n} - 1},$$

which concludes the proof. \square

8.2.4 Proof of Theorem 8.1.1

Let Y^r and Y be jump Markov processes on D with rates \tilde{q}_r and \tilde{q}_∞ respectively. The last needed result is the convergence in total variation distance of Y^r towards Y . This is a general result on jump Markov processes whose jump rates converge.

Lemma 8.2.7. *Under Assumption 8.1.1*

$$\lim_{r \rightarrow \infty} \|\mathcal{L}aw(Y_0^r) - \mathcal{L}aw(Y_0)\|_{TV} = 0 \implies \forall t \geq 0, \lim_{r \rightarrow \infty} \|\mathcal{L}aw(Y_t^r) - \mathcal{L}aw(Y_t)\|_{TV} = 0.$$

Proof. We have that for all $x, y \in D$,

$$\lim_{r \rightarrow \infty} \tilde{q}_r(x, y) = \tilde{q}_\infty(x, y),$$

and for all $x \in D$,

$$\sum_{y \in D} \sup_{r \in \mathbb{N}} \tilde{q}_r(x, y) < \infty.$$

Hence, [99, Theorem 19.25, p. 385] concludes. \square

We are now in position to prove Theorem 8.1.1.

Proof of Theorem 8.1.1. Recall the jump rates:

$$\tilde{q}_r(x, y) = \begin{cases} nq(x, y) \frac{\alpha_{x,y,r} - 1}{\alpha_{x,y,r}^n - 1} & \text{if } \alpha_{x,y,r} \neq 1, \\ q(x, y) & \text{otherwise,} \end{cases}$$

and let Y^r be the Markov process with jump rates $(\tilde{q}_r(x, y))_{x, y \in D}$ and initial condition Y_0^r such that the law of $\delta_{Y_0^r}$ is $\mathcal{L}aw(\pi_\tau^0)$. Write $p_x^r(t) = \mathbb{P}(Y_t^r = x)$, for $x \in D$. The $(p_x^r)_{x \in D}$ satisfy:

$$\sum_{x \in D} p_x^r = 1,$$

and the Kolmogorov equations:

$$\partial_t p_x^r = \sum_{y \neq x} (\tilde{q}_r(y, x) p_y^r - \tilde{q}_r(x, y) p_x^r).$$

Denote by $u(t) = (\mathbb{P}(\pi_t = \xi))_{\xi \in \mathcal{M}_n^1(D)}$ the law of the empirical measure of the Fleming-Viot process (which depends on r , even though this is not indicated explicitly for the sake of notation)

and define the conjectured equivalent by:

$$u_0(t) = \sum_{x \in D} p_x^r(t) \mathbb{1}_x,$$

which corresponds to the law of $\delta_{Y_t^r}$. Lemma 8.2.4 yields that for all $t \geq 0$:

$$L_0^* u_0(t) = 0.$$

The goal now is to solve (8.16) using Lemma 8.2.5. In order to do so, let us show that

$$\partial_t u_0 - L_m^* u_0 \in (\text{Ker} L_0)^\perp.$$

Fix $x \in D$. First:

$$\langle \partial_t u_0, \psi_x^r \rangle = \partial_t p_x^r.$$

For all $f \in \ell^1(\mathcal{M}_n^1(D))$:

$$L_m^* f(\xi) = \sum_{x \neq y} \left((n\xi(y) + 1) q(y, x) f\left(\xi + \frac{\delta_y - \delta_x}{n}\right) - n\xi(x) q(x, y) f(\xi) \right),$$

hence for all $x \neq y$, $n \geq 3$:

$$L_m^* u_0(\eta) = \begin{cases} -n \sum_{z \neq x} q(x, z) p_x^r & \text{if } \eta = \delta_x, \\ nq(x, y) p_x^r & \text{if } \eta = \delta_{x;y}, \\ 0 & \text{otherwise.} \end{cases}$$

In the case $n = 2$, the formula is adapted by $L_m^* u_0(\delta_{x;y}) = nq(x, y) p_x^r + nq(y, x) p_y^r$. Using Lemma 8.2.6, this yields that:

$$\begin{aligned} & \langle L_m^* u_0, \psi_x^r \rangle \\ &= L_m^* u_0(\delta_x) \psi_x^r(\delta_x) + \sum_{y \neq x} (L_m^* u_0(\delta_y) \psi_x^r(\delta_y) + L_m^* u_0(\delta_{x;y}) \psi_x^r(\delta_{x;y}) + L_m^* u_0(\delta_{y;x}) \psi_x^r(\delta_{y;x})) \\ &= -n \sum_{z \neq x} q(x, z) p_x^r + \sum_{y \neq x} nq(x, y) p_x^r \alpha_{x,y,r} \frac{\alpha_{x,y,r}^{n-1} - 1}{\alpha_{x,y,r}^n - 1} + nq(y, x) p_y^r \alpha_{x,y,r}^{n-1} \frac{\alpha_{x,y,r} - 1}{\alpha_{x,y,r}^n - 1} \\ &= \sum_{y \neq x} (-\tilde{q}_r(x, y) p_x^r + \tilde{q}_r(y, x) p_y^r). \end{aligned}$$

Finally we get that for all $x \in D$:

$$\langle \partial_t u_0 - L_m^* u_0, \psi_x^r \rangle = \partial_t p_x^r - \sum_{y \neq x} (\tilde{q}_r(y, x) p_y^r - \tilde{q}_r(x, y) p_x^r) = 0.$$

Lemma 8.2.4 then yields that $\partial_t u_0 - L_m^* u_0 \in (\text{Ker} L_0)^\perp$. Thus, Lemma 8.2.5 yields that, for any $t \geq 0$, there exists $u_1(t) \in (\text{Ker} L_0)^\perp$ such that

$$\partial_t u_0(t) - L_m^* u_0(t) = L_0^* u_1(t),$$

with the explicit representation

$$u_1(t) = \int_0^\infty (\partial_t u_0(t) - L_m^* u_0(t)) e^{sL_0} ds.$$

From this representation and the regularity of $u_0(t)$ provided by its definition, one gets that u_1 is a \mathcal{C}^1 function of t , and that $\partial_t u_1$ solves the Poisson equation

$$\partial_t^2 u_0(t) - L_m^* \partial_t u_0(t) = L_0^* \partial_t u_1(t).$$

As a conclusion, using Lemma 8.2.5 again, we deduce that

$$\|u_1(t)\|_1 \leq C \|\partial_t u_0(t) - L_m^* u_0(t)\|_1, \quad \|\partial_t u_1(t)\|_1 \leq C \|\partial_t^2 u_0(t) - L_m^* \partial_t u_0(t)\|_1.$$

The Kolmogorov equations yield that $\|\partial_t u_0\|_1 \leq Q$, and $\|\partial_t^2 u_0\|_1 \leq Q^2$, and since L_m^* is a bounded operator, we have that:

$$\sup_{r \in \mathbb{N}} \sup_{t \geq 0} \|u_1(t)\|_1 < \infty, \quad \sup_{r \in \mathbb{N}} \sup_{t \geq 0} \|\partial_t u_1(t)\|_1 < \infty.$$

Write

$$u = u_0 + \frac{1}{\lambda_r} u_1 + v.$$

Then v satisfies the following equation:

$$\partial_t v = L^* v + \frac{1}{\lambda_r} (L_m^* u_1 - \partial_t u_1), \quad v(0) = u(0) - u_0(0) - \frac{1}{\lambda_r} u_1(0).$$

In the case where there exists $z \in D$ such that $\pi(\mathbf{X}_0) = \delta_z$, then $\tau = 0$ so $Y_0^r = z$, and we have $v(0) = -u_1(0)/\lambda_r$. Thus we can write:

$$v(t) = -\frac{1}{\lambda_r} e^{tL^*} u_1(0) + \frac{1}{\lambda_r} \int_0^t e^{(t-s)L^*} (L_m^* u_1 - \partial_t u_1) ds, \quad (8.31)$$

where for any $w \in \ell^1(\mathcal{M}_n^1(D))$, $\eta \in \mathcal{M}_n^1(D)$

$$e^{tL^*} w(\eta) = \sum_{\xi \in \mathcal{M}_n^1(D)} w(\xi) \mathbb{P}_\xi(\pi_t = \eta).$$

Thanks to the bounds on $\|u_1\|_1$ and $\|\partial_t u_1\|_1$, Equation (8.31) yields that for any $T > 0$, there exists $C > 0$ such that:

$$\sup_{t \in [0, T]} \|v(t)\|_1 \leq C/\lambda_r.$$

As a conclusion, for any $t \in [0, T]$,

$$\|\mathcal{L}aw(\pi(\mathbf{X}_t)) - \mathcal{L}aw(\delta_{Y_t^r})\|_1 \leq \|v(t)\|_1 + \frac{\|u_1(t)\|_1}{\lambda_r},$$

which concludes the proof of the second statement of Theorem 8.1.1.

To prove the first statement, with an initial condition which is not necessarily a Dirac mass,

we first write

$$\|\mathcal{L}aw(\pi(\mathbf{X}_t)) - \mathcal{L}aw(\delta_{Y_t})\|_1 \leq \|\mathcal{L}aw(\pi(\mathbf{X}_t)) - \mathcal{L}aw(\delta_{Y_t^r})\|_1 + \|\mathcal{L}aw(\delta_{Y_t^r}) - \mathcal{L}aw(\delta_{Y_t})\|_1,$$

where Y is the continuous-time Markov chain with initial condition η_∞ given by Lemma 8.2.3 and jump rates $\tilde{q}_\infty(x, y)$. For the first term of the right-hand side, we integrate the equation on v between time $1/\sqrt{\lambda_r}$ and t to get:

$$v(t) = e^{(t-1/\sqrt{\lambda_r})L^*} v\left(\frac{1}{\sqrt{\lambda_r}}\right) + \frac{1}{\lambda_r} \int_{\frac{1}{\sqrt{\lambda_r}}}^t e^{(t-s)L^*} (L_m^* u_1 - \partial_t u_1) ds.$$

The second term of this last equality still goes to 0 at speed $1/\lambda_r$, and we are just left with showing that:

$$v\left(\frac{1}{\sqrt{\lambda_r}}\right) = u\left(\frac{1}{\sqrt{\lambda_r}}\right) - u_0\left(\frac{1}{\sqrt{\lambda_r}}\right) - \frac{1}{\lambda_r} u_1\left(\frac{1}{\sqrt{\lambda_r}}\right) \xrightarrow{r \rightarrow \infty} 0,$$

in the ℓ^1 distance. Since u_1 is bounded in $\ell^1(\mathcal{M}_n^1(D))$, uniformly in $t \geq 0$ and $r \in \mathbb{N}$, we have that:

$$\lim_{r \rightarrow \infty} \left\| \frac{1}{\lambda_r} u_1\left(\frac{1}{\sqrt{\lambda_r}}\right) \right\|_1 = 0.$$

Moreover, Y^r is a continuous-time Markov chain with initial condition Y_0^r , where Y_0^r is such that $\mathcal{L}aw(\delta_{Y_0^r}) = \mathcal{L}aw(\pi_\tau^0)$, and jump rates uniformly bounded with respect to r , hence $\lambda_r \rightarrow \infty$ yields that:

$$\lim_{r \rightarrow \infty} \left\| \mathcal{L}aw(\pi_\tau^0) - u_0\left(\frac{1}{\sqrt{\lambda_r}}\right) \right\|_1 = 0.$$

Let us now show that

$$\lim_{r \rightarrow \infty} \|u(1/\sqrt{\lambda_r}) - \mathcal{L}aw(\pi_\tau^0)\|_1 = 0,$$

even though $u(0) = \eta$ for all $r \in \mathbb{N}$. Write

$$\tau_1 = \inf \{t \geq 0, \pi_t \in \Delta\}, \quad (8.32)$$

and S_1 for the first jump of a particles due to the mutation mechanism. Using the notation of Lemma 8.2.1, write $\Theta = \text{supp}(\eta)$, $b_r = 1$, $L_r^2 = L_m$, $L_r^1 = L_0^{\text{supp}(\eta)}$, where

$$L_0^{\text{supp}(\eta)} f(\xi) = \sum_{x, y \in \text{supp}(\eta)} \alpha_r(x) \xi(x) \xi(y) \left(f\left(\xi + \frac{\delta_y - \delta_x}{n}\right) - f(\xi) \right)$$

as well as $a_r = \lambda_r$, and $c_r = \sqrt{\lambda_r}$. In this case, we have $\mathbb{M}^1 = \Delta$, and Lemma 8.2.1 yields that:

$$\lim_{r \rightarrow \infty} \mathbb{P}_\eta \left(\tau_1 < \frac{1}{\sqrt{\lambda_r}} < S_1 \right) = 1. \quad (8.33)$$

For all $\xi \in \mathcal{M}_n^1(D)$, we may write:

$$\begin{aligned} u\left(\frac{1}{\sqrt{\lambda_r}}\right)(\xi) &= \mathbb{P}_\eta\left(\pi_{\frac{1}{\sqrt{\lambda_r}}} = \xi, \tau_1 < \frac{1}{\sqrt{\lambda_r}} < S_1\right) + \mathbb{P}_\eta\left(\pi_{\frac{1}{\sqrt{\lambda_r}}} = \xi, \left(\tau_1 < \frac{1}{\sqrt{\lambda_r}} < S_1\right)^c\right) \\ &= \mathbb{P}_\eta\left(\pi_\tau^0 = \xi, \tau_1 < \frac{1}{\sqrt{\lambda_r}} < S_1\right) + \mathbb{P}_\eta\left(\pi_{\frac{1}{\sqrt{\lambda_r}}} = \xi, \left(\tau_1 < \frac{1}{\sqrt{\lambda_r}} < S_1\right)^c\right), \end{aligned}$$

and thus

$$\|u\left(1/\sqrt{\lambda_r}\right) - \mathcal{L}aw(\pi_\tau^0)\|_1 \leq 2\mathbb{P}_\eta\left(\left(\tau_1 < \frac{1}{\sqrt{\lambda_r}} < S_1\right)^c\right) \xrightarrow{r \rightarrow \infty} 0.$$

Finally, Lemma 8.2.3 and Lemma 8.2.7 imply the convergence of $\|\mathcal{L}aw(\delta_{Y_t^r}) - \mathcal{L}aw(\delta_{Y_t})\|_1$ towards 0, and conclude the proof of Theorem 8.1.1. \square

8.3 Proof of Theorem 8.1.2

We are now interested in the convergence of the trajectories. As stated in the introduction, there is no hope of having convergence in the Skorohod topology. Instead, we use the L_{TV}^1 topology. As the projection

$$\pi \in \mathcal{D}([0, T], \mathcal{M}^1(D)) \mapsto \pi_t \in \mathcal{M}^1(D)$$

is not continuous for this topology, it is not enough to show compactness of the probability measures of the trajectories, because an accumulation point would not be characterised by its time marginal. Instead, we proceed as follows. First, let $F : \mathcal{D}([0, T], \mathcal{M}^1(D)) \rightarrow \mathbb{R}$ be bounded and Lipschitz continuous for the L_{TV}^1 distance (8.10). We decompose

$$\begin{aligned} \mathbb{E}\left(F\left(\left(\pi(\mathbf{X}_t^r)\right)_{t \in [0, T]}\right)\right) - \mathbb{E}\left(F\left(\left(\delta_{Y_t}\right)_{t \in [0, T]}\right)\right) \\ = \left(\mathbb{E}\left(F\left(\left(\pi(\mathbf{X}_t^r)\right)_{t \in [0, T]}\right)\right) - \mathbb{E}\left(F\left(\left(\delta_{Y_t^r}\right)_{t \in [0, T]}\right)\right)\right) \\ + \left(\mathbb{E}\left(F\left(\left(\delta_{Y_t^r}\right)_{t \in [0, T]}\right)\right) - \mathbb{E}\left(F\left(\left(\delta_{Y_t}\right)_{t \in [0, T]}\right)\right)\right), \end{aligned}$$

with $\mathcal{L}aw(Y_0^r) = \mathcal{L}aw(\pi_\tau^0)$ and $\mathcal{L}aw(Y_0) = \eta_\infty$. Thus, the conclusion of Theorem 8.1.2 follows from the combination of Lemmas 8.3.1 and 8.3.2.

Lemma 8.3.1. *The process $(\delta_{Y_t^r})_{t \in [0, T]}$ converges in distribution, in $\mathcal{D}([0, T], \mathcal{M}^1(D))$, to the process $(\delta_{Y_t})_{t \in [0, T]}$.*

Proof. Let us endow the set D with the distance $\rho(x, y) = \mathbb{1}_{x \neq y}$, and the set $\mathcal{D}([0, T], D)$ of cadlag trajectories $[0, T] \rightarrow D$ with the associated Skorohod J_1 -topology. By [99, Theorem 19.25, p. 385] (see the proof of Lemma 8.2.7), the process $(Y_t^r)_{t \in [0, T]}$ converges in distribution to $(Y_t)_{t \in [0, T]}$ in this space. To conclude, we now check that the mapping

$$\begin{aligned} \mathcal{D}([0, T], D) &\rightarrow \mathcal{D}([0, T], \mathcal{M}^1(D)) \\ (y_t)_{t \in [0, T]} &\mapsto (\delta_{y_t})_{t \in [0, T]} \end{aligned}$$

is continuous. Let $((y_t^k)_{t \in [0, T]})_{k \geq 1}$ be a sequence of elements of $\mathcal{D}([0, T], D)$ which converges to

$(y_t)_{t \in [0, T]}$ in the J_1 -topology. We have

$$\|(\delta_{y_t^k})_{t \in [0, T]} - (\delta_{y_t})_{t \in [0, T]}\|_{L^1_{TV}} = 2 \int_0^T \mathbb{1}_{y_t^k \neq y_t} dt = 2 \int_0^T \rho(y_t^k, y_t) dt.$$

By [16, p. 125], the convergence of $(y_t^k)_{t \in [0, T]}$ in the J_1 -topology implies the convergence of $\rho(y_t^k, y_t)$ to 0 for almost every $t \in [0, T]$, and therefore the conclusion follows from the dominated convergence theorem. \square

Lemma 8.3.2. *There exists a coupling of the processes $(\pi(\mathbf{X}_t^r))_{t \in [0, T]}$ and $(\delta_{Y_t^r})_{t \in [0, T]}$ such that*

$$\lim_{r \rightarrow \infty} \mathbb{E} \left[\int_0^T \|\pi(\mathbf{X}_t^r) - \delta_{Y_t^r}\|_{TV} dt \right] = 0.$$

Proof. Fix $T > 0$. The proof of Lemma 8.3.2 is divided in five steps. The first one is dedicated to the definition of the coupling.

Step 1. Write $\sigma_0 = 0$,

$$\tau_k = \inf \{t \geq \sigma_k, \pi_t \in \Delta\},$$

and

$$\sigma_{k+1} = \inf \{t \geq \tau_k, \pi_t \notin \Delta\},$$

for all $k \in \mathbb{N}$. We define an intermediate process, which is not Markov:

$$\bar{\eta}_t = \pi_{\tau_{N(t)}}, \quad N(t) = \max \{k, \tau_k \leq t\},$$

and for $t \in [0, \tau_0]$, write $\bar{\eta}_t = \pi_{\tau_0}$. This is a process living in Δ , and we will get a Markov process by a time re-scaling and conditioning. Define the change of time:

$$s(t) = \inf \left\{ s \geq 0, \int_0^s \mathbb{1}_{\pi_u \in \Delta} du > t \right\}.$$

Write $\tilde{N}(t) = \max \{k, \sigma_k \leq t\}$, and

$$\begin{aligned} & \mathcal{A}_r(T) \\ &= \left\{ \text{For all } k \in \llbracket 0, \tilde{N}(T) \rrbracket, \text{ there are no jumps from the mutation mechanism between } \sigma_k \text{ and } \tau_k \right\}. \end{aligned}$$

If $\pi_{\tau_k} = \delta_x$, then $\sigma_{k+1} - \tau_k$ is an exponential random variable with rate $n \sum_{y \neq x} q(x, y)$. Additionally, on $\mathcal{A}_r(T)$, Lemma 8.2.6 yields that the Dirac mass goes from x to y with probability

$$\frac{q(x, y)}{\sum_{y \neq x} q(x, y)} \alpha_{y, x, r}^{n-1} \frac{\alpha_{y, x, r} - 1}{\alpha_{y, x, r}^n - 1}.$$

Hence, writing

$$\delta_{Y_t^{r,1}} = \bar{\eta}_{s(t)},$$

we have that on $\mathcal{A}_r(T)$, $Y^{r,1}$ is exactly a continuous-time Markov chain with jump rates \tilde{q}_r and initial condition π_{τ_0} . Let $Y^{r,2}$ be another continuous-time Markov chain on D with jump rates \tilde{q}_r , initial condition with distribution $\mathcal{L}aw(\pi_\tau^0)$, independent of the Fleming-Viot process, and

write:

$$Y^r = Y^{r,1} \mathbb{1}_{\mathcal{A}_r(T)} + Y^{r,2} \mathbb{1}_{\mathcal{A}_r^c(T)}.$$

The process Y^r is a jump Markov process with jump rates \tilde{q}_r and initial condition with distribution $\mathcal{L}aw(\pi_r^0)$. In Step 2, we show that the probability of $\mathcal{A}_r(T)$ converges to 1. In Step 3, we show that π is close to $\bar{\eta}$, and finally in Steps 4 and 5, we show that $\bar{\eta}$ is close to $Y^{r,1}$ in the L^1 distance defined in (8.10), and thus to Y^r .

Step 2. Let us show that for all $T > 0$,

$$\lim_{r \rightarrow \infty} \mathbb{P}(\mathcal{A}_r(T)) = 1.$$

For any $k \geq 0$, the events $\{\tilde{N}(T) \geq k\}$ and $\{\text{there is a mutation jump between } \sigma_k \text{ and } \tau_k\}$ are independent. Thus we have:

$$\begin{aligned} & \mathbb{P}(\mathcal{A}_r(T)^c) \\ & \leq \sum_{k=0}^{\infty} \mathbb{P}(\tilde{N}(T) \geq k, \text{ there is a mutation jump between } \sigma_k \text{ and } \tau_k) \\ & \leq \sup_{k \in \mathbb{N}} \mathbb{P}(\text{there is a mutation jump between } \sigma_k \text{ and } \tau_k) \sum_{k=0}^{\infty} \mathbb{P}(\tilde{N}(T) \geq k). \end{aligned}$$

Because $\sigma_{k+1} - \tau_k$ is an exponential random variable with parameter bounded by nQ , \tilde{N} is bounded by a Poisson random variable with parameter nQT , and hence:

$$\sum_{k=0}^{\infty} \mathbb{P}(\tilde{N}(T) \geq k) = \mathbb{E}(\tilde{N}(T)) \leq nQT.$$

The convergence (8.17) and the strong Markov property at time σ_k yield that

$$\lim_{r \rightarrow \infty} \sup_{k \in \mathbb{N}} \mathbb{P}(\text{there is a mutation jump between } \sigma_k \text{ and } \tau_k) = 0,$$

which concludes the proof.

Step 3. Let us now prove that the L^1_{TV} distance between π and $\bar{\eta}$ goes to 0 when r goes to infinity. We have:

$$\|\pi - \bar{\eta}\|_{L^1_{TV}} \mathbb{1}_{\mathcal{A}_r(T)} \leq 2 \mathbb{1}_{\mathcal{A}_r(T)} \sum_{k=0}^{\tilde{N}(T)} \bar{\tau}_k - \sigma_k \leq 2 \sum_{k=0}^{\infty} (\bar{\tau}_k - \sigma_k) \mathbb{1}_{\sigma_k \leq T},$$

where

$$\bar{\tau}_k = \inf \{t \geq \sigma_k, \bar{\pi}_t^k \in \Delta\}, \tag{8.34}$$

and $\bar{\pi}^k$ is equal to π on $[0, \sigma_k]$, then the particles are subject to the same jump, but only from the selection part. The application of Lemma 8.2.1 to $(\bar{\pi}_{t+\sigma_k}^k)_{t \geq 0}$ yields that there exist $C, c > 0$, independent of $k \in \mathbb{N}$, such that for all $t \geq 0$:

$$\mathbb{P}(\bar{\tau}_k - \sigma_k > t | \sigma_k \leq T) \leq C e^{-c\lambda_r t},$$

yielding that

$$\lim_{r \rightarrow \infty} \sup_{k \in \mathbb{N}} \mathbb{E}(\bar{\tau}_k - \sigma_k | \sigma_k \leq T) = 0.$$

Using again that $\tilde{N}(T)$ is bounded by a Poisson random variable with parameter nQT we get:

$$\begin{aligned} \mathbb{E}(\|\pi - \bar{\eta}\|_{L^1_{TV}}) &\leq 2T\mathbb{P}(\mathcal{A}_r(T)^c) + \sup_{k \in \mathbb{N}} \mathbb{E}(\bar{\tau}_k - \sigma_k | \sigma_k \leq T) \sum_{k \geq 0} \mathbb{P}(\tilde{N}(T) \geq k) \\ &= 2T\mathbb{P}(\mathcal{A}_r(T)^c) + \sup_{k \in \mathbb{N}} \mathbb{E}(\bar{\tau}_k - \sigma_k | \sigma_k \leq T) \mathbb{E}(\tilde{N}(T)) \\ &\leq 2T\mathbb{P}(\mathcal{A}_r(T)^c) + nQT \sup_{k \in \mathbb{N}} \mathbb{E}(\bar{\tau}_k - \sigma_k | \sigma_k \leq T) \xrightarrow{r \rightarrow \infty} 0. \end{aligned}$$

Step 4. In order to show that the distance between $\bar{\eta}$ and $(\delta_{Y_t^{r,1}})_{0 \leq t \leq T}$ goes to zero as well, let us define the event

$$\mathcal{B}_r(T) = \left\{ \sum_{k=0}^{\tilde{N}(T)} \tau_k - \sigma_k < \min_{0 \leq k \leq \tilde{N}(T)} \sigma_{k+1} - \tau_k \right\},$$

and show that

$$\lim_{r \rightarrow \infty} \mathbb{P}(\mathcal{A}_r(T), \mathcal{B}_r(T)) = 1.$$

Fix $\varepsilon > 0$, and $N_0 \in \mathbb{N}$ such that $\mathbb{P}(\tilde{N}(T) > N_0) < \varepsilon$. Then

$$\mathbb{P}(\mathcal{B}_r(T)^c, \mathcal{A}_r(T)) \leq \varepsilon + \mathbb{P}\left(\sum_{k=0}^{N_0} \tau_k - \sigma_k > \min_{0 \leq k \leq N_0} \sigma_{k+1} - \tau_k, \mathcal{A}_r(T)\right).$$

On the event $\mathcal{A}_r(T)$, the random variable $\min_{0 \leq k \leq N_0} \sigma_{k+1} - \tau_k$ is lower bounded by a exponential random variable E with parameter $N_0 nQ$, independent of the family of random variable $(\tau_k - \sigma_k)_{0 \leq k \leq N_0}$. This implies that

$$\begin{aligned} \mathbb{P}\left(\sum_{k=0}^{N_0} \tau_k - \sigma_k > \min_{0 \leq k \leq N_0} \sigma_{k+1} - \tau_k, \mathcal{A}_r(T)\right) &\leq \mathbb{P}(\exists 1 \leq k \leq N_0, \tau_k - \sigma_k > E/N_0) \\ &\leq N_0 \sup_{k \in \mathbb{N}} \mathbb{P}(\tau_k - \sigma_k > E/N_0). \end{aligned}$$

Lemma 8.2.1 then yields that

$$\limsup_{r \rightarrow \infty} \mathbb{P}(\mathcal{A}_r(T), \mathcal{B}_r(T)^c) \leq \varepsilon,$$

for all $\varepsilon > 0$, which concludes Step 4.

Step 5. Now, using Step 4, all is left to do is show that

$$\lim_{r \rightarrow \infty} \|\bar{\eta} - (\delta_{Y_t^{r,1}})_{0 \leq t \leq T}\|_{L^1_{TV}} = 0.$$

First notice that for all $s \geq 0$

$$\int_0^s \mathbb{1}_{\pi_u \in \Delta} du = s - \sum_{k=0}^{\tilde{N}(s)} s \wedge \tau_k - \sigma_k,$$

so that

$$s(t) = t + \sum_{k=0}^{\tilde{N}(s(t))} \tau_k - \sigma_k \geq t.$$

Additionally, $\delta_{Y_t} \neq \bar{\eta}_t$ only if there is $p \in \mathbb{N}$ such that $t \leq \sigma_p \leq s(t)$, and on the event $\mathcal{B}_r(T)$, $t \leq \sigma_p < s(t)$ implies that $\tilde{N}(s(t)) = p$. Hence

$$t \geq \sigma_p - \sum_{k=0}^p \tau_k - \sigma_k.$$

Hence the total amount of time where $\delta_{Y_r} \neq \bar{\eta}$ is bounded as follow

$$\mathbb{1}_{\mathcal{A}_r(T), \mathcal{B}_r(T)} \int_0^T \mathbb{1}_{\delta_{Y_t} \neq \bar{\eta}_t} dt \leq \mathbb{1}_{\mathcal{A}_r(T), \mathcal{B}_r(T)} \sum_{p=0}^{\tilde{N}(T)} \sum_{k=0}^p \tau_k - \sigma_k \leq \sum_{k=0}^{\tilde{N}(T)} (\tilde{N}(T) - k) (\bar{\tau}_k - \sigma_k),$$

where $\bar{\tau}_k$ was defined in (8.34). We have:

$$\|\delta_{Y_r} - \bar{\eta}\|_{L^1_{TV}} \mathbb{1}_{\mathcal{A}_r(T)} \mathbb{1}_{\mathcal{B}_r(T)} = \|\delta_{Y_{r,1}} - \bar{\eta}\|_{L^1_{TV}} \mathbb{1}_{\mathcal{A}_r(T)} \mathbb{1}_{\mathcal{B}_r(T)} \leq 2 \sum_{k=0}^{\infty} \tilde{N}(T) (\bar{\tau}_k - \sigma_k) \mathbb{1}_{\sigma_k \leq T}.$$

Using Cauchy-Schwarz inequality, one gets:

$$\begin{aligned} \mathbb{E} \left(\sum_{k=0}^{\infty} \tilde{N}(T) (\bar{\tau}_k - \sigma_k) \mathbb{1}_{\sigma_k \leq T} \right) &\leq \sum_{k=0}^{\infty} \mathbb{E} \left(\tilde{N}(T)^2 \right) \mathbb{E} \left((\bar{\tau}_k - \sigma_k)^2 \mathbb{1}_{\sigma_k \leq T} \right) \\ &\leq \mathbb{E} \left(\tilde{N}(T)^2 \right) \mathbb{E} \left(\tilde{N}(T) \right) \sup_{k \in \mathbb{N}} \mathbb{E} \left((\bar{\tau}_k - \sigma_k)^2 \mid \sigma_k \leq T \right). \end{aligned}$$

Hence:

$$\mathbb{E} \left(\|\delta_{Y_r} - \bar{\eta}\|_{L^1_{TV}} \right) \leq 2T \mathbb{P}(\mathcal{A}_r(T) \cup \mathcal{B}_r(T)^c) + 2 \sup_{k \in \mathbb{N}} \mathbb{E} \left((\bar{\tau}_k - \sigma_k)^2 \mid \sigma_k \leq T \right) \mathbb{E} \left(\tilde{N}(T)^2 \right) \mathbb{E} \left(\tilde{N}(T) \right).$$

yielding that

$$\lim_{r \rightarrow \infty} \mathbb{E} \left(\|\delta_{Y_r} - \bar{\eta}\|_{L^1_{TV}} \right) = 0,$$

which concludes the proof. \square

8.4 Proof of Theorem 8.1.3

The aim of this section is to prove Theorem 8.1.3, and we therefore suppose that Assumption 8.1.2 holds for the remainder of this work. In this case, we can write:

$$\lambda_r = \underline{\lambda}_r + m_r,$$

where $\underline{\lambda}_r = \inf_D \lambda_r$, $m_r \geq 0$ and

$$\|m\|_{\infty} := \sup_{r \in \mathbb{N}} \sup_{x \in D} m_r(x) < \infty.$$

We start by showing that π_t converges to a Dirac mass. Denote still for $z \in D$:

$$\pi_t(z) = \pi(\mathbf{X}_t^r)(z). \quad (8.35)$$

Lemma 8.4.1. *Under Assumption 8.1.2, we have for all $t \geq 0$:*

$$\lim_{r \rightarrow \infty} \sum_{x \neq y \in D} \mathbb{E}(\pi_t(x)\pi_t(y)) \rightarrow 0, \quad \lim_{r \rightarrow \infty} \mathbb{E}(\|\pi_t\|_\infty) = 1.$$

Moreover, if $\pi(\mathbf{X}_0) = \delta_z$ for some $z \in D$ and all $r \in \mathbb{N}$, then:

$$\sum_{x \neq y \in D} \mathbb{E}(\pi_t(x)\pi_t(y)) \leq (Q + 2\|m\|_\infty) \frac{n_r}{\lambda_r}, \quad \|\pi_t\|_\infty \geq 1 - (Q + 2\|m\|_\infty) \frac{n_r}{\lambda_r}.$$

Proof. Write, for a given probability measure ξ on D ,

$$g_2(\xi) = \sum_{x \in D} \xi(x)^2. \quad (8.36)$$

We have:

$$\begin{aligned} Lg_2(\xi) &= \sum_{x \neq y} n_r \xi(x) \left(q(x, y) + \lambda_r(x) \frac{n_r}{n_r - 1} \xi(y) \right) \\ &\quad \left(\left(\xi(x) - \frac{1}{n_r} \right)^2 - \xi(x)^2 + \left(\xi(y) + \frac{1}{n_r} \right)^2 - \xi(y)^2 \right) \\ &= 2 \sum_{x \neq y} n_r \xi(x) \left(q(x, y) + \lambda_r(x) \frac{n_r}{n_r - 1} \xi(y) \right) \left(\frac{1}{n_r^2} + \frac{\xi(y) - \xi(x)}{n_r} \right) \\ &\geq \frac{2}{n_r} \sum_{x \neq y} \lambda_r(x) \xi(x) \xi(y) - 2 \sum_{x \neq y} \xi(x)^2 q(x, y) + \frac{2n_r}{n_r - 1} \sum_{x \neq y} \lambda_r(x) \xi(x) \xi(y) (\xi(y) - \xi(x)) \\ &\geq \frac{2\lambda_r}{n_r} (1 - g_2(\xi)) - 2Qg_2(\xi) - \frac{n_r}{n_r - 1} \sum_{x \neq y} (\lambda_r(y) - \lambda_r(x)) \xi(x) \xi(y) (\xi(y) - \xi(x)) \\ &\geq \frac{2\lambda_r}{n_r} (1 - g_2(\xi)) - (2Q + 4\|m\|_\infty). \end{aligned}$$

Using the Kolmogorov equation, this yields that for all $t \geq 0$:

$$\partial_t \mathbb{E}(g_2(\pi_t)) \geq \frac{2\lambda_r}{n_r} (1 - \mathbb{E}(g_2(\pi_t))) - (2Q + 4\|m\|_\infty)$$

and hence

$$\mathbb{E}(g_2(\pi_t)) \geq 1 - e^{-\frac{2\lambda_r}{n_r} t} (1 - \mathbb{E}(g_2(\pi_0))) - (2Q + 4\|m\|_\infty) \frac{n_r}{2\lambda_r}. \quad (8.37)$$

Now, since $\sum_{x \in D} \xi(x) = 1$ for all $\xi \in \mathcal{M}^1(D)$, we have:

$$g_2(\pi_t) \leq \|\pi_t\|_\infty,$$

which implies the result on $\|\pi_t\|_\infty$. We also have:

$$\sum_{x \neq y \in D} \mathbb{E}(\pi_t(x)\pi_t(y)) = 1 - \mathbb{E}(g_2(\pi_t)),$$

which concludes the proof. \square

The preceding Lemma showed that π_t converges towards a Dirac measure as $r \rightarrow \infty$. The goal of the next Lemma is to determine the law of this limiting Dirac mass.

Lemma 8.4.2. *Recall that $\pi_t(x) = \pi(\mathbf{X}_t^r)(x)$. Under Assumption 8.1.2, we have:*

$$\lim_{r \rightarrow 0} \sum_{x \in D} |\mathbb{E}(\pi_t(x)) - \mathbb{P}(Y_t = x)| = 0,$$

where $(Y_t)_{t \geq 0}$ is the Markov process with jump rates $(q(x, y))_{x, y \in D}$ and initial condition η . Moreover, if $\pi(\mathbf{X}_0^r) = \delta_z$ for some $z \in D$ and all $r \in \mathbb{N}$, then for all $T > 0$, there exists $C > 0$ such that for all $t \in [0, T]$:

$$\sum_{x \in D} |\mathbb{E}(\pi_t(x)) - \mathbb{P}(Y_t = x)| \leq C \frac{n_r}{\lambda_r}.$$

Proof. The Kolmogorov equation yields that for all $x \in D$:

$$\begin{aligned} \partial_t \mathbb{E}(\pi_t(x)) &= \sum_{y \neq x} \mathbb{E}(\pi_t(y))q(y, x) - \mathbb{E}(\pi_t(x)) \sum_{y \neq x} q(x, y) \\ &\quad + \frac{n_r}{n_r - 1} \sum_{y \neq x} \mathbb{E}(\pi_t(x)\pi_t(y)) (\lambda_r(y) - \lambda_r(x)). \end{aligned}$$

Let $(\nu_t)_{t \geq 0}$ be the unique solution to the following system:

$$\partial_t \nu_t(x) = \sum_{y \neq x} \nu_t(y)q(y, x) - \nu_t(x) \sum_{y \neq x} q(x, y) = L_m^*(\nu_t)(x),$$

with initial condition $\nu_0 = \eta$. We can identify $\nu_t(x) = \mathbb{P}_\eta(Y_t = x)$. Besides, L_m^* is a linear operator, and we have:

$$\partial_t (\mathbb{E}(\pi_t) - \nu_t) = L_m^*(\mathbb{E}(\pi_t) - \nu_t) + g_t,$$

where

$$g_t(x) = \sum_{y \neq x} \frac{n_r}{n_r - 1} \mathbb{E}(\pi_t(x)\pi_t(y)) (\lambda_r(y) - \lambda_r(x)),$$

for all $x \in D$. We get:

$$\mathbb{E}(\pi_t) - \eta_t = e^{tL_m^*} (\pi(\mathbf{X}_0^r) - \eta) + \int_0^t e^{sL_m^*} g_{t-s} ds.$$

We have that for all $t \geq 0$:

$$\|g_t\|_1 \leq \frac{n_r}{n_r - 1} \|m\|_\infty \sum_{x \neq y \in D} \mathbb{E}(\pi_t(x)\pi_t(y)) \leq 2\|m\|_\infty (1 - \mathbb{E}(g_2(\pi_t))),$$

where g_2 is defined in (8.36). Since L_m is a Markov generator, Lemma 8.4.1 (and more precisely

equation (8.37)) yields that

$$\lim_{r \rightarrow \infty} \|\mathbb{E}(\pi_t) - \nu_t\|_1 = 0,$$

as well as, if $\eta = \pi(X_0)$:

$$\|\mathbb{E}(\pi_t) - \nu_t\|_1 \leq C \frac{n_r}{\Delta_r},$$

for all $0 < t < T$ and some $C > 0$, which concludes the proof. \square

We are now in position to conclude the proof of Theorem 8.1.3.

Proof of Theorem 8.1.3. Let $F : \mathcal{M}^1(D) \rightarrow \mathbb{R}$ bounded, and $\varepsilon > 0$. Write

$$\left| \mathbb{E}(F(\pi(\mathbf{X}_t^r))) - \sum_{z \in D} F(\delta_z) \mathbb{P}(\|\pi(\mathbf{X}_t^r) - \delta_z\|_{TV} \leq \varepsilon) \right| \leq \sum_{z \in D} \varepsilon \|F\|_\infty \mathbb{P}(\|\pi(\mathbf{X}_t^r) - \delta_z\|_{TV} \leq \varepsilon) + R_{r,t},$$

where

$$R_{r,t} \leq \|F\|_\infty \mathbb{P}(d(\pi(\mathbf{X}_t^r), \Delta) > \varepsilon).$$

Using the fact that $\|\pi_t - \delta_z\|_{TV} = 2(1 - \pi_t^z)$, we get

$$R_{r,t} \leq \|F\|_\infty \mathbb{P}(\|\pi(\mathbf{X}_t^r)\|_\infty < 1 - \varepsilon/2) \leq \frac{2\|F\|_\infty}{\varepsilon} \mathbb{E}(1 - \|\pi(\mathbf{X}_t^r)\|_\infty),$$

and finally

$$\left| \mathbb{E}(F(\pi(\mathbf{X}_t^r))) - \sum_{x \in D} F(\delta_x) \mathbb{P}(\|\pi(\mathbf{X}_t^r) - \delta_x\|_{TV} \leq \varepsilon) \right| \leq \|F\|_\infty \left(\varepsilon + \frac{2}{\varepsilon} \mathbb{E}(1 - \|\pi(\mathbf{X}_t^r)\|_\infty) \right). \quad (8.38)$$

Using Markov inequality, we have:

$$\mathbb{P}(\|\pi(\mathbf{X}_t^r) - \delta_z\|_{TV} \leq \varepsilon) = \mathbb{P}(\pi_t^z \geq 1 - \varepsilon/2) \leq (1 - \varepsilon/2)^{-1} \mathbb{E}(\pi_t(z)) \leq (1 + \varepsilon) \mathbb{E}(\pi_t(z)),$$

as soon as $\varepsilon < 1$. On the other side, we have that

$$\mathbb{E}(\pi_t(z)) = \mathbb{E}(\pi_t(z) \mathbb{1}_{\pi_t(z) \geq 1 - \varepsilon/2} + \mathbb{1}_{\pi_t(z) < 1 - \varepsilon/2}) \leq \mathbb{P}(\pi_t^z \geq 1 - \varepsilon/2) + \mathbb{E}(\pi_t(z) \mathbb{1}_{\pi_t(z) < 1 - \varepsilon/2}).$$

Moreover,

$$\begin{aligned} \sum_{x \in D} \mathbb{E}(\pi_t(z) \mathbb{1}_{\pi_t(z) < 1 - \varepsilon/2}) &= \sum_{x \in D} \mathbb{E}(\pi_t(x) \mathbb{1}_{\pi_t(x) < 1 - \varepsilon/2} (\mathbb{1}_{\|\pi\|_\infty \leq 1 - \varepsilon/2} + \mathbb{1}_{\|\pi\|_\infty > 1 - \varepsilon/2})) \\ &\leq \mathbb{P}(\|\pi(\mathbf{X}_t)\|_\infty < 1 - \varepsilon/2) + \frac{\varepsilon}{2}, \end{aligned}$$

yielding that

$$\left| \sum_{x \in D} F(\delta_x) \mathbb{P}(\|\pi(\mathbf{X}_t^r) - \delta_x\|_{TV} \leq \varepsilon) - \sum_{x \in D} F(\delta_x) \mathbb{E}(\pi_t(x)) \right| \leq \|F\|_\infty \left(\varepsilon + \frac{2}{\varepsilon} \mathbb{E}(1 - \|\pi(\mathbf{X}_t^r)\|_\infty) \right). \quad (8.39)$$

Lastly, we have that:

$$\left| \sum_{x \in D} F(\delta_x) \mathbb{E}(\pi_t(x)) - \sum_{x \in D} F(\delta_x) \mathbb{E}(\nu_t(x)) \right| \leq \|F\|_\infty \sum_{x \in D} |\mathbb{E}(\pi_t(x)) - \mathbb{P}(Y_t = x)|. \quad (8.40)$$

Equations (8.38), (8.39) and (8.40) together yield

$$\begin{aligned} & \left| \mathbb{E}(F(\pi(\mathbf{X}_t^r))) - \sum_{x \in D} F(\delta_x) \mathbb{E}(\nu_t(x)) \right| \\ & \leq 2\|F\|_\infty \left(\varepsilon + \frac{2}{\varepsilon} \mathbb{E}(1 - \|\pi(\mathbf{X}_t^r)\|_\infty) \right) + \|F\|_\infty \sum_{x \in D} |\mathbb{E}(\pi_t(x)) - \mathbb{P}(Y_t = x)|, \end{aligned} \quad (8.41)$$

and Lemma 8.4.1 and Lemma 8.4.2 yield

$$\limsup_{r \rightarrow \infty} \left| \mathbb{E}(F(\pi(\mathbf{X}_t^r))) - \sum_{x \in D} F(\delta_x) \mathbb{E}(\nu_t(x)) \right| \leq 2\|F\|_\infty \varepsilon.$$

Letting $\varepsilon \rightarrow 0$ yields the first part of the theorem. In the case where the initial condition is a Dirac mass, plugging $\varepsilon = \sqrt{n_r/\lambda_r}$ in equation (8.41) and Lemma 8.4.2 yields for all $T > 0$ and $0 < t < T$:

$$\begin{aligned} & \left| \mathbb{E}(F(\pi(\mathbf{X}_t^r))) - \sum_{x \in D} F(\delta_x) \mathbb{E}(\nu_t(x)) \right| \\ & \leq \|F\|_\infty \left(\sqrt{\frac{n_r}{\lambda_r}} + \sqrt{\frac{\lambda_r}{n_r}} (Q + 2\|m\|_\infty) \frac{n_r}{\lambda_r} + C \frac{n_r}{\lambda_r} \right) \leq C' \sqrt{\frac{n_r}{\lambda_r}}, \end{aligned}$$

for some $C' > 0$, and this concludes the proof. \square

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LONG-TIME BEHAVIOR OF SOME MARKOV PROCESSES, AND APPLICATION TO STOCHASTIC ALGORITHMS

Abstract

This thesis is devoted to the study of the long-time behavior of some Markov processes arising in stochastic algorithms. These algorithms are variations of Monte Carlo methods, which constitute a class of techniques for sampling probability measures based on Markov processes. The thesis is structured into three parts, each addressing a different type of algorithm:

1. Chapters 2 and 3 focus on sampling Gibbs measures using two distinct kinetic processes.
2. Chapter 4 explores non-convex and high-dimensional optimization through simulated annealing, while Chapter 5 investigates optimization using a switched process.
3. Chapters 6, 7, and 8 delve into sampling quasi-stationary distributions based on the Fleming-Viot process, a Moran-type particle system.

The motivation for these algorithms, and thus much of the research conducted for this thesis, stems from molecular dynamics and statistics applications. By applying coupling and partial differential equation methods, we aim to establish convergence guarantees for these algorithms.

Keywords: probability theory, stochastic calculus, coupling methods, long time behavior of markov processes, poincaré inequality, stochastic algorithm, hypocoercivity.

Résumé

Cette thèse est consacrée à l'étude du comportement à long terme de certains processus de Markov apparaissant dans les algorithmes stochastiques. Ces algorithmes sont des variations autour des méthodes de Monte Carlo, qui constituent une classe de techniques d'échantillonnage de mesures de probabilité basées sur des processus de Markov. La thèse est structurée en trois parties, chacune traitant d'un type d'algorithme différent :

1. Les chapitres 2 et 3 portent sur l'échantillonnage des mesures de Gibbs à l'aide de deux processus cinétiques différents.
2. Le chapitre 4 traite de l'optimisation non-convexe en grande dimension par recuit simulé, tandis que le chapitre 5 étudie l'optimisation à l'aide d'un processus commuté.
3. Les chapitres 6, 7 et 8 traitent de l'échantillonnage de mesures quasi-stationnaires basé sur le processus de Fleming-Viot, un système de particules de type Moran.

La motivation pour ces algorithmes, et donc pour la plupart des recherches menées dans le cadre de cette thèse, provient de dynamique moléculaire et d'applications en statistiques. En appliquant des méthodes de couplage et d'équations aux dérivées partielles, nous établirons des garanties de convergence pour ces algorithmes.

Mots clés : probabilités, calcul stochastique, méthodes de couplage, comportement en temps long de processus de markov, inégalité de poincaré, algorithme stochastique, hypocoercivité.



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