



HAL
open science

Computation of sensitivities for the invariant measure of a parameter dependent diffusion

Roland Assaraf, Benjamin Jourdain, Tony Lelièvre, Raphaël Roux

► **To cite this version:**

Roland Assaraf, Benjamin Jourdain, Tony Lelièvre, Raphaël Roux. Computation of sensitivities for the invariant measure of a parameter dependent diffusion. *Stochastics and Partial Differential Equations: Analysis and Computations*, 2017, June 2018, 6 (2), pp.125-183. 10.1007/s40072-017-0105-6 . hal-01192862

HAL Id: hal-01192862

<https://hal.science/hal-01192862v1>

Submitted on 3 Sep 2015

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

Computation of sensitivities for the invariant measure of a parameter dependent diffusion

Roland Assaraf^{*}, Benjamin Jourdain[†], Tony Lelièvre[‡], Raphaël Roux[§]

September 4, 2015

Abstract

We consider the solution to a stochastic differential equation with a drift function which depends smoothly on some real parameter λ , and admitting a unique invariant measure for any value of λ around $\lambda = 0$. Our aim is to compute the derivative with respect to λ of averages with respect to the invariant measure, at $\lambda = 0$. We analyze a numerical method which consists in simulating the process at $\lambda = 0$ together with its derivative with respect to λ on long time horizon. We give sufficient conditions implying uniform-in-time square integrability of this derivative. This allows in particular to compute efficiently the derivative with respect to λ of the mean of an observable through Monte Carlo simulations.

Keywords: Stochastic differential equations, invariant measure, variance reduction, Feynman-Kac formulae.

1 Introduction

We are interested in methods to compute the response of a Brownian dynamics to an infinitesimal change of a parameter $\lambda \in \mathbb{R}$. More precisely, we consider the dynamics in \mathbb{R}^d :

$$\begin{cases} dX_t^\lambda = F_\lambda(X_t^\lambda)dt + \sqrt{2}dW_t, \\ X_0^\lambda = X_0, \end{cases} \quad (1)$$

for $\lambda \in \mathbb{R}$ close to 0, where $(W_t)_{t \geq 0}$ is a standard d -dimensional Brownian motion independent of $X_0 \in \mathbb{R}^d$. Note that neither the initial condition X_0 nor the Brownian motion depend on λ . The family of vector fields $F_\lambda : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is indexed by a real parameter λ . We assume that when $\lambda = 0$, the vector field derives from some potential energy $V : \mathbb{R}^d \rightarrow \mathbb{R}$, namely

$$F_0 = -\nabla V,$$

^{*}Laboratoire de Chimie Théorique, CNRS-UMR 7616 et Université Pierre et Marie Curie, 75252 Paris Cedex, France, assaraf@lct.jussieu.fr

[†]Université Paris-Est, CERMICS (ENPC), INRIA, F-77455 Marne-la-Vallée, France, jourdain@cermics.enpc.fr

[‡]Université Paris-Est, CERMICS (ENPC), INRIA, F-77455 Marne-la-Vallée, France, lelievre@cermics.enpc.fr

[§]Laboratoire de Probabilités et Modèles Aléatoires, UMR 7599, UPMC, Case 188, 4 pl. Jussieu, F-75252 Paris Cedex 5, France, raphael.roux@upmc.fr

where ∇ denotes the gradient operator with respect to the space variables. For λ close to zero, one can think of $(X_t^\lambda)_{t \geq 0}$ as a physical system undergoing a potential energy V to which one applies an external force $\lambda \partial_\lambda^0 F_\lambda$. Here and in all the following, the notation ∂_λ^0 denotes the derivative with respect to λ computed at $\lambda = 0$.

Concerning the potential V , we assume that the following assumption holds.

Assumption (Pot). *The function V satisfies the following assumptions:*

(i) $V : \mathbb{R}^d \rightarrow \mathbb{R}$ is a C^2 function such that $x \mapsto \nabla^2 V(x)$ is locally Lipschitz.

(ii) $\int_{\mathbb{R}^d} e^{-V(x)} dx = 1$ and $\int_{\mathbb{R}^d} |\nabla V|^2(x) e^{-V(x)} dx < \infty$.

(iii) Pathwise existence and uniqueness hold for the process $(X_t^0)_{t \geq 0}$.

Since ∇V is assumed to be locally Lipschitz, pathwise uniqueness is automatically ensured. Pathwise existence is ensured for instance as soon as there exists a finite constant C such that for all $x \in \mathbb{R}^d$, $\nabla V(x) \cdot x \leq C(1 + |x|^2)$.

At $\lambda = 0$, the dynamics (1) is of the following gradient form

$$dX_t^0 = -\nabla V(X_t^0) dt + \sqrt{2} dW_t. \quad (2)$$

Under the above assumptions, it can be checked that $e^{-V(x)} dx$ is the unique invariant probability measure (see Lemma 18 below) denoted in the following:

$$d\pi_0 = e^{-V(x)} dx.$$

Then, from classical results in ergodic theory, for any f in $\mathbb{L}^1(\pi_0)$, almost surely,

$$\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t f(X_s^0) ds = \int_{\mathbb{R}^d} f d\pi_0. \quad (3)$$

Let us now introduce the assumptions we need on the drift $(F_\lambda)_{\lambda \in \mathbb{R}}$.

Assumption (Drift). *There exists $\lambda_0 > 0$ such that, for all $\lambda \in [0, \lambda_0]$,*

(i) *The function $F_\lambda - F_0$ is bounded by $C\lambda$ for some constant C not depending on x . Moreover, as $\lambda \rightarrow 0^+$, $\frac{F_\lambda(x) - F_0(x)}{\lambda}$ converges locally uniformly for $x \in \mathbb{R}^d$ to some limit $\partial_\lambda^0 F_\lambda$. Note that $\partial_\lambda^0 F_\lambda$ is bounded by C .*

(ii) *The function $x \mapsto F_\lambda(x)$ is locally Lipschitz. The function $x \mapsto \partial_\lambda^0 F_\lambda(x)$ is differentiable on \mathbb{R}^d and $\nabla \cdot \partial_\lambda^0 F_\lambda$ is in $\mathbb{L}^2(\pi_0)$.*

Under these assumptions, we will show (see Lemma 18 below) that the dynamics (1) is ergodic with respect to a probability measure π_λ : for any $f \in \mathbb{L}^1(\pi_\lambda)$, almost surely,

$$\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t f(X_s^\lambda) ds = \int_{\mathbb{R}^d} f d\pi_\lambda. \quad (4)$$

The aim of this paper is to study the quantity: for a given observable f ,

$$\lim_{\lambda \rightarrow 0} \frac{\int_{\mathbb{R}^d} f d\pi_\lambda - \int_{\mathbb{R}^d} f d\pi_0}{\lambda} = \partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right). \quad (5)$$

In particular, we will exhibit sufficient conditions for the existence of this derivative, derive various explicit formulae for this quantity, and discuss numerical techniques in order to approximate it.

The estimation of derivatives of the form (5) is useful in various applications, in particular in molecular simulations (see for example the recent work [34]): optimization procedure to fit a force

field to some observations, study of phase transitions, estimate of forces in Variational Monte Carlo methods (see [2]), or computation of transport coefficients. Transport coefficients are computed as the ratio of the magnitude of the response of the system submitted to a perturbation in its steady-state to the magnitude of the perturbation. These coefficients are related to macroscopic properties of the system through fluctuation dissipation theorems [6, 14]. Examples include the mobility or the thermal conductivity.

It is well-known that it is possible to approximate $\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right)$ by considering a simulation at $\lambda = 0$. For example, the celebrated Green-Kubo formula [6, 14] writes (see Theorem 37 in Section 4 for a proof in our specific context):

$$\partial_\lambda^0 \int_{\mathbb{R}^d} f d\pi_\lambda = \int_0^\infty \mathbb{E}_{\pi_0} [f(X_0) (\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(X_s^0)] ds$$

where the subscript π_0 indicates that the initial condition X_0 is distributed according to π_0 . The derivative $\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right)$ can thus be approximated by considering infinite-time integrals of auto-correlation functions for the stationary process at $\lambda = 0$. This formula can be used to approximate $\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right)$ numerically, which requires at least in some cases to be careful when choosing the truncation time in the integral, see for example [7]. Let us also mention another technique discussed in [34], based on the use of Malliavin weights and the Bismut Elworthy Li formula (see [3, 19, 13]).

In this work, we are interested in so-called non-equilibrium molecular dynamics (NEMD) methods which consists in simulating two trajectories with $\lambda = 0$ and $\lambda = \varepsilon$ small, and then considering the finite difference when $\varepsilon \rightarrow 0$ (see for example [8, 9]):

$$\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right) \simeq \frac{\frac{1}{t} \int_0^t f(X_s^\varepsilon) ds - \frac{1}{t} \int_0^t f(X_s^0) ds}{\varepsilon} \text{ when } \varepsilon \rightarrow 0 \text{ and } t \rightarrow \infty.$$

Note that the consistency of this estimate is based on the ergodic properties (3) and (4). To reduce the variance of the computation, it is natural to use the same driving Brownian motion for the two processes $(X_s^\varepsilon)_{s \geq 0}$ and $(X_s^0)_{s \geq 0}$ (see [8]) and we therefore end up with the natural following estimate:

$$\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right) \simeq \frac{1}{t} \int_0^t \partial_\lambda^0(f(X_s^\lambda)) ds \text{ when } t \rightarrow \infty. \quad (6)$$

As will be shown below (see Proposition 19), it is easy to simulate $\partial_\lambda^0(f(X_t^\lambda))$ by using the formula

$$\partial_\lambda^0(f(X_t^\lambda)) = T_t \cdot \nabla f(X_t^0)$$

where the so-called tangent vector $T_t \in \mathbb{R}^d$ is defined by

$$T_t = \partial_\lambda^0 X_t^\lambda.$$

Indeed, the couple (X_t^0, T_t) is a Markov process which satisfies the following extended version of the stochastic differential equation (2):

$$\begin{cases} dX_t^0 = -\nabla V(X_t^0) dt + \sqrt{2} dW_t, \\ dT_t = (\partial_\lambda^0 F_\lambda(X_t^0) - \nabla^2 V(X_t^0) T_t) dt, \end{cases} \quad (7)$$

with initial conditions $X_0^0 = X_0$ and $T_0 = 0$ (since, we recall, X_0 does not depend on λ). The estimate (6) thus leads to a practical numerical method to evaluate the derivative $\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right)$.

The main theoretical result of this paper consists in exhibiting sufficient conditions such that the following equalities hold true (see Theorem 40):

$$\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right) = \lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \partial_\lambda^0(f(X_s^\lambda)) ds \quad \text{a.s.} \quad (8)$$

and

$$\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right) = \lim_{t \rightarrow \infty} \mathbb{E} \left[\partial_\lambda^0(f(X_t^\lambda)) \right]. \quad (9)$$

Therefore, two natural estimators of $\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right)$ are

$$\frac{1}{t} \int_0^t \partial_\lambda^0(f(X_s^\lambda)) ds \quad (10)$$

and

$$\mathbb{E} \left[\partial_\lambda^0(f(X_t^\lambda)) \right]. \quad (11)$$

The second estimator is derived from the expected ergodic property on the time marginals: $\lim_{t \rightarrow \infty} \mathbb{E}(f(X_t^\lambda)) = \int_{\mathbb{R}^d} f d\pi_\lambda$. For both estimators, Theorem 40 can be seen as a rigorous justification of the interversion of the derivative ∂_λ^0 with the limit $\lim_{t \rightarrow \infty}$ and an average in time for the first estimator and over the underlying probability space for the second one, since $\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right) = \partial_\lambda^0 \left(\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t f(X_s^\lambda) ds \right)$ and $\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right) = \partial_\lambda^0 \left(\lim_{t \rightarrow \infty} \mathbb{E} [f(X_t^\lambda)] \right)$. In addition, we also study the variance of the random variable $\partial_\lambda^0(f(X_t^0)) = T_t \cdot \nabla f(X_t^0)$ which influences the statistical errors associated with the two estimators (10) and (11).

The proof of (8) and (9) is based on two main ideas. First, the long-time limit (in law) of the couple (X_t^0, T_t) is identified using a time-reversal argument (see Lemma 42) in the spirit of the argument used in [15] to study the long-time behavior of two interacting stochastic vortices. We are then able to identify the long-time limit of the estimators using the Green-Kubo formula which we prove in our setting in Section 4. Second, the justification of the interversion of the derivative with the long-time limit and the integrals requires some integrability results, which are based on the study of the long-time behaviour of $\mathbb{E} \left[e^{-\int_0^t \varphi(Y_s^x) ds} \right]$ for $\varphi = \min \text{Spec}(\nabla^2 V)$, where $(Y_s^x)_{s \geq 0}$ satisfies (2) with x as an initial condition:

$$\begin{cases} dY_t^x = -\nabla V(Y_t^x) dt + \sqrt{2} dW_t, \\ Y_0^x = x. \end{cases} \quad (12)$$

Let us emphasize that we prove all these results in a rather general setting: the state space is non compact (namely \mathbb{R}^d), the coefficients are only assumed to be locally Lipschitz and the potential V is not necessarily strictly convex. The study of the long-time behaviour of the couple (X_t^0, T_t) is very much related to the study of the long-time behaviour of the couple (Y_t^x, DY_t^x) , (see Lemma 21) which may be also useful to analyze other related numerical methods, see [30].

The paper is organized as follows. In Section 2, we give preliminary results on the stochastic differential equations (1) and (2), in particular on their ergodic properties and the long-time behaviour of the associated Kolmogorov equations. In Section 3, we then introduce the tangent vector T_t and study its integrability. In Section 4, we derive and prove finite-time and infinite-time Green-Kubo formulae. We are then in position to prove the long-time convergence of the estimators (10) and (11) in Section 5. Finally, the theoretical results are illustrated through various numerical experiments in Section 6.

In all the following, we assume that Assumptions **(Pot)** and **(Drift)** hold, and we do not mention them explicitly in the statements of the mathematical results.

2 Preliminary results on (1) and (2) and the associated Kolmogorov equations

In this section, we introduce partial differential equations related to the stochastic differential equations (1) and (2), and study their long-time behaviors. These preliminary results will be crucial to

analyze the numerical methods aimed at evaluating $\partial_\lambda^0 (\int_{\mathbb{R}^d} f d\pi_\lambda)$ that we study.

Let us introduce a few notations. For any positive Borel measure μ on \mathbb{R}^d , we denote by $\mathbb{L}^2(\mu)$ the space of real valued measurable functions on \mathbb{R}^d which are square integrable with respect to μ . We denote by $\mathbb{L}_0^2(e^{-V(x)} dx)$ the space of zero-mean square integrable functions:

$$\mathbb{L}_0^2(e^{-V(x)} dx) = \left\{ f \in \mathbb{L}^2(e^{-V(x)} dx), \int_{\mathbb{R}^d} f(x) e^{-V(x)} dx = 0 \right\}, \quad (13)$$

and by $\mathbb{H}^1(e^{-V(x)} dx)$ the first order Sobolev space associated with the measure $e^{-V(x)} dx$:

$$\mathbb{H}^1(e^{-V(x)} dx) = \left\{ f \in \mathbb{L}^2(e^{-V(x)} dx), \nabla f \in \mathbb{L}^2(e^{-V(x)} dx) \right\},$$

where ∇f is to be understood in the distributional sense.

2.1 About the solution to (1) and the regularity of the law of X_t^λ

Let us first start by an existence and uniqueness result for the process $(X_t^\lambda)_{t \geq 0}$ solution to (1).

Lemma 1. *There exists a unique strong solution to (1).*

Proof. The proof is rather standard. The existence of a weak solution to (1) is obtained thanks to the Girsanov theorem and the existence assumption for the process $(X_t^0)_{t \geq 0}$ (see Assumption **(Pot)**-iii)). Indeed,

$$\begin{aligned} dX_t^0 &= -\nabla V(X_t^0) dt + \sqrt{2} dW_t \\ &= F_\lambda(X_t^0) dt + \sqrt{2} d \left(\int_0^t \frac{1}{\sqrt{2}} (F_0 - F_\lambda)(X_s^0) ds + W_t \right). \end{aligned}$$

Indeed, under the probability \mathbb{Q} such that, for all $t \geq 0$, $((\mathcal{F}_t)_{t \geq 0})$ being the natural filtration for $(W_t)_{t \geq 0}$,

$$\frac{d\mathbb{Q}}{d\mathbb{P}} \Big|_{\mathcal{F}_t} = \exp \left(- \int_0^t \frac{1}{\sqrt{2}} (F_0 - F_\lambda)(X_s^0) dW_s - \frac{1}{4} \int_0^t |F_0 - F_\lambda|^2(X_s^0) ds \right)$$

the process $\widetilde{W}_t = \int_0^t \frac{1}{\sqrt{2}} (F_0 - F_\lambda)(X_s^0) ds + W_t$ is a Brownian motion and therefore the triple $(X_t^0, \widetilde{W}_t, \mathbb{Q})$ is a weak solution to (1). Note that thanks to the Assumption **(Drift)**-(i), the Novikov conditions are satisfied which justifies the use of the Girsanov theorem [21, Section 3.5-D].

Moreover, it is standard to check that trajectorial uniqueness holds for the stochastic differential equation (1), since from Assumption **(Drift)**-(ii), $x \mapsto F_\lambda(x)$ is locally Lipschitz (see [21, Section 5.2-B, Theorem 2.5]). As a consequence, by the Yamada-Watanabe theorem (see for example [21, Section 5.3-D]), the stochastic differential equation (1) admits a unique strong solution. \square

In the sequel, we will need some results about the Radon-Nikodym density of the distribution of the process with respect to the equilibrium measure. These properties are given in the two following Lemmas.

Lemma 2. *Whatever the choice of X_0 , for each $\lambda \in [0, \lambda_0]$ and $t > 0$, X_t^λ admits a positive density with respect to the Lebesgue measure on \mathbb{R}^d .*

Let us now consider $\lambda = 0$ and $(Y_t^x)_{t \geq 0}$ solution to (12). For all $t > 0$, the law of Y_t^x admits a density $y \mapsto p(t, x, y)$ with respect to the Lebesgue measure which satisfies the reversibility property:

$$\forall t > 0, e^{-V(x)} p(t, x, y) = e^{-V(y)} p(t, y, x), dx \otimes dy \text{-a.e.} \quad (14)$$

Remark 3. A well-known corollary of (14) is that if X_0 is distributed according to π_0 , then the process $(X_t^0)_{t \geq 0}$ solution to (2) is reversible: for any $t > 0$,

$$(X_s^0)_{s \in [0, t]} \text{ has the same law as } (X_{t-s}^0)_{s \in [0, t]}.$$

Proof. Let $\psi : \mathbb{R}^d \rightarrow \mathbb{R}$ be a bounded measurable function. By the Girsanov theorem,

$$\mathbb{E}[\psi(X_t^\lambda)] = \mathbb{E} \left[\psi(X_0 + \sqrt{2}W_t) e^{\frac{1}{\sqrt{2}} \int_0^t F_\lambda(X_0 + \sqrt{2}W_s) dW_s - \frac{1}{4} \int_0^t |F_\lambda(X_0 + \sqrt{2}W_s)|^2 ds} \right].$$

Here, the assumptions of the Girsanov theorem are satisfied. Indeed, according to [29, Theorem 2.1] these assumptions are satisfied if global-in-time existence and uniqueness in law hold for both Equation (1) (see Lemma 1) and its driftless counterpart

$$dY_t = \sqrt{2}dW_t,$$

which is a mere Brownian motion. The first assertion of Lemma 2 is thus proved. For $\lambda = 0$, we follow [16, page 91] to deduce that

$$\mathbb{E}[\psi(X_t^0)] = \mathbb{E} \left[\psi(X_0 + \sqrt{2}W_t) e^{-\frac{1}{2}V(X_0 + \sqrt{2}W_t)} e^{\frac{1}{2}V(X_0)} e^{\frac{1}{4} \int_0^t (2\Delta V - |\nabla V|^2)(X_0 + \sqrt{2}W_s) ds} \right]. \quad (15)$$

Now, if one considers the Brownian bridge:

$$\forall s \in [0, t], B_s^{x,y} = x + \sqrt{2}W_s + \frac{s}{t} (y - x - \sqrt{2}W_t)$$

one obtains by conditioning with respect to W_t :

$$\mathbb{E}(\psi(Y_t^x)) = \mathbb{E} \left(\psi(x + \sqrt{2}W_t) e^{-\frac{1}{2}V(x + \sqrt{2}W_t)} e^{\frac{1}{2}V(x)} g(x, x + \sqrt{2}W_t) \right)$$

where $g(x, y) = \mathbb{E} \left(e^{\frac{1}{4} \int_0^t (2\Delta V - |\nabla V|^2)(B_s^{x,y}) ds} \right)$. This shows that Y_t^x admits a density with respect to the Lebesgue measure:

$$p(t, x, y) = e^{-\frac{1}{2}V(y)} e^{\frac{1}{2}V(x)} g(x, y) \frac{e^{-\frac{|x-y|^2}{4t}}}{(4\pi t)^{d/2}}. \quad (16)$$

From the formula (16), it is straightforward to check that

$$e^{-V(x)} p(t, x, y) = e^{-V(y)} p(t, y, x) \quad (17)$$

by using the fact that $g(x, y) = g(y, x)$ which is a direct consequence of the fact that $(B_s^{x,y})_{s \in [0, t]}$ has the same law as $(B_{t-s}^{y,x})_{s \in [0, t]}$. This concludes the proof of Lemma 2. \square

Let us now state a few additional results on the dynamics when $\lambda = 0$ and when $(X_t^0)_{t \geq 0}$ starts from a general random variable instead of a deterministic point.

Lemma 4. Let X_0 be distributed according to some probability measure μ_0 , and let $(X_t^0)_{t \geq 0}$ evolve according to Equation (2). Denote by μ_t the distribution of the random variable X_t^0 .

For all $t > 0$, μ_t has a density $r(t, \cdot)$ with respect to $d\pi_0 = e^{-V(x)} dx$:

$$\mu_t(dx) = r(t, x) e^{-V(x)} dx.$$

Moreover, for $0 < s \leq t$, for dx-a.e. $x \in \mathbb{R}^d$,

$$r(t, x) = \mathbb{E}(r(s, Y_{t-s}^x)) \quad (18)$$

where Y_t^x satisfies (12). Equation (18) holds for $s = 0$ if μ_0 has a density $r(0, \cdot)$ with respect to $d\pi_0 = e^{-V(x)} dx$.

If there exists $s \geq 0$ such that $\|r(s, \cdot)\|_{\mathbb{L}^\infty} < \infty$, then, for all $t \geq s$,

$$\operatorname{ess\,inf}_{x \in \mathbb{R}^d} r(s, x) \leq \operatorname{ess\,inf}_{x \in \mathbb{R}^d} r(t, x) \leq \operatorname{ess\,sup}_{x \in \mathbb{R}^d} r(t, x) \leq \operatorname{ess\,sup}_{x \in \mathbb{R}^d} r(s, x). \quad (19)$$

Finally, for any $q \in [1, \infty)$, if there exists $s \geq 0$ such that $r(s, \cdot) \in \mathbb{L}^q(e^{-V(x)} dx)$, then for all $t \geq s$, $r(t, \cdot) \in \mathbb{L}^q(e^{-V(x)} dx)$ and

$$\forall t \geq s, \|r(t, \cdot)\|_{\mathbb{L}^q(e^{-V(x)} dx)} \leq \|r(s, \cdot)\|_{\mathbb{L}^q(e^{-V(x)} dx)}. \quad (20)$$

Proof. Let $\psi : \mathbb{R}^d \rightarrow \mathbb{R}$ be a bounded measurable function. By conditioning with respect to X_0 , and using the function $p(t, x, y)$ introduced in Lemma 2

$$\begin{aligned} \mathbb{E}(\psi(X_t^0)) &= \int \int \psi(y) p(t, x, y) dy d\mu_0(x) \\ &= \int \psi(y) e^{-V(y)} e^{V(y)} \int p(t, x, y) d\mu_0(x) dy. \end{aligned} \quad (21)$$

This shows that the law μ_t of X_t^0 is $r(t, y) e^{-V(y)} dy$ with

$$r(t, y) = e^{V(y)} \int p(t, x, y) d\mu_0(x).$$

Likewise, for any $s \in [0, t]$, by conditioning with respect to X_s^0 , it is easy to check that $\mathbb{E}(\psi(X_t^0)) = \int \psi(y) e^{-V(y)} e^{V(y)} \int p(t-s, x, y) d\mu_s(x) dy$. Now by taking $0 < s \leq t$ and using the reversibility property (14), we get

$$\begin{aligned} \mathbb{E}(\psi(X_t^0)) &= \int \psi(y) e^{-V(y)} \int e^{V(y)} p(t-s, x, y) d\mu_s(x) dy \\ &= \int \psi(y) e^{-V(y)} \int e^{V(x)} p(t-s, y, x) r(s, x) e^{-V(x)} dx dy. \end{aligned}$$

Since the law of X_t^0 is $r(t, y) e^{-V(y)} dy$, this shows that,

$$\text{dy-a.e.}, r(t, y) = \int p(t-s, y, x) r(s, x) dx = \mathbb{E}(r(s, Y_{t-s}^y)). \quad (22)$$

This integral is well defined since $x \mapsto p(t-s, y, x)$ and $x \mapsto r(s, x)$ are non negative measurable functions. This shows formula (18).

The maximum principle (19) is then a direct consequence from this representation formula (22).

Finally, if $r(s, \cdot) \in \mathbb{L}^q(e^{-V(x)} dx)$, then, for $t > s$, $r(t, \cdot) \in \mathbb{L}^q(e^{-V(x)} dx)$ since (using the fact that $x \mapsto p(t-s, y, x)$ is a probability density function and the reversibility property (14))

$$\begin{aligned} \int |r(t, y)|^q e^{-V(y)} dy &= \int \left| \int p(t-s, y, x) r(s, x) dx \right|^q e^{-V(y)} dy \\ &\leq \int \int p(t-s, y, x) |r(s, x)|^q dx e^{-V(y)} dy \\ &= \int \int p(t-s, x, y) e^{-V(x)} |r(s, x)|^q dx dy \\ &= \int e^{-V(x)} |r(s, x)|^q dx < \infty. \end{aligned}$$

□

Remark 5. In Appendix A, we discuss a stronger assumption on V under which we are able to get more precise bounds on $p(t, x, y)$.

2.2 A Feynman-Kac formula and the Fokker-Planck equation

For two measurable functions $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}$, with φ locally integrable with respect to the Lebesgue measure, consider the Kolmogorov equation associated with the infinitesimal generator of the stochastic differential equation (1):

$$\begin{cases} \partial_t u(t, x) = \Delta u(t, x) + F_\lambda(x) \cdot \nabla u(t, x) - \varphi(x)u(t, x), & t > 0, x \in \mathbb{R}^d, \\ u(0, x) = f(x), & x \in \mathbb{R}^d. \end{cases} \quad (23)$$

In all this section, λ is a fixed parameter in the interval $[0, \lambda_0]$.

In the following, we will consider solutions to Equation (23) in the following weak sense:

Definition 6. Let u be a function in the space

$$\mathbb{L}^\infty \left([0, T], \mathbb{L}^2(e^{-V(x)} dx) \right) \cap \mathbb{L}^2 \left([0, T], \mathbb{L}^2(|\varphi(x)|e^{-V(x)} dx) \right) \cap \mathbb{L}^2 \left([0, T], \mathbb{H}^1(e^{-V(x)} dx) \right)$$

for any $T > 0$. For $f \in \mathbb{L}^2(e^{-V(x)} dx)$, we say that u is a weak solution to (23) if $u(0, \cdot) = f$ and for any function v in $\mathbb{H}^1(e^{-V(x)} dx) \cap \mathbb{L}^2(|\varphi(x)|e^{-V(x)} dx)$,

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^d} u(t, x)v(x)e^{-V(x)} dx &= - \int_{\mathbb{R}^d} \nabla u(t, x) \cdot \nabla v(x)e^{-V(x)} dx - \int_{\mathbb{R}^d} \varphi(x)u(t, x)v(x)e^{-V(x)} dx \\ &\quad + \int_{\mathbb{R}^d} (F_\lambda(x) - F_0(x)) \cdot \nabla u(t, x)v(x)e^{-V(x)} dx \end{aligned} \quad (24)$$

in distributional sense.

Note that the last term in (24) is well defined since for $\lambda \in [0, \lambda_0]$, from Assumption **(Drift)**-(i), $\|F_\lambda - F_0\|_{\mathbb{L}^\infty(\mathbb{R}^d)} \leq C\lambda$. Moreover, note that the condition $u(0, \cdot) = f$ makes sense, since a function u satisfying

$$u \in \mathbb{L}^2([0, T], \mathbb{H}^1(e^{-V(x)} dx)) \text{ and } \partial_t u \in \mathbb{L}^2([0, T], \mathbb{H}^{-1}(e^{-V(x)} dx))$$

actually lies in $\mathcal{C}([0, T], \mathbb{L}^2(e^{-V(x)} dx))$ (see for example [31, Lemma 1.2 p. 261]).

Proposition 7. Assume $f \in \mathbb{L}^2(e^{-V(x)} dx)$ and that the function φ is locally integrable with respect to the Lebesgue measure and bounded from below. Then, Equation (23) admits a unique solution in the sense of Definition 6. Moreover, this solution is in $\mathcal{C}([0, +\infty), \mathbb{L}^2(e^{-V(x)} dx))$.

In addition, if $f \in \mathbb{H}^1(e^{-V(x)} dx) \cap \mathbb{L}^2(|\varphi(x)|e^{-V(x)} dx)$, the solution u is more regular: for any $T > 0$,

$$u \in \mathbb{L}^\infty \left([0, T], \mathbb{H}^1(e^{-V(x)} dx) \cap \mathbb{L}^2(|\varphi(x)|e^{-V(x)} dx) \right) \cap \mathbb{H}^1 \left([0, T], \mathbb{L}^2(e^{-V(x)} dx) \right).$$

Proof. By Assumption **(Drift)**-(i), there exists $C_0 > 0$ such that $\|F_\lambda - F_0\|_{\mathbb{L}^\infty(\mathbb{R}^d)} \leq C_0$. Let C be a positive constant such that $\varphi + C - \frac{C_0^2}{2}$ is nonnegative. From [31, Lemma 1.2 p. 261], one can

take $e^{-Ct}u(t, x)$ as a test function in (24) and obtain the following estimate

$$\begin{aligned}
& \frac{d}{dt} \left(\frac{e^{-Ct}}{2} \int_{\mathbb{R}^d} |u(t, x)|^2 e^{-V(x)} dx \right) \\
&= -e^{-Ct} \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx - e^{-Ct} \int_{\mathbb{R}^d} |u(t, x)|^2 (\varphi(x) + C) e^{-V(x)} dx \\
&\quad + e^{-Ct} \int_{\mathbb{R}^d} (F_\lambda - F_0) \cdot \nabla u(t, x) u(t, x) e^{-V(x)} dx \\
&\leq -e^{-Ct} \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx - e^{-Ct} \int_{\mathbb{R}^d} |u(t, x)|^2 (\varphi(x) + C) e^{-V(x)} dx \\
&\quad + \frac{e^{-Ct}}{2} \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx + \frac{e^{-Ct}}{2} C_0^2 \int_{\mathbb{R}^d} |u(t, x)|^2 e^{-V(x)} dx \\
&\leq -\frac{e^{-Ct}}{2} \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx - \int_{\mathbb{R}^d} e^{-Ct} |u(t, x)|^2 \left(\varphi(x) + C - \frac{C_0^2}{2} \right) e^{-V(x)} dx.
\end{aligned}$$

Therefore, by integrating in time, one obtains the following estimate:

$$\begin{aligned}
& \frac{e^{-Ct}}{2} \int_{\mathbb{R}^d} |u(t, x)|^2 e^{-V(x)} dx + \frac{1}{2} \int_0^t \int_{\mathbb{R}^d} e^{-Cs} |\nabla u(s, x)|^2 e^{-V(x)} dx ds \\
&+ \int_0^t \int_{\mathbb{R}^d} e^{-Cs} |u(s, x)|^2 \left(\varphi(x) + C - \frac{C_0^2}{2} \right) e^{-V(x)} dx ds = \frac{1}{2} \int_{\mathbb{R}^d} |f(x)|^2 e^{-V(x)} dx.
\end{aligned} \tag{25}$$

From this estimate, the uniqueness result follows from linearity by taking $f = 0$ in (25). And thanks to this a priori estimate, existence can be proved by using a Galerkin method on a countable family of smooth functions dense in $\mathbb{H}^1(e^{-V(x)} dx) \cap \mathbb{L}^2(|\varphi(x)|e^{-V(x)} dx)$, which exists since the measure $|\varphi(x)|e^{-V(x)} dx$ is finite on compact sets (see for example [25, chapter II, Theorem 3.5]). As explained above, the fact that $u \in \mathcal{C}([0, T], \mathbb{L}^2(e^{-V(x)} dx))$ is then a standard result, see for example [31, Lemma 1.2 p. 261].

In order to obtain the additional regularity, let us take $\partial_t u(t, x)$ as a test function in (24):

$$\begin{aligned}
\int_{\mathbb{R}^d} |\partial_t u(t, x)|^2 e^{-V(x)} dx &= -\frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx - \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} |u(t, x)|^2 \varphi(x) e^{-V(x)} dx \\
&\quad + \int_{\mathbb{R}^d} (F_\lambda - F_0) \cdot \nabla u(t, x) \partial_t u(t, x) e^{-V(x)} dx \\
&\leq -\frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx - \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} |u(t, x)|^2 \varphi(x) e^{-V(x)} dx \\
&\quad + C_0^2 \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx + \frac{1}{4} \int_{\mathbb{R}^d} |\partial_t u(t, x)|^2 e^{-V(x)} dx.
\end{aligned}$$

Therefore, for a constant $C_1 > 0$ such that $\varphi + C_1$ is nonnegative,

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx + \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} |u(t, x)|^2 (\varphi(x) + C_1) e^{-V(x)} dx + \frac{3}{4} \int_{\mathbb{R}^d} |\partial_t u(t, x)|^2 e^{-V(x)} dx \\
&\leq C_0^2 \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 + C_1 \int_{\mathbb{R}^d} u(t, x) \partial_t u(t, x) e^{-V(x)} dx \\
&\leq C_0^2 \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 + C_1^2 \int_{\mathbb{R}^d} |u(t, x)|^2 e^{-V(x)} dx + \frac{1}{4} \int_{\mathbb{R}^d} |\partial_t u(t, x)|^2 e^{-V(x)} dx.
\end{aligned}$$

Using Grönwall's Lemma, one obtains the estimate after integration in time:

$$\begin{aligned} & e^{-2C_0^2 t} \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx + e^{-2C_0^2 t} \int_{\mathbb{R}^d} |u(t, x)|^2 (\varphi(x) + C_1) e^{-V(x)} dx \\ & + \int_0^t \int_{\mathbb{R}^d} e^{-2C_0^2 s} |\partial_t u(s, x)|^2 e^{-V(x)} dx ds \leq \int_{\mathbb{R}^d} |\nabla f(x)|^2 e^{-V(x)} dx \\ & + \int_{\mathbb{R}^d} |f(x)|^2 (\varphi(x) + C_1) e^{-V(x)} dx + 2C_1^2 \int_0^t \int_{\mathbb{R}^d} e^{-2C_0^2 s} |u(s, x)|^2 e^{-V(x)} dx ds. \end{aligned}$$

The last term is bounded from above over finite time intervals by a constant times $\int_{\mathbb{R}^d} |f(x)|^2 e^{-V(x)} dx$ thanks to (25). Again, this a priori estimate can be made rigorous through a Galerkin procedure, and yields the additional regularity stated in the Proposition (see for example [26, Proposition 11.1.1] for a similar reasoning). \square

Proposition 8. *Let u be a solution to the partial differential equation (23) in the sense of Definition 6, and assume that the initial condition f is of class C^2 with locally Lipschitz second order derivatives. If φ is locally Lipschitz, then u , $\partial_t u$, ∇u and $\nabla^2 u$ are continuous functions and u is a classical solution to (23).*

Proof. We use a bootstrap argument based on $\mathbb{L}_t^p \mathbb{L}_x^q$ regularity results for parabolic partial differential equations. In order to apply standard results which require 0 as an initial condition, we consider $v = u - f$, which satisfies (in the weak sense, see Definition 6) the partial differential equation:

$$\begin{cases} \partial_t v(t, x) = \Delta v(t, x) + F_\lambda(x) \cdot \nabla v(t, x) - \varphi(x)v(t, x) + g(x), & t > 0, x \in \mathbb{R}^d, \\ v(0, x) = 0, & x \in \mathbb{R}^d, \end{cases} \quad (26)$$

where

$$g(x) = \Delta f(x) + F_\lambda(x) \cdot \nabla f(x) - \varphi(x)f(x)$$

is a locally Lipschitz function.

In this proof, we use the following notation

$$\mathbb{L}_t^p \mathbb{L}_x^q = \bigcap_{T>0} \mathbb{L}^p([0, T], \mathbb{L}^q(\mathbb{R}^d)),$$

where $\mathbb{L}^q(\mathbb{R}^d)$ is the \mathbb{L}^q space associated with the Lebesgue measure. We will also use the notations $\mathbb{L}_t^p \mathbb{W}_x^{s,p}$ where \mathbb{W} stands for the usual Sobolev space. We moreover introduce the notation

$$\mathbb{L}^{\infty-} = \bigcap_{2 \leq q < \infty} \mathbb{L}^q.$$

Last, we set

$$\mathbb{W}_t^{1,p} \mathbb{L}_x^q = \{u \in \mathbb{L}_t^p \mathbb{L}_x^q, \partial_t u \in \mathbb{L}_t^p \mathbb{L}_x^q\}.$$

Let χ be some function in the space C_0^∞ of smooth, compactly supported functions on \mathbb{R}^d . The function χv satisfies, in the weak sense, the equation

$$\begin{cases} \partial_t(\chi v) - \Delta(\chi v) = \Phi^\chi \text{ on } (0, +\infty) \times \mathbb{R}^d, \\ (\chi v)(0, x) = 0, \quad x \in \mathbb{R}^d, \end{cases}$$

where

$$\Phi^\chi = (\chi F_\lambda - 2\nabla \chi) \cdot \nabla v - (\Delta \chi + \chi \varphi)v + \chi g.$$

From parabolic regularity results, see for example [33, Theorem III.1], one has the implication:

$$(\Phi^\chi \in \mathbb{L}_t^2 \mathbb{L}_x^p) \Rightarrow (\chi v \in \mathbb{L}_t^2 \mathbb{W}_x^{2,p} \cap \mathbb{W}_t^{1,2} \mathbb{L}_x^p). \quad (27)$$

In addition, from the definition of Φ^χ , one has

$$(\forall \chi \in \mathcal{C}_0^\infty, \chi v \in \mathbb{L}_t^2 \mathbb{W}_x^{2,p}) \Rightarrow (\forall \chi \in \mathcal{C}_0^\infty, \Phi^\chi \in \mathbb{L}_t^2 \mathbb{W}_x^{1,p}) \quad (28)$$

since φ and F_λ are locally Lipschitz functions (see Assumption **(Drift)**-(ii)).

Now, by Definition 6, the function v lies in $\mathbb{L}^\infty([0, T], \mathbb{L}^2(e^{-V(x)} dx)) \cap \mathbb{L}^2([0, T], \mathbb{H}^1(e^{-V(x)} dx))$, so that Φ^χ lies in $\mathbb{L}_t^2 \mathbb{L}_x^2$, for any function $\chi \in \mathcal{C}_0^\infty$. First assume $d > 1$, and let \bar{p} be the supremum of all those p such that Φ^χ lies in $\mathbb{L}_t^2 \mathbb{L}_x^p$ for all χ . Assume $\bar{p} < \infty$. Since

$$\frac{d\bar{p}}{d + \bar{p}} < \min(\bar{p}, d),$$

one can find some $p \in \left(\frac{d\bar{p}}{d + \bar{p}}, d\right)$, such that Φ^χ belongs to $\mathbb{L}_t^2 \mathbb{L}_x^p$ for any χ (note that $\frac{d\bar{p}}{d + \bar{p}} \geq 1$, since $\frac{1}{d} + \frac{1}{\bar{p}} \leq \frac{1}{2} + \frac{1}{2} = 1$). From (27) χv lies in $\mathbb{L}_t^2 \mathbb{W}_x^{2,p}$, and hence from (28), Φ^χ lies in $\mathbb{L}_t^2 \mathbb{W}_x^{1,p}$. However, Sobolev embeddings yield

$$\Phi^\chi \in \mathbb{L}_t^2 \mathbb{W}_x^{1,p} \subset \mathbb{L}_t^2 \mathbb{L}_x^{\frac{dp}{d-p}}, \text{ where } \frac{dp}{d-p} > \bar{p} \text{ since } p > \frac{d\bar{p}}{d + \bar{p}},$$

which contradicts the definition of \bar{p} . As a conclusion, Φ^χ lies in $\mathbb{L}_t^2 \mathbb{L}_x^{\infty-}$ for any χ . In the case $d = 1$, one can directly deduce from $\Phi^\chi \in \mathbb{L}_t^2 \mathbb{L}_x^2$ that χv is in $\mathbb{L}_t^2 \mathbb{W}_x^{2,2} \subset \mathbb{L}_t^2 \mathbb{W}_x^{1,\infty-}$ for any χ , and thus $\Phi^\chi \in \mathbb{L}_t^2 \mathbb{L}_x^{\infty-}$ for any χ . In any case, χv lies in $\mathbb{L}_t^2 \mathbb{W}_x^{2,\infty-}$ for any χ .

Now consider the equation satisfied by $\chi \partial_i v$, for any coordinate i . One obtains

$$\begin{cases} \partial_t(\chi \partial_i v) - \Delta(\chi \partial_i v) = \Psi^\chi \text{ on } (0, +\infty) \times \mathbb{R}^d, \\ (\chi \partial_i v)(0, x) = 0, \quad x \in \mathbb{R}^d, \end{cases} \quad (29)$$

where

$$\Psi^\chi = (\chi F_\lambda - 2\nabla \chi) \cdot \nabla(\partial_i v) + (\chi \partial_i F_\lambda - (\Delta \chi + \chi \varphi) e_i) \cdot \nabla v - (\chi \partial_i \varphi) v + \chi \partial_i g.$$

Since χv lies in $\mathbb{L}_t^2 \mathbb{W}_x^{2,\infty-}$ for any $\chi \in \mathcal{C}_0^\infty$, the function Ψ^χ is in $\mathbb{L}_t^2 \mathbb{L}_x^{\infty-}$, from the boundedness of $\chi \partial_i \varphi$, $\chi \partial_i g$ and $\chi \partial_i F_\lambda$. Then, parabolic regularity (27) for the heat equation (29) implies

$$\forall i, \forall \chi \in \mathcal{C}_0^\infty, \chi \partial_i v \in \mathbb{L}_t^2 \mathbb{W}_x^{2,\infty-} \cap \mathbb{W}_t^{1,2} \mathbb{L}_x^{\infty-}.$$

In particular, for any $\chi \in \mathcal{C}_0^\infty$, χv is in $\mathbb{W}_t^{1,2} \mathbb{W}_x^{1,\infty-}$. From Sobolev embeddings, we deduce that χv lies in $\mathcal{C}_t^{1/2} \mathcal{C}_x^{1-\varepsilon}$, for any ε in $(0, 1)$ (\mathcal{C}^s stand for Hölder spaces). From the Hölder regularity of the initial condition, Hölder regularity theory for the heat equation now yields the desired regularity on v (and thus on u), see for example [22, Theorem 10.3.3]. \square

Proposition 9. *Assume $f \in \mathbb{L}^2(e^{-V(x)} dx)$ and that φ is locally Lipschitz and bounded from below. Then the solution $u(t, x)$ to the partial differential equation (23) given by Proposition 7 admits the following probabilistic representation formula: for all $t \geq 0$,*

$$dx\text{-a.e.}, u(t, x) = \mathbb{E} \left[f(Y_t^{\lambda,x}) e^{-\int_0^t \varphi(Y_s^{\lambda,x}) ds} \right] \quad (30)$$

where $(Y_t^{\lambda,x})_{t \geq 0}$ is defined by (notice that $(Y_t^{0,x})_{t \geq 0} = (Y_t^x)_{t \geq 0}$ is defined by (12))

$$\begin{cases} dY_t^{\lambda,x} = F_\lambda(Y_t^{\lambda,x}) dt + \sqrt{2} dW_t, \\ Y_0^{\lambda,x} = x. \end{cases} \quad (31)$$

Proof. Step 1: Let us first prove a maximum principle for solutions to Equation (23) in the sense of Definition 6. Assume that the initial condition f of Equation (23) is bounded from above by some nonnegative constant M . Let C be a constant such that $\varphi + C$ is nonnegative. From [31, Lemma 1.2 p. 261], and [17, Lemma 7.6], one can take $e^{-Ct}(e^{-Ct}u(t, x) - M)^+$ as the test function in the weak formulation (24), and obtain (using the fact that from Assumption **(Drift)**-(i), $\|F_\lambda - F_0\|_{\mathbb{L}^\infty(\mathbb{R}^d)} \leq C_0$ for some $C_0 > 0$)

$$\begin{aligned}
& \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} |(e^{-Ct}u(t, x) - M)^+|^2 e^{-V(x)} dx \\
&= - \int_{\mathbb{R}^d} |\nabla(e^{-Ct}u(t, x) - M)^+|^2 e^{-V(x)} dx \\
&\quad - \int_{\mathbb{R}^d} (\varphi(x) + C)e^{-Ct}u(t, x)(e^{-Ct}u(t, x) - M)^+ e^{-V(x)} dx \\
&\quad + \int_{\mathbb{R}^d} (F_\lambda(x) - F_0(x)) \cdot \nabla(e^{-Ct}u(t, x) - M)^+ (e^{-Ct}u(t, x) - M)^+ e^{-V(x)} dx \\
&\leq - \frac{1}{2} \int_{\mathbb{R}^d} |\nabla(e^{-Ct}u(t, x) - M)^+|^2 e^{-V(x)} dx \\
&\quad - \int_{\mathbb{R}^d} (\varphi(x) + C)e^{-Ct}u(t, x)(e^{-Ct}u(t, x) - M)^+ e^{-V(x)} dx \\
&\quad + \frac{C_0^2}{2} \int_{\mathbb{R}^d} |(e^{-Ct}u(t, x) - M)^+|^2 e^{-V(x)} dx.
\end{aligned}$$

By using Grönwall's Lemma, one therefore obtain after integration in time:

$$\begin{aligned}
& \frac{e^{-C_0^2 t}}{2} \int_{\mathbb{R}^d} |(e^{-Ct}u(t, x) - M)^+|^2 e^{-V(x)} dx \\
&\leq - \frac{1}{2} \int_0^t \int_{\mathbb{R}^d} e^{-C_0^2 s} |\nabla(e^{-Cs}u(s, x) - M)^+|^2 e^{-V(x)} dx ds \\
&\quad - \int_0^t \int_{\mathbb{R}^d} e^{-C_0^2 s} (\varphi(x) + C)e^{-Cs}u(s, x)(e^{-Cs}u(s, x) - M)^+ e^{-V(x)} dx ds \\
&\quad + \frac{1}{2} \int_{\mathbb{R}^d} |(f(x) - M)^+|^2 e^{-V(x)} dx \leq 0
\end{aligned}$$

so that the function $u(t, \cdot)$ is bounded from above by Me^{Ct} , for any positive t . By a similar argument, if f is bounded from below by $-M$, with M nonnegative, then $u(t, \cdot)$ is bounded from below by $-e^{-Ct}M$ for any positive t .

Step 2: Let us now prove the Feynman-Kac formula (30) under the assumption $f \in \mathcal{C}^\infty \cap \mathbb{L}^\infty(\mathbb{R}^d)$. Let $x \in \mathbb{R}^d$, $t > 0$ and $M > 0$. Let τ_M be the first exit time from $B(x, M)$ (namely the ball centered at x and of radius M) for the process $(Y_s^{\lambda, x})_{s \geq 0}$. Since $s \mapsto Y_s^{\lambda, x}$ is continuous, τ_M goes to ∞ as M goes to ∞ . Let us consider the solution $(t, x) \mapsto u(t, x)$ to (23), which is \mathcal{C}^1 with respect to t and \mathcal{C}^2 with respect to x thanks to Proposition 8. Applying Itô's formula to $u(t - s, Y_s^{\lambda, x})$ in the time interval $[0, t \wedge \tau_M]$, one obtains

$$u((t - \tau_M)^+, Y_{t \wedge \tau_M}^{\lambda, x}) e^{-\int_0^{t \wedge \tau_M} \varphi(Y_s^{\lambda, x}) ds} = u(t, x) + \sqrt{2} \int_0^{t \wedge \tau_M} \nabla u(t - s, Y_s^{\lambda, x}) e^{-\int_0^s \varphi(Y_u^{\lambda, x}) du} dW_s.$$

On the interval $[0, t \wedge \tau_M]$, the integrand in the stochastic integral remains bounded, so that this integral has zero mean. Taking the expectation, one obtains

$$u(t, x) = \mathbb{E} \left[u((t - \tau_M)^+, Y_{t \wedge \tau_M}^{\lambda, x}) e^{-\int_0^{t \wedge \tau_M} \varphi(Y_s^{\lambda, x}) ds} \right].$$

By the above maximum principle the function u is bounded on $[0, t] \times \mathbb{R}^d$. With the lower bound on φ , the dominated convergence theorem yields, letting $M \rightarrow \infty$,

$$u(t, x) = \mathbb{E} \left[f(Y_t^{\lambda, x}) e^{-\int_0^t \varphi(Y_s^{\lambda, x}) ds} \right].$$

Step 3: Let us now assume that f is in $\mathbb{L}^\infty(\mathbb{R}^d)$. Let f_n be a sequence of C^∞ functions such that $\sup_{n \geq 1} \|f_n\|_{\mathbb{L}^\infty(\mathbb{R}^d)} \leq \|f\|_{\mathbb{L}^\infty(\mathbb{R}^d)}$, and converging to f almost everywhere. In particular, f_n converges to f in $\mathbb{L}^2(e^{-V(x)} dx)$ by Lebesgue's theorem. Therefore, the solution u_n to Equation (23) starting from f_n is such that $u_n(t, \cdot)$ converges to $u(t, \cdot)$ as $n \rightarrow \infty$ in $\mathbb{L}^2(e^{-V(x)} dx)$, from the a priori estimate (25). Moreover, one has

$$\forall x \in \mathbb{R}^d, u_n(t, x) = \mathbb{E} \left[f_n(Y_t^{\lambda, x}) e^{-\int_0^t \varphi(Y_s^{\lambda, x}) ds} \right] = \mathbb{E}[f_n(Y_t^{\lambda, x}) \Gamma(Y_t^{\lambda, x})],$$

where Γ is a bounded function satisfying $\Gamma(Y_t^{\lambda, x}) = \mathbb{E} \left[e^{-\int_0^t \varphi(Y_s^{\lambda, x}) ds} \middle| Y_t^{\lambda, x} \right]$. For the remaining of the proof, we assume that $t > 0$ (the formula (30) clearly holds for $t = 0$). From Lemma 2, the distribution of $Y_t^{\lambda, x}$ admits a density $p^\lambda(t, x, y)$ with respect to the Lebesgue measure. Therefore, by the Lebesgue theorem, $\mathbb{E}[f_n(Y_t^{\lambda, y}) \Gamma(Y_t^{\lambda, y})]$ converges to $\mathbb{E}[f(Y_t^{\lambda, y}) \Gamma(Y_t^{\lambda, y})]$ as $n \rightarrow \infty$. This shows the equality $u(t, x) = \mathbb{E} \left[f(Y_t^{\lambda, x}) e^{-\int_0^t \varphi(Y_s^{\lambda, x}) ds} \right]$ for dx-a.e. x .

Step 4: Let us now assume that f is in $\mathbb{L}^2(e^{-V(x)} dx)$ and let us write $f = f^+ - f^-$ where $f^+ = \max(f, 0)$ and $f^- = \max(-f, 0)$. For $n \in \mathbb{N}$, the functions $f_n^+ = \min(f^+, n)$ (resp. $f_n^- = \min(f^-, n)$) are in $\mathbb{L}^\infty(\mathbb{R}^d)$ and converge in $\mathbb{L}^2(e^{-V(x)} dx)$ to f^+ (resp. f^-). Let us consider the solution u_n^+ (resp. u_n^-) to Equation (23) starting from f_n^+ (resp. f_n^-). Since $f_n^+ - f_n^-$ converges as $n \rightarrow \infty$ to f in $\mathbb{L}^2(e^{-V(x)} dx)$, for every $t \geq 0$, $u_n^+(t, \cdot) - u_n^-(t, \cdot)$ converges in $\mathbb{L}^2(e^{-V(x)} dx)$ to $u(t, \cdot)$, where u is the solution to Equation (23) starting from f . Moreover, one has

$$\text{dx-a.e.}, u_n^\pm(t, x) = \mathbb{E} \left[f_n^\pm(Y_t^{\lambda, x}) e^{-\int_0^t \varphi(Y_s^{\lambda, x}) ds} \right] = \mathbb{E}[f_n^\pm(Y_t^{\lambda, x}) \Gamma(Y_t^{\lambda, x})],$$

where Γ is the bounded function defined above. By the monotone convergence theorem, $\mathbb{E}[f_n^\pm(Y_t^{\lambda, x}) \Gamma(Y_t^{\lambda, x})]$ converges to $\mathbb{E}[f^\pm(Y_t^{\lambda, x}) \Gamma(Y_t^{\lambda, x})]$. This shows the equality $u(t, x) = \mathbb{E} \left[f(Y_t^{\lambda, x}) e^{-\int_0^t \varphi(Y_s^{\lambda, x}) ds} \right]$ for dx-a.e. x . \square

As a corollary of the previous result, we obtain that the law of X_t^0 satisfies a partial differential equation (the Fokker-Planck equation).

Corollary 10. *Let X_0 be distributed according to some probability measure μ_0 , and let $(X_t^0)_{t \geq 0}$ evolve according to Equation (2). Let us assume that μ_0 has a density r_0 with respect to $d\pi_0 = e^{-V(x)} dx$ such that $r_0 \in \mathbb{L}^2(e^{-V(x)} dx)$. Denote by μ_t the distribution of the random variable X_t^0 , and by $x \mapsto r(t, x)$ the density of μ_t with respect to $d\pi_0 = e^{-V(x)} dx$ which exists by Lemma 4.*

Then, $r(t, x)$ is the unique solution to the partial differential equation

$$\begin{cases} \partial_t r(t, x) = \Delta r(t, x) - \nabla V(x) \cdot \nabla r(t, x), & t > 0, x \in \mathbb{R}^d, \\ r(0, x) = r_0(x), & x \in \mathbb{R}^d, \end{cases} \quad (32)$$

in the sense of Definition 6.

Proof. From Lemma 4, we know that

$$\forall t \geq 0, \text{dx-a.e.}, r(t, x) = \mathbb{E}(r_0(Y_t^x)).$$

The conclusion is then a consequence of the Feynman-Kac representation formula (30). \square

2.3 Long-time behavior of the partial differential equation (23) when $\lambda = 0$

In this section, we are interested in the long-time behavior of the partial differential equation (23) when $\lambda = 0$, which is related to the stochastic differential equation (2) through the Feynman-Kac formula (30).

2.3.1 The case $\varphi = 0$

To study the long-time behavior of the solution to (23) with $\lambda = \varphi = 0$, we introduce the following hypothesis (defined for any $\eta > 0$).

Assumption (Poinc(η)). *The measure e^{-V} satisfies a Poincaré inequality with constant $\eta > 0$: for any function v in $\mathbb{L}_0^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx)$,*

$$\eta \int_{\mathbb{R}^d} |v|^2(x) e^{-V(x)} dx \leq \int_{\mathbb{R}^d} |\nabla v|^2(x) e^{-V(x)} dx. \quad (33)$$

Recall that $\mathbb{L}_0^2(e^{-V(x)} dx)$ denotes the functions in $\mathbb{L}^2(e^{-V(x)} dx)$ with zero mean with respect to π_0 (see (13)).

Proposition 11. *Let Assumption (Poinc(η)) be satisfied for some positive η , and let u be a solution to (23) in the sense of Definition 6, in the case $\lambda = \varphi = 0$, with an initial condition $f \in \mathbb{L}^2(e^{-V(x)} dx)$. Then u converges exponentially fast to the constant function $\int_{\mathbb{R}^d} f(x) e^{-V(x)} dx$ in the following sense:*

$$\forall t \geq 0, \left\| u(t, \cdot) - \int_{\mathbb{R}^d} f(x) e^{-V(x)} dx \right\|_{\mathbb{L}^2(e^{-V(x)} dx)} \leq e^{-\eta t} \left\| f - \int_{\mathbb{R}^d} f(x) e^{-V(x)} dx \right\|_{\mathbb{L}^2(e^{-V(x)} dx)}.$$

Proof. Taking the constant function $\mathbf{1}$ as the test function in (24), one obtains that $\int_{\mathbb{R}^d} u(t, x) e^{-V(x)} dx = \int_{\mathbb{R}^d} f(x) e^{-V(x)} dx$ for any $t \geq 0$. In particular, $u(t, \cdot) - \int_{\mathbb{R}^d} f(x) e^{-V(x)} dx \in \mathbb{L}_0^2(e^{-V(x)} dx)$. In addition, from [31, Lemma 1.2 p. 261], one can take $u(t, \cdot) - \int_{\mathbb{R}^d} f(x) e^{-V(x)} dx$ as the test function in (24), which yields, using the Poincaré inequality,

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} \left| u(t, x) - \int_{\mathbb{R}^d} f(x) e^{-V(x)} dx \right|^2 e^{-V(x)} dx &= - \int_{\mathbb{R}^d} |\nabla u(t, x)|^2 e^{-V(x)} dx \\ &\leq -\eta \int_{\mathbb{R}^d} \left| u(t, x) - \int_{\mathbb{R}^d} f(x) e^{-V(x)} dx \right|^2 e^{-V(x)} dx. \end{aligned}$$

One concludes from Grönwall's lemma. \square

This Proposition shows that, under the assumption of Corollary 10 (namely $d\mu_0 = r(0, x) e^{-V(x)} dx$ with $r(0, \cdot) \in \mathbb{L}^2(e^{-V(x)} dx)$), the density $r(t, x)$ of X_t^0 with respect to π_0 converges exponentially fast to 1 if (Poinc(η)) is satisfied for some positive η . Actually, the convergence of $d\mu_t$ to $e^{-V(x)} dx$ holds in total variation norm for any initial condition μ_0 .

Corollary 12. *Let Assumption (Poinc(η)) be satisfied for some positive η , and let $(X_t^0)_{t \geq 0}$ evolve according to Equation (2). Let us assume that X_0 is distributed according to some probability measure μ_0 . Denote by μ_t the distribution of the random variable X_t^0 , and for all $t > 0$, denote by $q(t, x)$ the density of μ_t with respect to the Lebesgue measure (which exists according to Lemma 2). Then*

$$\lim_{t \rightarrow \infty} \|q(t, \cdot) - e^{-V}\|_{\mathbb{L}^1(dx)} = 0.$$

Proof. From Equation (21), for all $t > 0$, one has

$$\text{dy-a.e.}, q(t, y) = \int p(t, x, y) \mu_0(dx).$$

Let us fix a positive ε . Let us consider $t_0 > 0$ (to be fixed later on) and $q^\varepsilon(t_0, x)$ a function in $\mathbb{L}^\infty(\mathbb{R}^d)$ which is non-negative, with compact support, such that $\int q^\varepsilon(t_0, x) dx = 1$ and

$$\int_{\mathbb{R}^d} |q(t_0, x) - q^\varepsilon(t_0, x)| dx \leq \varepsilon.$$

To build such a function $q^\varepsilon(t_0, \cdot)$, one could for example consider for n large enough $\frac{\min(q(t_0, x), n) 1_{|x| \leq n}}{\int \min(q(t_0, x), n) 1_{|x| \leq n}}$ which indeed converges to $q(t, x)$ in $\mathbb{L}^1(dx)$ when $n \rightarrow \infty$. Let us define the function

$$q^\varepsilon(t, y) = \int p(t - t_0, x, y) q^\varepsilon(t_0, x) dx \quad \forall t \geq t_0, \forall y \in \mathbb{R}^d.$$

For $t \geq t_0$, $q^\varepsilon(t, \cdot)$ is the density at time t of the process $(X_t^{0, \varepsilon})_{t \geq t_0}$ solution to (2), with $X_{t_0}^{0, \varepsilon}$ distributed according to $q^\varepsilon(t_0, x) dx$. Let us now set $r^\varepsilon(t, x) = e^{V(x)} q^\varepsilon(t, x)$, the density of $X_t^{0, \varepsilon}$ with respect to $e^{-V(x)} dx$. Since $r^\varepsilon(t_0, x) = e^{V(x)} q^\varepsilon(t_0, x) \in \mathbb{L}^2(e^{-V(x)} dx)$, from Corollary 10, $(s, x) \mapsto r^\varepsilon(t_0 + s, x)$ satisfies the following partial differential equation (with unknown r)

$$\begin{cases} \partial_t r(s, x) = \Delta r(s, x) - \nabla V(x) \cdot \nabla r(s, x), & s \geq 0, x \in \mathbb{R}^d, \\ r(0, x) = r^\varepsilon(t_0, x), & x \in \mathbb{R}^d, \end{cases}$$

in the sense of Definition 6. In particular, from Proposition 11, since $\int r^\varepsilon(t_0, x) e^{-V(x)} dx = 1$,

$$\forall t \geq t_0, \|r^\varepsilon(t, \cdot) - 1\|_{\mathbb{L}^2(e^{-V(x)} dx)} \leq e^{-\eta(t-t_0)} \|r^\varepsilon(t_0, \cdot) - 1\|_{\mathbb{L}^2(e^{-V(x)} dx)}$$

which is equivalent to

$$\forall t \geq t_0, \|q^\varepsilon(t, \cdot) - e^{-V}\|_{\mathbb{L}^2(e^{V(x)} dx)} \leq e^{-\eta(t-t_0)} \|q^\varepsilon(t_0, \cdot) - e^{-V}\|_{\mathbb{L}^2(e^{V(x)} dx)}.$$

By Cauchy-Schwarz inequality, we deduce that $\forall t \geq t_0$

$$\begin{aligned} \|q^\varepsilon(t, \cdot) - e^{-V}\|_{\mathbb{L}^1(dx)} &= \int_{\mathbb{R}^d} |q^\varepsilon(t, x) - e^{-V(x)}| e^{V(x)/2} \times e^{-V(x)/2} dx \\ &\leq \|q^\varepsilon(t, \cdot) - e^{-V}\|_{\mathbb{L}^2(e^{V(x)} dx)} \leq e^{-\eta(t-t_0)} \|q^\varepsilon(t_0, \cdot) - e^{-V}\|_{\mathbb{L}^2(e^{V(x)} dx)}. \end{aligned}$$

Moreover, we also have: $\forall t \geq t_0$

$$\begin{aligned} \|q(t, \cdot) - q^\varepsilon(t, \cdot)\|_{\mathbb{L}^1(dx)} &= \int_{\mathbb{R}^d} \left| \int_{\mathbb{R}^d} (q(t_0, x) - q^\varepsilon(t_0, x)) p(t - t_0, x, y) dx \right| dy \\ &\leq \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} |q(t_0, x) - q^\varepsilon(t_0, x)| p(t - t_0, x, y) dx dy \\ &= \int_{\mathbb{R}^d} |q(t_0, x) - q^\varepsilon(t_0, x)| dx \leq \varepsilon. \end{aligned}$$

We thus obtain: $\forall t \geq t_0$,

$$\begin{aligned} \|q(t, \cdot) - e^{-V}\|_{\mathbb{L}^1(dx)} &\leq \|q(t, \cdot) - q^\varepsilon(t, \cdot)\|_{\mathbb{L}^1(dx)} + \|q^\varepsilon(t, \cdot) - e^{-V}\|_{\mathbb{L}^1(dx)} \\ &\leq \varepsilon + e^{-\eta(t-t_0)} \|q^\varepsilon(t_0, \cdot) - e^{-V}\|_{\mathbb{L}^2(e^{V(x)} dx)} \end{aligned}$$

and the right-hand side is smaller than 2ε for t sufficiently large. This concludes the proof. \square

2.3.2 The case $\varphi \neq 0$

In this section, we are going to investigate the long-time behavior of the function u defined by

$$u(t, x) = \mathbb{E} \left[e^{-\int_0^t \varphi(Y_s^x) ds} \right], \quad (34)$$

for a generic function φ where, we recall, $(Y_s^x)_{s \geq 0}$ satisfies (12). When $\varphi \geq \alpha$ for some positive constant α , u converges to 0 exponentially fast as $t \rightarrow \infty$. We now look for hypotheses on φ under which this convergence is preserved in the case $\inf \varphi \leq 0$.

Notice that by ergodicity, almost surely, $\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \varphi(Y_s^x) ds = \int \varphi e^{-V(x)} dx$ and therefore, the almost sure exponential decay to zero is ensured if $\int_{\mathbb{R}^d} \varphi(x) e^{-V(x)} dx > 0$, at any rate in $(0, \int_{\mathbb{R}^d} \varphi(x) e^{-V(x)} dx)$. The exponential decay to zero in L^1 is more complicated to establish. In Proposition 13 below, we prove this exponential decay under a sufficient condition which contains the assumption $\int_{\mathbb{R}^d} \varphi(x) e^{-V(x)} dx > 0$.

When φ is bounded from below and locally Lipschitz, from Proposition 9, the function u defined by (34) is solution (in the sense of Definition 6) to the partial differential equation (23) with $f = 1$ and $\lambda = 0$. As a consequence, the long-time behavior of (34) is related to the spectrum of the operator $\Delta - \nabla V \cdot \nabla - \varphi$ which is self-adjoint in $L^2(e^{-V(x)} dx)$.

One way to study this spectrum is to perform the change of variable $v(t, x) = e^{-\frac{1}{2}V(x)} u(t, x)$, making Equation (23) become

$$\partial_t v = \Delta v + \frac{1}{4} (2\Delta V - |\nabla V|^2 - 4\varphi) v.$$

As a consequence, the long-time behavior of v is characterized by the spectrum of the Schrödinger operator $\Delta + \frac{1}{4} (2\Delta V - |\nabla V|^2 - 4\varphi)$, which can be controlled by the Cwikel-Lieb-Rozenblum bound (see for example [10, 24, 28]). Indeed, for $d \geq 3$, this bound states that the number N of nonnegative eigenvalues of $\Delta + W$ satisfies

$$N \leq L_d \int_{\mathbb{R}^d} \max(W(x), 0)^{d/2} dx,$$

where L_d is some constant independent of W . In particular, if there exists $\varepsilon > 0$ such that

$$\int_{\mathbb{R}^d} \max \left(\varepsilon + \frac{1}{2} \Delta V(x) - \frac{1}{4} |\nabla V(x)|^2 - \varphi(x), 0 \right)^{d/2} dx < \frac{1}{L_d}, \quad (35)$$

then the spectrum of $\Delta + \frac{1}{4} (2\Delta V - |\nabla V|^2 - 4\varphi)$ is included in $(-\infty, -\varepsilon)$.

There are two main concerns with this approach. First, the constant L_d is unknown, so that the criterion is not quantitative. Moreover, by Jensen's inequality, the exponential convergence to 0 of

$$\mathbb{E} \left[e^{-\delta \int_0^t \varphi(X_s^0) ds} \right]$$

for $\delta > 1$ implies the exponential convergence of the function $u(t, x)$ in (34). However, in some cases, the criterion (35) may apply to $\delta\varphi$ for some $\delta > 1$ and not to φ . We are going to present another criterion which does not present these flaws.

Proposition 13. *Assume that **(Poinc)(η)** holds for some positive η , and that*

$$-\infty < \inf \varphi \leq 0, \quad \int_{\mathbb{R}^d} \varphi(x) e^{-V(x)} dx > 0, \quad \int_{\mathbb{R}^d} \varphi(x)^2 e^{-V(x)} dx < \infty, \quad (36)$$

$$\text{and } -(\inf \varphi) \frac{\int_{\mathbb{R}^d} \varphi^2(x) e^{-V(x)} dx}{\left(\int_{\mathbb{R}^d} \varphi(x) e^{-V(x)} dx \right)^2} < \eta. \quad (37)$$

Let $\mathbf{E} = \int_{\mathbb{R}^d} \varphi(x) e^{-V(x)} dx$, $\mathbf{V} = \int_{\mathbb{R}^d} (\varphi(x) - \mathbf{E})^2 e^{-V(x)} dx$ and let u be the weak solution to Equation (23) in the sense of Definition 6 for $\lambda = 0$, with an initial condition $f \in \mathbb{L}^2(e^{-V(x)} dx)$. The quantity $\int_{\mathbb{R}^d} u^2 e^{-V}$ converges exponentially fast to 0 as $t \rightarrow \infty$:

$$\exists C > 0, \forall t > 0, \int_{\mathbb{R}^d} u^2(t, x) e^{-V(x)} dx \leq C e^{-\beta t},$$

with a rate β given by

$$\beta = \left(\eta + \inf \varphi + \frac{\mathbf{E}^2 + \mathbf{V}}{2\mathbf{E}} \right) - \sqrt{\left(\eta + \inf \varphi - \frac{\mathbf{E}^2 + \mathbf{V}}{2\mathbf{E}} \right)^2 + 2\frac{\eta\mathbf{V}}{\mathbf{E}}} > 0. \quad (38)$$

Note that the positivity of the rate (38) is equivalent to the condition (37). Moreover, note that the left-hand side in condition (37) is homogeneous of order 1 in φ , unlike the criterion (35) obtained using the Cwikel-Lieb-Rozenblum bound. As a consequence, if the criterion (37) applies to $\delta\varphi$ for some real number $\delta > 1$, then it applies to φ , as expected.

Proof of Proposition 13. In this proof, for notational simplicity, we omit the time and space variables in the integrals, which are all considered with respect to the Lebesgue measure on \mathbb{R}^d .

From [31, Lemma 1.2 p. 261], one can take u as the test function in (24), obtaining

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} u^2 e^{-V} &= - \int_{\mathbb{R}^d} |\nabla u|^2 e^{-V} - \int_{\mathbb{R}^d} \varphi u^2 e^{-V} \\ &\leq - \int_{\mathbb{R}^d} |\nabla u|^2 e^{-V} - \inf \varphi \int_{\mathbb{R}^d} u^2 e^{-V}. \end{aligned}$$

Using (33), one deduces that

$$\frac{1}{2} \frac{d}{dt} \int_{\mathbb{R}^d} u^2 e^{-V} \leq -(\eta + \inf \varphi) \int_{\mathbb{R}^d} u^2 e^{-V} + \eta \left(\int_{\mathbb{R}^d} u e^{-V} \right)^2. \quad (39)$$

On the other hand, taking the constant function $\mathbf{1}$ as the test function in (24),

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \left(\int_{\mathbb{R}^d} u e^{-V} \right)^2 &= - \int_{\mathbb{R}^d} u e^{-V} \int_{\mathbb{R}^d} \varphi u e^{-V} \\ &= - \int_{\mathbb{R}^d} \varphi e^{-V} \left(\int_{\mathbb{R}^d} u e^{-V} \right)^2 + \int_{\mathbb{R}^d} u e^{-V} \left(\int_{\mathbb{R}^d} \varphi e^{-V} \int_{\mathbb{R}^d} u e^{-V} - \int_{\mathbb{R}^d} \varphi u e^{-V} \right). \end{aligned}$$

By Cauchy-Schwarz inequality,

$$\begin{aligned} \left| \int_{\mathbb{R}^d} \varphi e^{-V} \int_{\mathbb{R}^d} u e^{-V} - \int_{\mathbb{R}^d} \varphi u e^{-V} \right| &= \left| \int_{\mathbb{R}^d} \left(\varphi - \int_{\mathbb{R}^d} \varphi e^{-V} \right) \left(u - \int_{\mathbb{R}^d} u e^{-V} \right) e^{-V} \right| \\ &\leq \mathbf{V}^{1/2} \left(\int_{\mathbb{R}^d} \left(u - \int_{\mathbb{R}^d} u e^{-V} \right)^2 e^{-V} \right)^{1/2}. \end{aligned} \quad (40)$$

Therefore, from the inequality $2ab \leq a^2 + b^2$,

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \left(\int_{\mathbb{R}^d} u e^{-V} \right)^2 &\leq -\frac{\mathbf{E}}{2} \left(\int_{\mathbb{R}^d} u e^{-V} \right)^2 + \frac{\mathbf{V}}{2\mathbf{E}} \left(\int_{\mathbb{R}^d} \left(u - \int_{\mathbb{R}^d} u e^{-V} \right)^2 e^{-V} \right) \\ &= -\frac{\mathbf{E}^2 + \mathbf{V}}{2\mathbf{E}} \left(\int_{\mathbb{R}^d} u e^{-V} \right)^2 + \frac{\mathbf{V}}{2\mathbf{E}} \int_{\mathbb{R}^d} u^2 e^{-V}. \end{aligned} \quad (41)$$

By combining (39) and (41), one obtains for $\delta \geq 0$,

$$\frac{1}{2} \frac{d}{dt} \left(\int_{\mathbb{R}^d} u^2 e^{-V} + \delta \left(\int_{\mathbb{R}^d} u e^{-V} \right)^2 \right) \leq -c_1(\delta) \int_{\mathbb{R}^d} u^2 e^{-V} - c_2(\delta) \left(\int_{\mathbb{R}^d} u e^{-V} \right)^2 \quad (42)$$

with

$$c_1(\delta) = \eta + \inf \varphi - \frac{\delta \mathbf{V}}{2\mathbf{E}} \text{ and } c_2(\delta) = -\eta + \frac{\delta \mathbf{V} + \mathbf{E}^2}{2\mathbf{E}}. \quad (43)$$

We want to find $\delta \geq 0$ such that (42) ensures exponential convergence to 0 of $\int_{\mathbb{R}^d} u^2 e^{-V}$ as $t \rightarrow +\infty$. If $\delta = 0$, one has $c_2(0) = -\eta < 0$, so we need $\delta > 0$. We look for $\delta > 0$ such that both $c_1(\delta)$ and $c_2(\delta)$ are positive.

From (43), $c_1(\delta)$ is positive if and only if

$$\frac{\delta}{2\mathbf{E}} < \frac{\eta + \inf \varphi}{\mathbf{V}}$$

and $c_2(\delta)$ is positive if and only if

$$\frac{\delta}{2\mathbf{E}} > \frac{\eta}{\mathbf{V} + \mathbf{E}^2}.$$

One concludes by checking that condition (37) is necessary and sufficient for the interval $\left(\frac{\eta}{\mathbf{V} + \mathbf{E}^2}, \frac{\eta + \inf \varphi}{\mathbf{V}} \right)$ to be nonempty.

For a given $\delta > 0$, Equation (42) gives a convergence rate of $2 \min(c_1(\delta), \frac{c_2(\delta)}{\delta})$. From the definition of c_1 and c_2 , one can see that $c_1(\delta)$ is nonincreasing and, under (37), $\frac{c_2(\delta)}{\delta}$ is nondecreasing in δ . As a consequence, $\min(c_1(\delta), \frac{c_2(\delta)}{\delta})$ is maximized for $\delta c_1(\delta) = c_2(\delta)$. This last equation is quadratic, and one can check that its unique positive solution is

$$\delta = \frac{\mathbf{E}}{\mathbf{V}} \left(\eta + \inf \varphi - \frac{\mathbf{V} + \mathbf{E}^2}{2\mathbf{E}} + \sqrt{\left(\eta + \inf \varphi - \frac{\mathbf{V} + \mathbf{E}^2}{2\mathbf{E}} \right)^2 + 2 \frac{\eta \mathbf{V}}{\mathbf{E}}} \right),$$

giving the rate (38). □

One can see that Equation (37) is necessary and sufficient for the existence of $\delta > 0$ such that $c_1(\delta) > 0$ and $c_2(\delta) > 0$. One can naturally wonder whether introducing more flexibility in the inequalities used in the proof of Proposition 13 could lead to a weaker condition. Actually, keeping track of the positive term $\int_{\mathbb{R}^d} |\nabla u|^2 e^{-V}$ in (39), using inequality (33) in (40), and using the inequality $2ab \leq \gamma a^2 + \frac{1}{\gamma} b^2$ in (41) leads to the exact same necessary and sufficient condition to ensure exponential convergence to 0.

Remark 14. *One can use the theory of large deviations to prove that the long-time behavior of quantities of the form (34) is necessarily exponential, with a rate given by a variational formula.*

Let $(X_t)_{t \geq 0}$ evolve according to Equation (2). According to Donsker-Varadhan's lemma, the random probability measure μ_t defined by the formula

$$\mu_t(A) = \frac{1}{t} \int_0^t \mathbf{1}_{X_s \in A} ds,$$

satisfies a large deviation principle with rate function

$$I(\nu) = \begin{cases} \int_{\mathbb{R}^d} |\nabla \sqrt{f}|^2 e^{-V(x)} dx & \text{if } \exists f : \mathbb{R}^d \rightarrow \mathbb{R}, \nu = f(x) e^{-V(x)} dx, \\ \infty & \text{otherwise,} \end{cases}$$

see for example [11, Chapter IV.4]. As a consequence, in the long-time limit,

$$-\frac{1}{t} \log \left(\mathbb{E} \left[e^{-\int_0^t \varphi(X_s) ds} \right] \right) = -\frac{1}{t} \log \left(\mathbb{E} \left[e^{-t \langle \varphi, \mu_t \rangle} \right] \right)$$

converges to the constant α defined by

$$\alpha = \inf_f \int_{\mathbb{R}^d} |\nabla \sqrt{f}|^2(x) e^{-V(x)} dx + \int_{\mathbb{R}^d} \varphi(x) f(x) e^{-V(x)} dx$$

where the infimum is taken over all probability densities with respect to the measure $e^{-V(x)} dx$, from Varadhan's lemma in large deviations theory. By the change of variables $g^2 = f$, α is equal to

$$\inf_g \frac{\int_{\mathbb{R}^d} |\nabla g|^2(x) e^{-V(x)} dx + \int_{\mathbb{R}^d} \varphi(x) g^2(x) e^{-V(x)} dx}{\int_{\mathbb{R}^d} g^2(x) e^{-V(x)} dx},$$

which is the bottom of the spectrum of the operator $-\Delta + \nabla V \cdot \nabla + \varphi$ which is self-adjoint in $\mathbb{L}^2(e^{-V(x)} dx)$, already discussed at the beginning of this section.

Let us give two examples where the result from Proposition 13 applies.

Example 15. A first example is given by the double-well potential in dimension 1, defined by

$$V_\gamma(x) = x^4 - \gamma x^2 + C_\gamma,$$

where $\gamma > 0$ and $C_\gamma = \ln \left(\int_{\mathbb{R}} \exp(-x^4 + \gamma x^2) dx \right)$. We want to apply Proposition 13 to the case where the function φ is a multiple of $\min \text{Spec} \nabla^2 V_\gamma(x)$ (see Section 3.3 for a justification of this choice for φ). In the present case, this writes $\varphi_{\gamma, \delta}(x) = \delta(12x^2 - 2\gamma)$, where δ is the positive multiplicative factor.

Denote by η_γ the optimal Poincaré constant associated to the potential V_γ . As γ goes to 0, the limit potential x^4 satisfies a Poincaré inequality with constant $\eta_0 > 0$, owing to its convexity. As a consequence, the Poincaré constants η_γ converge to a positive limit. On the other hand, as γ goes to 0, the quantity

$$-(\inf \varphi_{\gamma, \delta}) \frac{\int_{\mathbb{R}} \varphi_{\gamma, \delta}^2(x) e^{-V_\gamma(x)} dx}{\left(\int_{\mathbb{R}} \varphi_{\gamma, \delta}(x) e^{-V_\gamma(x)} dx \right)^2}$$

goes to 0, since $\inf \varphi_{\gamma, \delta}$ goes to 0 while $\frac{\int_{\mathbb{R}} \varphi_{\gamma, \delta}^2(x) e^{-V_\gamma(x)} dx}{\left(\int_{\mathbb{R}} \varphi_{\gamma, \delta}(x) e^{-V_\gamma(x)} dx \right)^2}$ converges to some positive constant. As a consequence, for any $\delta > 0$ the inequality (37) is satisfied for γ smaller than some critical value depending on δ . Notice that the inequalities (36) are satisfied for any $\gamma > 0$ since, for any smooth potential $V : \mathbb{R} \mapsto \mathbb{R}$, $\int_{\mathbb{R}} V''(x) e^{-V(x)} dx > 0$ holds from a mere integration by parts.

Example 16. The second example is given by an identically vanishing potential $V(x) = 0$, with the equation considered on the one-dimensional torus, identified with the segment $[0, 2\pi]$ with periodic boundary conditions. The invariant measure is then the uniform measure on the torus. Consider the function $\varphi(x) = \sin(x) + \alpha$ with $\alpha \geq 0$. In that cases, the mean value of φ is given by α , and $\varphi(x)$ is not nonnegative for all values of x as soon as $\alpha < 1$.

In that case, the Poincaré constant is given by $\eta = 1$ and $\inf \varphi$ is given by $\alpha - 1$. As a consequence, Equation (37) writes

$$(1 - \alpha) \frac{1 + 2\alpha^2}{2\alpha^2} < 1$$

The condition is thus satisfied if $\alpha > \alpha_0$ where α_0 is the unique real root of the equation

$$\alpha^3 + \frac{1}{2}\alpha - \frac{1}{2} = 0,$$

given by $\alpha_0 \simeq 0.590$. As a consequence, for $\alpha \in (\alpha_0, 1)$, one has exponential convergence of (34) to zero while the function φ is not uniformly positive.

2.4 Existence and uniqueness of an invariant measure π_λ for (1)

In all this section, we assume that Assumption **(Poinc(η))** holds for some positive η . We would like to show that the stochastic differential equation (1) admits a unique invariant probability measure that we denote in the following π_λ , and to give an explicit formula for this measure. Of course, for $\lambda = 0$, we have

$$d\pi_0 = e^{-V(x)} dx$$

and one result of this section is that it is the unique invariant measure for (2). We will use π_0 as a reference measure to build functional spaces, and to construct the invariant measure π_λ by perturbative arguments, using the crucial assumption on the boundedness of $F_\lambda + \nabla V = F_\lambda - F_0$ (see Assumption **(Drift)-(i)**): for $\lambda \in [0, \lambda_0]$,

$$\|F_\lambda - F_0\|_{\mathbb{L}^\infty(\mathbb{R}^d)} \leq C\lambda.$$

Let us begin with some notation. We denote by $\mathcal{L}_\lambda = F_\lambda \cdot \nabla + \Delta$ the generator of the process $(X_t^\lambda)_{t \geq 0}$. In particular, $\mathcal{L}_0 = -\nabla V \cdot \nabla + \Delta$. Also denote

$$\mathcal{T}_\lambda = \mathcal{L}_\lambda - \mathcal{L}_0 = (F_\lambda + \nabla V) \cdot \nabla \quad (44)$$

The space $\mathbb{L}_0^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx)$ endowed with the symmetric bilinear form

$$(u, v) \mapsto \int_{\mathbb{R}^d} \nabla u(x) \cdot \nabla v(x) e^{-V(x)} dx \quad (45)$$

is a Hilbert space by Assumption **(Poinc(η))**. A consequence of the Riesz theorem is that for any $u \in \mathbb{L}^2(e^{-V(x)} dx)$, there exists a unique function v in $\mathbb{L}_0^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx)$ such that

$$\forall w \in \mathbb{L}_0^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx), \int_{\mathbb{R}^d} \nabla v(x) \cdot \nabla w(x) e^{-V(x)} dx = \int_{\mathbb{R}^d} u(x) w(x) e^{-V(x)} dx.$$

This function is denoted $v = -\mathcal{L}_0^{-1}u$ since when v is smooth, $\int_{\mathbb{R}^d} \nabla v(x) \cdot \nabla w(x) e^{-V(x)} dx = -\int_{\mathbb{R}^d} \mathcal{L}_0 v(x) w(x) e^{-V(x)} dx$. We denote by $\mathcal{D}(\mathcal{L}_0)$ the domain of \mathcal{L}_0 , defined by

$$\mathcal{D}(\mathcal{L}_0) = \left\{ v \in \mathbb{L}_0^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx), \mathcal{L}_0 v \in \mathbb{L}_0^2(e^{-V(x)} dx) \right\}.$$

For a function $u \in \mathbb{L}^2(e^{-V(x)} dx)$, from the Poincaré inequality, one has

$$\begin{aligned} \eta \|\mathcal{L}_0^{-1}u\|_{\mathbb{L}^2(e^{-V(x)} dx)}^2 &\leq \int_{\mathbb{R}^d} |\nabla(\mathcal{L}_0^{-1}u)(x)|^2 e^{-V(x)} dx = - \int_{\mathbb{R}^d} (\mathcal{L}_0^{-1}u)(x) u(x) e^{-V(x)} dx, \\ &\leq \|\mathcal{L}_0^{-1}u\|_{\mathbb{L}^2(e^{-V(x)} dx)} \|u\|_{\mathbb{L}^2(e^{-V(x)} dx)} \end{aligned}$$

which implies

$$\eta \|\mathcal{L}_0^{-1}u\|_{\mathbb{L}^2(e^{-V(x)} dx)} \leq \|u\|_{\mathbb{L}^2(e^{-V(x)} dx)}. \quad (46)$$

In the following, we will use the orthogonal projection operator Π_0 from $\mathbb{L}^2(e^{-V(x)} dx)$ onto $\mathbb{L}_0^2(e^{-V(x)} dx)$ defined by:

$$\forall f \in \mathbb{L}^2(e^{-V(x)} dx), \Pi_0 f = f - \int_{\mathbb{R}^d} f(x) e^{-V(x)} dx. \quad (47)$$

Let us now explain formally how we obtain an explicit formula for the invariant measure π_λ of (1). For any test function φ and since $\mathcal{L}_\lambda 1 = 0$, $\int_{\mathbb{R}^d} \mathcal{L}_\lambda \Pi_0(\varphi) d\pi_\lambda = 0$. Thus, by considering $f = \mathcal{L}_0 \Pi_0(\varphi)$, for any test function f , $\int_{\mathbb{R}^d} \mathcal{L}_\lambda \mathcal{L}_0^{-1} \Pi_0 f d\pi_\lambda = 0$ which also writes $\int_{\mathbb{R}^d} (I + \mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0) \Pi_0 f d\pi_\lambda = 0$ where I denotes the identity operator. This is equivalent to: for any test function f , $\int_{\mathbb{R}^d} (I +$

$\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0) f \frac{d\pi_\lambda}{d\pi_0} d\pi_0 = \int_{\mathbb{R}^d} f d\pi_0$ which yields $(I + \mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^* \frac{d\pi_\lambda}{d\pi_0} = 1$, where $*$ denotes the dual operator on the Hilbert space $\mathbb{L}^2(e^{-V(x)} dx)$. As a consequence, we are naturally led to study the operator $\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0$ defined from $\mathbb{L}^2(e^{-V(x)} dx)$ to $\mathbb{L}^2(e^{-V(x)} dx)$. The aim of the next Lemma is to show rigorously that we can define an invariant measure π_λ of (1) by defining its Radon-Nikodym derivative with respect to π_0 as $(I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*)^{-1} \mathbf{1}$.

We can now state the result concerning the existence of an invariant measure for (1).

Lemma 17. *Let us assume that Assumption **(Poinc)(η)** holds for some positive η . Then there exists $\lambda_1 \in (0, \lambda_0]$ such that for $\lambda \in [0, \lambda_1]$, the dual operator $I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*$ on the Hilbert space $\mathbb{L}^2(e^{-V(x)} dx)$ of the operator $I + \mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0$ is invertible and has a bounded inverse.*

Let us then introduce, for $\lambda \in [0, \lambda_1]$, the function $g_\lambda \in \mathbb{L}^2(e^{-V(x)} dx)$ and the associated measure π_λ such that

$$d\pi_\lambda = g_\lambda d\pi_0 \text{ where } g_\lambda = (I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*)^{-1} \mathbf{1}. \quad (48)$$

The measure π_λ is a probability measure which is invariant for the process $(X_t^\lambda)_{t \geq 0}$ solution to (1).

Proof. Step 1: Let us first study the operator $\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0$. From the boundedness assumption on $\nabla V + F_\lambda = F_\lambda - F_0$ (see Assumption **(Drift)-(i)**), the definition of \mathcal{L}_0^{-1} and (46), for any $u \in \mathbb{L}_0^2(e^{-V(x)} dx)$,

$$\begin{aligned} \|\mathcal{T}_\lambda \mathcal{L}_0^{-1} u\|_{\mathbb{L}^2(e^{-V(x)} dx)}^2 &= \int_{\mathbb{R}^d} |(F_\lambda + \nabla V)(x) \cdot \nabla(\mathcal{L}_0^{-1} u)(x)|^2 e^{-V(x)} dx \\ &\leq C\lambda^2 \int_{\mathbb{R}^d} |\nabla(\mathcal{L}_0^{-1} u)(x)|^2 e^{-V(x)} dx \\ &= -C\lambda^2 \int_{\mathbb{R}^d} (\mathcal{L}_0^{-1} u)(x) u(x) e^{-V(x)} dx \\ &\leq C\lambda^2 \|\mathcal{L}_0^{-1} u\|_{\mathbb{L}^2(e^{-V(x)} dx)} \|u\|_{\mathbb{L}^2(e^{-V(x)} dx)} \leq C \frac{\lambda^2}{\eta} \|u\|_{\mathbb{L}^2(e^{-V(x)} dx)}^2. \end{aligned}$$

As a consequence, the operator $\mathcal{T}_\lambda \mathcal{L}_0^{-1}$ is bounded from $\mathbb{L}_0^2(e^{-V(x)} dx)$ to $\mathbb{L}^2(e^{-V(x)} dx)$, with:

$$\|\mathcal{T}_\lambda \mathcal{L}_0^{-1}\|_{\mathcal{L}(\mathbb{L}_0^2(e^{-V(x)} dx), \mathbb{L}^2(e^{-V(x)} dx))} \leq \sqrt{\frac{C}{\eta}} \lambda. \quad (49)$$

By composition, $\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0$ is thus a bounded operator from $\mathbb{L}^2(e^{-V(x)} dx)$ to itself, with a norm of order $\mathcal{O}(\lambda)$, and so is $(\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*$. As a consequence, for λ small enough, the operator $I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*$ is invertible from $\mathbb{L}^2(e^{-V(x)} dx)$ to itself.

Step 2: Let us now introduce the function $g_\lambda \in \mathbb{L}^2(e^{-V(x)} dx)$ defined by

$$g_\lambda = (I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*)^{-1} \mathbf{1}$$

and let us prove that $d\pi_\lambda = g_\lambda d\pi_0$ is invariant for the stochastic differential equation (1). Let $(Y_t^{\lambda, x})_{t \geq 0}$ be the solution to (1) with initial condition $Y_0^{\lambda, x} = x$ (see (31)). Using the Markov property, the aim is to prove that, for any \mathcal{C}^∞ bounded test function $f : \mathbb{R}^d \rightarrow \mathbb{R}$,

$$\int_{\mathbb{R}^d} \mathbb{E}(f(Y_t^{\lambda, x})) g_\lambda(x) e^{-V(x)} dx = \int_{\mathbb{R}^d} f(x) g_\lambda(x) e^{-V(x)} dx. \quad (50)$$

From Proposition 9, we know that $u(t, x) = \mathbb{E}(f(Y_t^{\lambda, x}))$ is the solution to (23) (with $\varphi = 0$), and from Proposition 7, we have for any $T > 0$,

$$u \in \mathbb{L}^\infty([0, T], \mathbb{H}^1(e^{-V(x)} dx)) \cap \mathbb{H}^1([0, T], \mathbb{L}^2(e^{-V(x)} dx)).$$

Moreover, from Proposition 8, u is a classical solution to (23). Therefore,

$$\begin{aligned} \frac{d}{dt} \int_{\mathbb{R}^d} \mathbb{E}(f(Y_t^{\lambda,x})) g_\lambda(x) e^{-V(x)} dx &= \frac{d}{dt} \int_{\mathbb{R}^d} u(t,x) g_\lambda(x) e^{-V(x)} dx \\ &= \int_{\mathbb{R}^d} \partial_t u(t,x) g_\lambda(x) e^{-V(x)} dx \\ &= \int_{\mathbb{R}^d} \mathcal{L}_\lambda u(t,x) g_\lambda(x) e^{-V(x)} dx, \end{aligned}$$

and $\mathcal{L}_\lambda u = \partial_t u \in \mathbb{L}^2(e^{-V(x)} dx)$. Now, notice that for any function ψ which is the sum of a \mathcal{C}^∞ function with compact support and a constant,

$$\mathcal{T}_\lambda \psi = \mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0 \mathcal{L}_0 \psi$$

holds true since \mathcal{T}_λ sends constant functions to 0. Therefore, for any such function ψ , one has

$$\begin{aligned} \int_{\mathbb{R}^d} \mathcal{L}_\lambda \psi g_\lambda d\pi_0 &= \int_{\mathbb{R}^d} [(\mathcal{L}_0 + \mathcal{T}_\lambda) \psi] g_\lambda d\pi_0 = \int_{\mathbb{R}^d} [(I + \mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0) \mathcal{L}_0 \psi] g_\lambda d\pi_0 \\ &= \int_{\mathbb{R}^d} [\mathcal{L}_0 \psi] (I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*) g_\lambda d\pi_0 \\ &= \int_{\mathbb{R}^d} \mathcal{L}_0 \psi d\pi_0. \end{aligned}$$

Since π_0 is invariant for the dynamics (2) with infinitesimal generator \mathcal{L}_0 , the right-hand side is zero. By density, the equality $\int_{\mathbb{R}^d} \mathcal{L}_\lambda \psi g_\lambda d\pi_0 = 0$ holds for any function ψ such that $\mathcal{L}_\lambda \psi \in \mathbb{L}^2(e^{-V(x)} dx)$. Therefore, $\frac{d}{dt} \int_{\mathbb{R}^d} \mathbb{E}(f(Y_t^{\lambda,x})) g_\lambda(x) e^{-V(x)} dx = 0$ which yields (50) after integration in time over $[0, t]$.

Step 3: Let us finally check that π_λ is a probability measure. First, one has

$$\int_{\mathbb{R}^d} g_\lambda d\pi_0 = \int_{\mathbb{R}^d} (I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*)^{-1} \mathbf{1} (I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)) \mathbf{1} d\pi_0 = \int_{\mathbb{R}^d} d\pi_0 = 1.$$

Second, one can prove that $g_\lambda \geq 0$. Indeed, from (50) and the fact that $Y_t^{\lambda,x}$ admits a density $p^\lambda(t, x, y)$ with respect to the Lebesgue measure (see Lemma 2), we have

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(y) p^\lambda(t, x, y) dy g_\lambda(x) e^{-V(x)} dx = \int_{\mathbb{R}^d} f(x) g_\lambda(x) e^{-V(x)} dx.$$

This equality holds for any smooth test function f and, by a density argument, one can apply it to the bounded function $f(x) = \text{sgn}(g_\lambda(x))$, where $\text{sgn}(y) = 1_{y \geq 0} - 1_{y < 0}$ denotes the sign function. One thus obtains

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (\text{sgn}(g_\lambda(y)) \text{sgn}(g_\lambda(x)) - 1) p^\lambda(t, x, y) dy |g_\lambda|(x) e^{-V(x)} dx = 0.$$

Thus, $(\text{sgn}(g_\lambda(y)) \text{sgn}(g_\lambda(x)) - 1) p^\lambda(t, x, y) |g_\lambda|(x) = 0$ $dx \otimes dy$ -a.e.. Since $p^\lambda(t, x, y) > 0$ $dx \otimes dy$ -a.e. (see Lemma 2) and $\int_{\mathbb{R}^d} |g_\lambda|(x) dx > 0$, this implies that dy -a.e., $\text{sgn}(g_\lambda(y)) = 1$ or dy -a.e. $\text{sgn}(g_\lambda(y)) = -1$. The conclusion then follows from the fact that $\int_{\mathbb{R}^d} g_\lambda d\pi_0 = 1$. \square

Notice that in the case $\lambda = 0$, we indeed have $g_0 = 1$. The next result states the uniqueness of the invariant measure for (1).

Lemma 18. *Let us assume that Assumption **(Poinc**(η)) holds for some positive η . For $\lambda \in [0, \lambda_1]$ (λ_1 being the constant introduced in Lemma 17), the unique invariant measure of the stochastic differential equation (1) is the probability measure π_λ defined by (48). This probability measure is equivalent to the Lebesgue measure on \mathbb{R}^d and for any initial condition X_0 ,*

$$\forall f \in \mathbb{L}^1(\pi_\lambda), \mathbb{P} \left(\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t f(X_s^\lambda) ds = \int_{\mathbb{R}^d} f d\pi_\lambda \right) = 1. \quad (51)$$

Proof. Let $\lambda \in [0, \lambda_1]$. Lemma 17 ensures that π_λ defined by (48) is an invariant probability measure for $dX_t^\lambda = F_\lambda(X_t^\lambda)dt + \sqrt{2}dW_t$. For X_0 distributed according to any invariant probability measure, Lemma 2 ensures that this measure is equivalent to the Lebesgue measure. As a consequence, all the invariant probability measures are equivalent and the dynamics admits exactly one invariant probability measure π_λ . Since π_λ is the only invariant probability measure, it is ergodic (see for example [27, Theorem 3.8 and Equation (52)]) and denoting by $(Y_t^{\lambda, x})_{t \geq 0}$ the solution to (1) started from $Y_0 = x \in \mathbb{R}^d$,

$$\forall f \in \mathbb{L}^1(\pi_\lambda), dx \text{ a.e.}, \mathbb{P} \left(\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t f(Y_s^{\lambda, x}) ds = \int_{\mathbb{R}^d} f d\pi_\lambda \right) = 1.$$

For any initial condition X_0 , since the law of X_1^λ is absolutely continuous with respect to the Lebesgue measure (see Lemma 2), (51) follows by the Markov property. \square

3 Tangent vector of the diffusion

In all this Section, $(X_t^\lambda)_{t \geq 0}$ denotes the process solution to (1), with an initial condition X_0 which, we recall, does not depend on λ . We establish various results on the tangent vector T_t defined by (52), which naturally appears in the estimators (10) and (11) to evaluate $\partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right)$.

3.1 Definition and interpretations of the tangent vector

If the function f is differentiable, one can write $\partial_\lambda^0 (f(X_t^\lambda)) = T_t \cdot \nabla f(X_t^0)$, where the process $(T_t)_{t \geq 0}$ is the so-called *tangent vector*, defined as

$$T_t = \partial_\lambda^0 X_t^\lambda, \quad (52)$$

and the existence of which is ensured by the following proposition.

Proposition 19. *For any $t \geq 0$, the function $\lambda \mapsto X_t^\lambda$ is almost surely differentiable, and the definition of the tangent vector (52) makes sense. Moreover, $(T_t)_{t \geq 0}$ almost surely satisfies the following ordinary differential equation whose coefficients depend on $(X_t^0)_{t \geq 0}$:*

$$\begin{cases} \frac{dT_t}{dt} = \partial_\lambda^0 F_\lambda(X_t^0) - \nabla^2 V(X_t^0) T_t, \\ T_0 = 0. \end{cases} \quad (53)$$

Proof. By **(Drift)**-(i) and the continuity of ∇V and $(X_t^0)_{t \geq 0}$, $t \mapsto |\partial_\lambda^0 F_\lambda(X_t^0)| + |\nabla^2 V(X_t^0)|$ is locally bounded. Hence (53) admits a unique solution $(T_t^0)_{t \geq 0}$ by the Cauchy-Lipschitz theorem. Let us prove that for $\bar{t} > 0$, $\lambda \mapsto X_{\bar{t}}^\lambda$ is differentiable at $\lambda = 0$ with derivative equal to $T_{\bar{t}}^0$. For $\lambda \in [0, \lambda_0]$, we set $\tau_\lambda = \inf\{t \geq 0 : |X_t^\lambda| \geq \sup_{t \in [0, \bar{t}]} |X_t^0| + 1\}$ with convention $\inf \emptyset = +\infty$. Let

$L_{\bar{t}}^{X^0} = \sup_{x \in \mathbb{R}^d; |x| \leq \sup_{t \in [0, \bar{t}]} |X_t^0| + 1} |\nabla^2 V(x)|$. For $t \in [0, \bar{t}]$, one has

$$\begin{aligned} \sup_{s \in [0, t]} |X_{s \wedge \tau_\lambda}^\lambda - X_{s \wedge \tau_\lambda}^0| &\leq \int_0^{t \wedge \tau_\lambda} \left| F_\lambda(X_s^\lambda) + \nabla V(X_s^\lambda) \right| + \left| \nabla V(X_s^0) - \nabla V(X_s^\lambda) \right| ds \\ &\leq C\lambda t + L_{\bar{t}}^{X^0} \int_0^t |X_{s \wedge \tau_\lambda}^\lambda - X_{s \wedge \tau_\lambda}^0| ds \end{aligned}$$

so that $\sup_{s \in [0, t]} |X_{s \wedge \tau_\lambda}^\lambda - X_{s \wedge \tau_\lambda}^0| \leq \frac{C(e^{L_{\bar{t}}^{X^0} t} - 1)}{L_{\bar{t}}^{X^0}} \lambda$. For $\lambda \leq \frac{L_{\bar{t}}^{X^0}}{C(e^{L_{\bar{t}}^{X^0} t} - 1)}$, one deduces that $\tau_\lambda \geq \bar{t}$

and $\sup_{s \in [0, t]} |X_s^\lambda - X_s^0| \leq \frac{C(e^{L_{\bar{t}}^{X^0} t} - 1)}{L_{\bar{t}}^{X^0}} \lambda$. In particular, X_t^λ converges to X_t^0 uniformly for $t \in [0, \bar{t}]$. Now, for $t \geq 0$,

$$X_t^\lambda - X_t^0 = \int_0^t (F_\lambda(X_s^\lambda) - F_0(X_s^\lambda)) ds + \int_0^t \nabla^2 V(\xi_s^\lambda) (X_s^0 - X_s^\lambda) ds,$$

where, by a slight abuse of notations, $\nabla^2 V(\xi_s^\lambda)$ stands for the matrix $(\partial_{ij} V(\xi_s^{\lambda, i}))_{1 \leq i, j \leq d}$ and $\forall i \in \{1, \dots, d\}$, $\xi_s^{\lambda, i} \in [X_s^0, X_s^\lambda]$. For $s \in [0, \bar{t}]$ and $\lambda \in \left(0, \lambda_0 \wedge \frac{L_{\bar{t}}^{X^0}}{C(e^{L_{\bar{t}}^{X^0} t} - 1)}\right]$, $|\xi_s^{\lambda, i}| \leq \sup_{t \in [0, \bar{t}]} |X_t^0| + 1$. Hence for $t \in [0, \bar{t}]$,

$$\begin{aligned} \sup_{s \in [0, t]} \left| \frac{X_s^\lambda - X_s^0}{\lambda} - T_s^0 \right| &\leq \int_0^t \left| \frac{F_\lambda(X_s^\lambda) - F_0(X_s^\lambda)}{\lambda} - \partial_\lambda^0 F_\lambda(X_s^0) \right| + |\nabla^2 V(X_s^0) - \nabla^2 V(\xi_s^\lambda)| |T_s^0| ds \\ &\quad + L_{\bar{t}}^{X^0} \int_0^t \left| \frac{X_s^\lambda - X_s^0}{\lambda} - T_s^0 \right| ds. \end{aligned}$$

By **(Drift)**-(i)-(ii) and the uniform convergence of X_t^λ to X_t^0 for $t \in [0, \bar{t}]$,

$$\lim_{\lambda \rightarrow 0} \int_0^{\bar{t}} \left| \frac{F_\lambda(X_s^\lambda) - F_0(X_s^\lambda)}{\lambda} - \partial_\lambda^0 F_\lambda(X_s^0) \right| + |\nabla^2 V(X_s^0) - \nabla^2 V(\xi_s^\lambda)| |T_s^0| ds = 0.$$

With Grönwall's lemma, one concludes that $\sup_{s \in [0, \bar{t}]} \left| \frac{X_s^\lambda - X_s^0}{\lambda} - T_s^0 \right|$ converges to 0 as $\lambda \rightarrow 0$. \square

We have the following expression of $(T_t)_{t \geq 0}$ as an integral:

Proposition 20. *Define the resolvent $(R_{X^0}(s, t))_{s, t \geq 0}$ associated with Equation (53) as the solution, with values in $\mathbb{R}^{d \times d}$, to the following ordinary differential equation:*

$$\begin{cases} \partial_t R_{X^0}(s, t) = -\nabla^2 V(X_t^0) R_{X^0}(s, t), & s, t \geq 0, \\ R_{X^0}(s, s) = I_d, & s \geq 0, \end{cases} \quad (54)$$

where I_d is the $d \times d$ identity matrix. The resolvent satisfies the following semigroup property

$$\forall r, s, t \in [0, \infty), \quad R_{X^0}(s, t) R_{X^0}(r, s) = R_{X^0}(r, t). \quad (55)$$

One can recover the tangent vector from the resolvent through the following formula:

$$\forall t \geq 0, \quad T_t = \int_0^t R_{X^0}(s, t) \partial_\lambda^0 F_\lambda(X_s^0) ds. \quad (56)$$

Proof. The semigroup property (55) is a consequence of uniqueness for Equation (54), satisfied by the two processes $(R_{X^0}(s, t))_{t \geq 0}$ and $(R_{X^0}(r, t)R_{X^0}(r, s)^{-1})_{t \geq 0}$.

In view of the differential equations satisfied by $(T_t)_{t \geq 0}$ and $(R_{X^0}(s, t))_{t \geq 0}$, one has, from the equality $R_{X^0}(t, 0) = R_{X^0}(0, t)^{-1}$,

$$\begin{aligned} \partial_t(R_{X^0}(t, 0)T_t) &= -R_{X^0}(t, 0)\partial_t(R_{X^0}(0, t))R_{X^0}(t, 0)T_t + R_{X^0}(t, 0)\partial_t T_t \\ &= R_{X^0}(t, 0)\nabla^2 V(X_t^0)R_{X^0}(0, t)R_{X^0}(t, 0)T_t \\ &\quad + R_{X^0}(t, 0)\partial_\lambda^0 F_\lambda(X_t^0) - R_{X^0}(t, 0)\nabla^2 V(X_t^0)T_t \\ &= R_{X^0}(t, 0)\partial_\lambda^0 F_\lambda(X_t^0). \end{aligned}$$

Integrating over $[0, t]$, one obtains

$$R_{X^0}(t, 0)T_t = \int_0^t R_{X^0}(s, 0)\partial_\lambda^0 F_\lambda(X_s^0)ds,$$

and the result follows by using the semigroup property (55). \square

Notice that the resolvent is also the differential of the trajectory with respect to its initial condition.

Lemma 21. *Let $(Y_t^x)_{t \geq 0}$ solve (12). Then for any $t \geq 0$, $x \mapsto Y_t^x$ is \mathcal{C}^1 on \mathbb{R}^d with Jacobian matrix $(DY_t^x)_{i,j} = \partial_{x_j} Y_t^{i,x}$ given by $DY_t^x = R_{Y^x}(0, t)$.*

Proof. By standard results on ordinary differential equations, $x \mapsto Y_t^x$ is \mathcal{C}^1 with Jacobian matrix DY_t^x solving the equation

$$\forall t \geq 0, \quad DY_t^x = I_d - \int_0^t \nabla^2 V(Y_s^x)DY_s^x ds,$$

obtained by spatial derivation of $Y_t^x = x - \int_0^t \nabla V(Y_s^x)ds + \sqrt{2}W_t$. By uniqueness for (54), one has $DY_t^x = R_{Y^x}(0, t)$. \square

In the following, we will need the following result about the link between the forward resolvent and its backward counterpart.

Lemma 22. *Let $(Y_s)_{0 \leq s \leq t}$ satisfy Equation (2) with Y_0 distributed according to π_0 . From the reversibility of the dynamics (2), the process $(Z_s)_{0 \leq s \leq t}$ defined by $Z_s = Y_{t-s}$ has the same law as $(Y_s)_{0 \leq s \leq t}$, and one has the relation*

$$R_Y(0, s) = R_Z^T(t - s, t),$$

where R_Z^T is the transposed matrix of the resolvent associated with Z .

Proof. Uniqueness holds for the ordinary differential equation satisfied by $s \mapsto R_Y(0, s)$:

$$\begin{cases} \frac{dR}{ds}(s) = -\nabla^2 V(Y_s)R(s), \\ R(0) = I_d. \end{cases} \quad (57)$$

One can check that $s \mapsto R_Z^T(t - s, t)$ also solves (57). Indeed, since, by the semigroup property, $R_Z(t - s, t) = R_Z(t, t - s)^{-1}$, one has, for $s \in [0, t]$,

$$\begin{aligned} \partial_s R_Z(t - s, t) &= -R_Z(t - s, t) (\partial_s R_Z(t, t - s)) R_Z(t - s, t) \\ &= -R_Z(t - s, t) \nabla^2 V(Z_{t-s}) R_Z(t, t - s) R_Z(t - s, t) \\ &= -R_Z(t - s, t) \nabla^2 V(Z_{t-s}) \\ &= -R_Z(t - s, t) \nabla^2 V(Y_s). \end{aligned}$$

This concludes the proof. \square

3.2 Almost sure boundedness of $R_{X^0}(0, t)$ and T_t

The tangent vector can take large values, since the second term in the right-hand side of (53) will provide exponential growth for $(T_t)_{t \geq 0}$, typically when the trajectory $(X_t^0)_{t \geq 0}$ is close to a local maximum of V , or when it crosses a saddle point of V . In the sequel, we need some assumptions on V to control this behavior.

3.2.1 Local-in-time boundedness of $R_{X^0}(s, t)$ and T_t

Let us first introduce an assumption which will be sufficient to get the local-in-time boundedness of $R_{X^0}(s, t)$ and T_t .

Assumption (min Spec). *The matrix-valued function $\nabla^2 V : \mathbb{R}^d \rightarrow \mathbb{R}^{d \times d}$ is bounded from below, in the sense that there exists $\alpha \in \mathbb{R}$ such that, for all $x, h \in \mathbb{R}^d$,*

$$h \cdot \nabla^2 V(x) h \geq \alpha |h|^2.$$

Equivalently, the spectrum of $\nabla^2 V(x)$ is bounded from below by α , uniformly in x .

Under Assumption **(min Spec)**, the random variables T_t and $R_{X^0}(s, t)$ are bounded:

Lemma 23. *One has*

$$\forall 0 \leq s < t, |R_{X^0}(s, t)| \leq e^{-\int_s^t \min \text{Spec}(\nabla^2 V(X_u^0)) du}, \quad (58)$$

$\mathbb{R}^{d \times d}$ being endowed with the matricial norm associated with the Euclidean norm on \mathbb{R}^d . In addition, if the Assumption **(min Spec)** is satisfied, for any $T > 0$, the random variables $\sup_{0 \leq s \leq t \leq T} |R_{X^0}(s, t)|$ and $\sup_{0 \leq t \leq T} |T_t|$ lie in $\mathbb{L}^\infty(\Omega)$.

Proof. For any vector x , one has

$$\begin{aligned} \partial_t |R_{X^0}(s, t)x|^2 &= -2(R_{X^0}(s, t)x)^T \nabla^2 V(X_t^0)(R_{X^0}(s, t)x) \\ &\leq -2 \min \text{Spec}(\nabla^2 V(X_t^0)) |R_{X^0}(s, t)x|^2. \end{aligned}$$

As a consequence, one has the estimation

$$|R_{X^0}(s, t)x|^2 \leq |x|^2 e^{-2 \int_s^t \min \text{Spec}(\nabla^2 V(X_u^0)) du}$$

so that (58) holds. If the Assumption **(min Spec)** is satisfied, this inequality proves that $R(s, t)$ is in $\mathbb{L}^\infty(\Omega)$ locally uniformly in time. From the expression (56) of T_t and the boundedness of $\partial_\lambda^0 F_\lambda$, one also concludes that $T_t \in \mathbb{L}^\infty(\Omega)$, locally uniformly in time. \square

3.2.2 Global-in-time boundedness of $R_{X^0}(0, t)$

We need some additional assumption on the convexity of the potential for $(R_{X^0}(0, t))_{t \geq 0}$ to be bounded globally in time.

Assumption (Conv). *The potential V is such that*

$$\int_{\mathbb{R}^d} \max(0, -\min \text{Spec}(\nabla^2 V(x))) e^{-V(x)} dx < \infty \text{ and } \int_{\mathbb{R}^d} \min \text{Spec}(\nabla^2 V(x)) e^{-V(x)} dx > 0. \quad (59)$$

In this assumption, the first inequality, always satisfied under **(min Spec)**, ensures that the integral $\int_{\mathbb{R}^d} \min \text{Spec} (\nabla^2 V(x)) e^{-V(x)} dx$ is well defined in $(-\infty, \infty]$. We refer to Appendix B for a discussion of this Assumption.

Lemma 24. *Under Assumptions **(min Spec)** and **(Conv)**, the resolvent matrix $R_{X^0}(0, t)$ almost surely converges to 0 as t goes to infinity, with exponential rate. Namely, for any β with*

$$0 < \beta < \int_{\mathbb{R}^d} \min \text{Spec} (\nabla^2 V(x)) e^{-V(x)} dx,$$

there exists an almost surely finite random variable $C > 0$ such that

$$\forall t \geq 0, |R_{X^0}(0, t)| \leq C e^{-\beta t}. \quad (60)$$

Proof. From Lemma 18, by ergodicity (see (51)), one has

$$\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \min \text{Spec} (\nabla^2 V(X_s^0)) ds = \int_{\mathbb{R}^d} \min \text{Spec} (\nabla^2 V(x)) e^{-V(x)} dx \quad \text{a.s.}$$

We conclude by combining this limit with Equation (58). \square

Remark 25 (On the Assumption **(Conv)**). *While Assumption **(Conv)** is automatically satisfied in dimension 1 from a mere integration by parts, this is not the case in higher dimension. Indeed, if one applies the integration by parts formula in this case, one only obtains that*

$$\int_{\mathbb{R}^d} \nabla^2 V(x) e^{-V(x)} dx = \int_{\mathbb{R}^d} \nabla V(x) \otimes \nabla V(x) e^{-V(x)} dx$$

is a positive definite matrix (because of the integrability of e^{-V} , for any y in \mathbb{R}^d , the function $x \mapsto \nabla V(x) \cdot y$ cannot be the zero function), so that the minimum of its spectrum is positive. A counterexample to Assumption **(Conv)** is given by a tensor potential $V(x) = U(x_1) + \dots + U(x_d)$ with a well chosen function U . Indeed, in this case the left hand side of equation (59) rewrites

$$\int_{\mathbb{R}^d} \min_{i \in \{1, \dots, d\}} (U''(x_i)) e^{-\sum_i U(x_i)} dx_1 \dots dx_d = \mathbb{E} \left[\min_{i \in \{1, \dots, d\}} U''(X_i) \right],$$

where X_i are i.i.d random variables with distribution $e^{-U(x)} dx$. If U is chosen so that U'' is bounded and has a strictly negative minimum, then the sequence $\left(\min_{i \in \{1, \dots, d\}} U''(X_i) \right)_{d \geq 1}$ converges almost surely as d goes to infinity to the negative constant $\min U''$. Then, from the dominated convergence theorem, the quantity $\mathbb{E} \left[\min_{i \in \{1, \dots, d\}} U''(X_i) \right]$ converges to $\min U''$, and is thus negative when d is large enough.

Remark 26 (On the assumptions of Lemma 24). *Assumption **(Conv)** is not necessary for (60) to hold. Indeed, if the matrices $\nabla^2 V(x)$ commute, the matrix R_{X^0} is given by*

$$R_{X^0}(0, t) = e^{-\int_0^t \nabla^2 V(X_s^0) ds}.$$

and the convergence of $\frac{1}{t} \int_0^t \nabla^2 V(X_s^0) ds$ to the positive definite matrix $\int_{\mathbb{R}^d} \nabla^2 V(x) e^{-V(x)} dx$ implies that (60) holds for $\beta < \min \text{Spec} \left(\int_{\mathbb{R}^d} \nabla^2 V(x) e^{-V(x)} dx \right)$, even in the cases when V does not satisfy Assumption **(Conv)**. An example where the matrices $\nabla^2 V(x)$ commute is the case of a tensor potential $V(x) = U(x_1) + \dots + U(x_d)$. As seen before, U and d can be chosen such that V does not satisfy Assumption **(Conv)**.

However, it is likely that Lemma 24 does not hold under the sole ergodicity property:

$$\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t (\nabla^2 V(X_s^0)) \, ds = \int_{\mathbb{R}^d} \nabla V(x) \otimes \nabla V(x) e^{-V(x)} \, dx \quad a.s.$$

Indeed, there exists some family of symmetric matrices $(A_t)_{t \geq 0}$ converging in the Cesàro sense to a positive-definite matrix, for which the solution to $\frac{d}{dt} R_t = -A_t R_t$, $R_0 = I_d$ does not converge to 0 as t goes to infinity. An example of this phenomenon is given by

$$A_t = \Omega_t \begin{pmatrix} -1 & 0 \\ 0 & 3 \end{pmatrix} \Omega_t^T, \quad \text{where } \Omega_t = \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix}.$$

Indeed, the family $(A_t)_{t \geq 0}$ converges in the Cesàro sense to I_d as t goes to infinity, but the associated matrix $(R_t)_{t \geq 0}$ diverges. To show this last point, consider the matrix $M_t = \Omega_t^T R_t$. Since $\partial_t \Omega_t = \Omega_t \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, then

$$\partial_t M_t = \begin{pmatrix} 1 & 1 \\ -1 & -3 \end{pmatrix} M_t$$

holds. As a consequence, $R_t = \Omega_t \exp \left(t \begin{pmatrix} 1 & 1 \\ -1 & -3 \end{pmatrix} \right)$. The eigenvalues of the matrix $\begin{pmatrix} 1 & 1 \\ -1 & -3 \end{pmatrix}$ are $-1 - \sqrt{3}$ and $-1 + \sqrt{3}$, the latter being positive, so that R_t diverges as t goes to infinity.

3.3 Boundedness of moments of $R_{X^0}(s, t)$ and T_t

In the sequel, we will need to control the moments of T_t . From Equation (56) and the boundedness of $\partial_\lambda^0 F_\lambda$ (see Assumption **(Drift)**-(i)), this boils down to estimating the moments of $R_{X^0}(s, t)$. For this purpose, from (58), it is enough control expectations of the form $\mathbb{E} \left[e^{-\beta \int_0^t \min \text{Spec}(\nabla^2 V)(Y_s^x) \, ds} \right]$, where β is a positive constant.

3.3.1 Preliminary result when $X_0 \sim \pi_0$

One can deduce from Proposition 13 a criterion for exponential convergence of the moments of $R_{X^0}(0, t)$ to 0 as $t \rightarrow \infty$. To state the result, we need to strengthen the assumptions **(min Spec)** and **(Conv)** which is the point of the following assumption. For any $\rho > 0$, let us consider:

Assumption (Spec(ρ)). Assume that

$$\begin{aligned} & -\infty < \inf_{x \in \mathbb{R}^d} \min \text{Spec}(\nabla^2 V(x)) \leq 0, \\ & \int_{\mathbb{R}^d} \min \text{Spec}(\nabla^2 V(x)) e^{-V(x)} \, dx > 0 \quad \text{and} \quad \int_{\mathbb{R}^d} (\min \text{Spec}(\nabla^2 V(x)))^2 e^{-V(x)} \, dx < \infty, \\ & -(\inf \min \text{Spec}(\nabla^2 V(x))) \frac{\int_{\mathbb{R}^d} (\min \text{Spec}(\nabla^2 V(x)))^2 e^{-V(x)} \, dx}{\left(\int_{\mathbb{R}^d} \min \text{Spec}(\nabla^2 V(x)) e^{-V(x)} \, dx \right)^2} < \rho. \end{aligned}$$

Notice that for $\eta > 0$ and $\beta > 0$ under assumptions **(Poinc(η))** and **(Spec(η/β))** then the assumptions (36) and (37) of Proposition 13 are satisfied with $\varphi(x) = \beta \min \text{Spec}(\nabla^2 V(x))$.

We are now in position to state a simple consequence of Proposition 13:

Proposition 27. Let $(X_t^0)_{t \geq 0}$ solve (2) starting from X_0 distributed according to π_0 . Assume that **(Poinc(η))** and **(Spec(η/β))** hold for some $\eta > 0$ and $\beta > 0$. Then there is a constant $C \in (0, +\infty)$ such that

$$\forall t \geq 0, \mathbb{E}_{\pi_0} [|R_{X^0}(0, t)|^\beta] \leq C e^{-t/C}.$$

Here and in the following, the notation \mathbb{E}_{π_0} means that the initial condition X_0 of the processes $(X_t^\lambda)_{t \geq 0}$ solution to (1) is distributed according to π_0 .

Proof of Proposition 27. To apply Proposition 9 to the function $\varphi(x) = \beta \min \text{Spec}(\nabla^2 V(x))$, we need this function to be locally Lipschitz. Since $\nabla^2 V$ is locally Lipschitz (see Assumption **(Pot)**-(i)), this is a consequence of the Lemma 28 given below. By Proposition 9, the function $u(t, x) = \mathbb{E} \left[e^{-\int_0^t \beta \min \text{Spec}(\nabla^2 V(Y_s^x)) ds} \right]$ is the solution to Equation (23) in the sense of Definition 6 for $\varphi(x) = \beta \min \text{Spec}(\nabla^2 V(x))$ and $f(x) = 1$.

Since conditions (36) and (37) hold for this choice of φ , Equation (58) and Proposition 13 give

$$\mathbb{E}_{\pi_0} \left[|R_{X^0}(0, t)|^\beta \right] \leq \int_{\mathbb{R}^d} u(t, x) e^{-V(x)} dx \leq \left(\int_{\mathbb{R}^d} u^2(t, x) e^{-V(x)} dx \right)^{1/2} \leq C e^{-t/C}$$

for some positive constant C . □

Lemma 28. *The function $A \mapsto \min \text{Spec}(A)$ is a Lipschitz function on the space of symmetric $d \times d$ matrices.*

Proof. Let A be a symmetric matrix, and let x be a vector in \mathbb{R}^d such that $|x| = 1$ and $\min \text{Spec}(A) = x \cdot Ax$. Then, for any symmetric matrix B , one has

$$\min \text{Spec}(B) \leq x \cdot Bx = x \cdot (B - A)x + x \cdot Ax \leq |A - B| + \min \text{Spec}(A),$$

$\mathbb{R}^{d \times d}$ being endowed with the matricial norm associated with the Euclidean norm on \mathbb{R}^d . By exchanging A and B in the previous inequality, one obtains

$$|\min \text{Spec}(A) - \min \text{Spec}(B)| \leq |A - B|.$$

□

3.3.2 Uniform-in-time boundedness of moments of T_t

Numerically, the computation of (5) through the long-time limit of a Monte Carlo approximation of the expression $\mathbb{E}[T_t \cdot \nabla f(X_t^0)]$ is only possible if T_t has a bounded variance uniformly in time.

A case where this fact is easily proved is when the function V is η -convex, where η is a positive constant. We recall that this means that the spectrum of $\nabla^2 V(x)$ is bounded from below by η , independently of x . More precisely, one has the following proposition.

Proposition 29. *Assume that the V is η -convex, for a positive constant η . Then, for any $\alpha \geq 1$,*

$$\sup_{t \geq 0} \mathbb{E}|T_t|^\alpha < \infty.$$

In particular, T_t has a bounded variance uniformly in time.

Proof. By (58) and the boundedness of $\partial_\lambda^0 F_\lambda$, one has

$$\mathbb{E}[|T_t|^\alpha] = \mathbb{E} \left[\left| \int_0^t R_{X^0}(s, t) \partial_\lambda^0 F_\lambda(X_s^0) ds \right|^\alpha \right] \leq \mathbb{E} \left[\left(C \int_0^t e^{-\alpha(t-s)} ds \right)^\alpha \right] < \infty,$$

so that T_t has a finite moment of order α . □

The convexity assumption on the potential can be loosened, as shown in the next Proposition.

Proposition 30. *Let $\alpha \in [1, +\infty)$. Assume that **(Poinc)(η)** holds for some positive η , that the initial condition X_0 is distributed according to a measure μ_0 having a density with respect to the measure $e^{-V(x)}dx$ which is in $\mathbb{L}^p(e^{-V(x)}dx)$ for some $p \in (1, \infty]$, and Assumption **(Spec)($\eta(p-1)/(\alpha p)$)** holds (with the convention $\eta(\infty-1)/(\alpha\infty) = \eta/\alpha$). Then,*

$$\sup_{t \geq 0} \mathbb{E}|T_t|^\alpha < \infty.$$

and, when $\alpha \geq 2$, T_t has a bounded variance uniformly in time.

Proof. By (56) and **(Drift)-(i)**,

$$\mathbb{E}^{1/\alpha}[|T_t|^\alpha] \leq \int_0^t \mathbb{E}^{1/\alpha}[|R_{X^0}(s, t) \partial_\lambda^0 F_\lambda(X_s^0)|^\alpha] ds \leq C \int_0^t \mathbb{E}^{1/\alpha}[|R_{X^0}(s, t)|^\alpha] ds$$

Let μ_s denote the law of X_s^0 for $s \geq 0$ and $(Y_t)_{t \geq 0}$ be a solution to (2) with Y_0 distributed according to π_0 . We notice that the Markov property gives: for $0 \leq s \leq t$,

$$\mathbb{E}[|R_{X^0}(s, t)|^\alpha] = \mathbb{E} \left[|R_Y(s, t)|^\alpha \frac{d\mu_s}{e^{-V(x)}dx}(Y_s) \right].$$

Using Hölder inequality with $q = p/(p-1)$ ($q = 1$ if $p = \infty$), Lemma 4 and Proposition 27, one deduces that for $t \geq s \geq 0$,

$$\mathbb{E}[|R_{X^0}(s, t)|^\alpha] \leq \mathbb{E}[|R_Y(s, t)|^{\alpha q}]^{1/q} \left\| \frac{d\mu_s}{e^{-V(x)}dx} \right\|_{\mathbb{L}^p(e^{-V(x)}dx)} \leq C e^{-\frac{t-s}{C}}.$$

This concludes the proof. □

We are now in position to give sufficient conditions for the finiteness of the variance of the two estimators (10) and (11).

Corollary 31. *Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be a C^1 function such that ∇f is bounded. Let us assume that either V is η -convex (for a positive constant η), or that there exists $\eta > 0$ and $p \in (1, \infty]$ such that **(Poinc)(η)** holds, X_0 is distributed according to a measure μ_0 having a density in $\mathbb{L}^p(e^{-V(x)}dx)$ with respect to $e^{-V(x)}dx$ and Assumption **(Spec)($\eta(p-1)/(2p)$)** holds. Then,*

$$\sup_{t \geq 0} \text{Var}(T_t \cdot \nabla f(X_t^0)) < \infty \text{ and } \sup_{t \geq 0} \text{Var} \left(\frac{1}{t} \int_0^t T_s \cdot \nabla f(X_s^0) ds \right) < \infty.$$

Proof. These results are simple consequences of the boundedness of ∇f and Proposition 30 for $\alpha = 2$. □

From the Central Limit Theorem for trajectorial averages (see for example [12, Section 2.1.3, Theorem 6.3.20]), it is expected that the variance of $\frac{1}{t} \int_0^t T_s \cdot \nabla f(X_s^0) ds$ actually scales like $1/t$ in the limit $t \rightarrow \infty$. This requires for example to prove the existence of a solution to the Poisson problem associated with the Markov process $(X_s^0, T_s)_{s \geq 0}$, which does not seem to be ensured under our set of assumptions. We leave the study of this issue to a future work.

Remark 32. *Under the additional assumption **(V)** given in Appendix A, it is possible to extend the previous results to more general initial conditions. Assume that the initial condition X_0 is distributed according to a measure μ_0 such that the measure $e^{\frac{1}{2}V}d\mu_0$ can be written as*

$$e^{\frac{1}{2}V(x)}d\mu_0 = f(x)dx + d\nu, \tag{61}$$

where f is some function in $\mathbb{L}^p(dx)$ with $p \in [1, 2]$ and ν is some finite measure on \mathbb{R}^d . From (82), for any $t > 0$, μ_t is absolutely continuous with respect to $e^{-V(x)}dx$ with $\frac{d\mu_t}{e^{-V(x)}dx} \in \mathbb{L}^2(e^{-V(x)}dx)$. Now, by the semi-group property satisfied by R_{X^0} , (58) and the fact that $-\min \text{Spec}(\nabla^2 V(x)) \leq C < \infty$, one has for $\varepsilon > 0$,

$$|R_{X^0}(s, t)| \leq |R_{X^0}(s \vee \varepsilon, t)R_{X^0}(s, s \vee \varepsilon)| \leq e^{C(\varepsilon-s)^+} |R_{X^0}(s \vee \varepsilon, t)|.$$

For $\alpha > 0$, using a similar change of measure as in the previous proof, the fact that $\frac{d\mu_\varepsilon}{e^{-V(x)}dx} \in \mathbb{L}^2(e^{-V(x)}dx)$ and Proposition 27, one deduces that under Assumptions **(Poinc)(η)** and **(Spec)($\eta/(2\alpha)$)**, for $t \geq s \vee \varepsilon$,

$$\begin{aligned} \mathbb{E}[|R_{X^0}(s, t)|^\alpha] &\leq e^{C(\varepsilon-s)^+} \mathbb{E}[|R_Y(s \vee \varepsilon, t)|^{2\alpha}]^{\frac{1}{2}} \mathbb{E}\left[\left(\frac{d\mu_\varepsilon}{e^{-V(x)}dx}(Y_\varepsilon)\right)^2\right]^{\frac{1}{2}} \\ &\leq Ce^{C(\varepsilon-s)^+} e^{-\frac{t-s\vee\varepsilon}{C}} \leq Ce^{C\varepsilon} e^{-\frac{t-s}{C}}. \end{aligned}$$

This estimation remains valid for $0 \leq s \leq t \leq \varepsilon$ up to increasing C , since then, by (58) and the fact that $-\min \text{Spec}(\nabla^2 V(x)) \leq C < \infty$, $|R_{X^0}(s, t)| \leq e^{C\varepsilon}$. In conclusion, for $\alpha \geq 1$, under Assumptions **(V)**, **(Poinc)(η)** and **(Spec)($\eta/(2\alpha)$)**, $\sup_{t \geq 0} \mathbb{E}[|T_t|^\alpha] < \infty$ if μ_0 satisfies (61).

4 The Green-Kubo formulae

A first way to compute the derivative (5) is to use the Green-Kubo formula (see for example [18] for a mathematical approach and [6, 14] for physical motivations). This formula gives an expression of (5) in terms of the time autocorrelations of $(X_t^0)_{t \geq 0}$, where $(X_t^0)_{t \geq 0}$ satisfies (2) with an initial condition X_0 being distributed according to the equilibrium measure π_0 .

4.1 Finite time Green-Kubo formula

We start with the Green-Kubo formula in finite time, which will not be used in the sequel of the paper, but motivates the infinite horizon Green-Kubo formula.

Theorem 33. *Let $f \in \mathbb{L}^1(e^{-V(x)}dx)$ be a Lipschitz function and let ∇f be its gradient in the sense of distributions which can be identified with its almost everywhere gradient. Suppose that the initial condition X_0 is distributed according to the equilibrium measure π_0 and that Assumption **(min Spec)** is satisfied. Then, for any $t \geq 0$, for any $\lambda \in [0, \lambda_0]$, $f(X_t^\lambda)$ is integrable and $\lambda \mapsto \mathbb{E}_{\pi_0}[f(X_t^\lambda)]$ is differentiable at 0 with derivative*

$$\partial_\lambda^0 \mathbb{E}_{\pi_0}[f(X_t^\lambda)] = \int_0^t \mathbb{E}_{\pi_0} \left[\nabla f(X_0) \cdot R_{X^0}^T(0, s) \partial_\lambda^0 F_\lambda(X_s^0) \right] ds. \quad (62)$$

Proof. Since X_t^0 is distributed according to $e^{-V(x)}dx$, Proposition 19 and the chain rule ensure that $\lambda \mapsto f(X_t^\lambda)$ is a.s. differentiable at $\lambda = 0$ with derivative $\nabla f(X_t^0) \cdot T_t$.

To justify the interchange between the derivation and the expectation, we need some integrability property. For $\lambda \in (0, \lambda_0]$ and $t \geq 0$, one has, using **(min Spec)** and **(Drift)-(i)** for the inequality:

$$\begin{aligned} |X_t^\lambda - X_t^0|^2 &= 2 \int_0^t (F_\lambda(X_s^\lambda) + \nabla V(X_s^\lambda)) \cdot (X_s^\lambda - X_s^0) ds + 2 \int_0^t (\nabla V(X_s^0) - \nabla V(X_s^\lambda)) \cdot (X_s^\lambda - X_s^0) ds \\ &\leq C\lambda^2 t + (1 - 2\alpha) \int_0^t |X_s^\lambda - X_s^0|^2 ds. \end{aligned}$$

As a consequence,

$$\forall \lambda \in (0, \lambda_0], \frac{|X_t^\lambda - X_t^0|^2}{\lambda^2} \leq C \frac{e^{(1-2\alpha)t} - 1}{1 - 2\alpha} \quad (63)$$

with the convention that the last ratio is equal to t if $1 - 2\alpha = 0$. With the Lipschitz continuity of f , one deduces that the random variable $\frac{f(X_t^\lambda) - f(X_t^0)}{\lambda}$ is bounded by a deterministic constant not depending on λ . The integrability of $f(X_t^\lambda)$ then follows from the integrability of $f(X_t^0)$ where X_t^0 is distributed according to $e^{-V(x)} dx$ and $f \in \mathbb{L}^1(e^{-V(x)} dx)$.

Moreover, by Lebesgue's theorem, $\lambda \mapsto \mathbb{E}_{\pi_0}[f(X_t^\lambda)]$ is differentiable at 0 with derivative

$$\partial_\lambda^0 \mathbb{E}_{\pi_0}[f(X_t^\lambda)] = \mathbb{E}_{\pi_0}[\nabla f(X_t^0) \cdot T_t] = \int_0^t \mathbb{E}_{\pi_0}[\nabla f(X_t^0) \cdot R_{X^0}(s, t) \partial_\lambda^0 F_\lambda(X_s^0)] ds, \quad (64)$$

where we used (56) for the second equality. All terms in Equation (64) are well defined thanks to Lemma 23. Let us now rewrite the right-hand side of (64). By introducing the process $(Y_s)_{0 \leq s \leq t} = (X_{t-s}^0)_{0 \leq s \leq t}$ (which has the same law as $(X_s^0)_{0 \leq s \leq t}$), using a change of variable $s \rightarrow t - s$ and Lemma 22, we get

$$\begin{aligned} \int_0^t \mathbb{E}_{\pi_0}[\nabla f(X_t^0) \cdot R_{X^0}(s, t) \partial_\lambda^0 F_\lambda(X_s^0)] ds &= \int_0^t \mathbb{E}_{\pi_0}[\nabla f(X_t^0) \cdot R_{X^0}(t - s, t) \partial_\lambda^0 F_\lambda(X_{t-s}^0)] ds \\ &= \int_0^t \mathbb{E}_{\pi_0}[\nabla f(Y_0) \cdot R_Y^T(0, s) \partial_\lambda^0 F_\lambda(Y_s)] ds \\ &= \int_0^t \mathbb{E}_{\pi_0}[\nabla f(X_0) \cdot R_{X^0}^T(0, s) \partial_\lambda^0 F_\lambda(X_s^0)] ds. \end{aligned}$$

This completes the proof of (62). \square

Remark 34. *The conclusion of Theorem 33 still holds if $f \in \mathbb{L}^1(e^{-V(x)} dx)$ is a \mathcal{C}^1 function such that ∇f is uniformly continuous on \mathbb{R}^d and $\nabla f \in \mathbb{L}^1(e^{-V(x)} dx)$.*

It is possible to give another expression of the right-hand side in (62).

Proposition 35. *Let $f \in \mathbb{L}^2(e^{-V(x)} dx)$ be a Lipschitz function. Assume **(min Spec)** and consider the process $(X_t^0)_{t \geq 0}$ satisfying (2) with an initial condition X_0 being distributed according to the equilibrium measure π_0 . For almost every $s \geq 0$*

$$\mathbb{E}_{\pi_0}[\nabla f(X_0) \cdot R_{X^0}^T(0, s) \partial_\lambda^0 F_\lambda(X_s^0)] = \mathbb{E}_{\pi_0}[f(X_0) (\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(X_s^0)]. \quad (65)$$

Proof. Since $f \in \mathbb{L}^2(e^{-V(x)} dx)$, by Proposition 7, the partial differential equation

$$\begin{cases} \partial_t u(t, x) = \Delta u(t, x) - \nabla V(x) \cdot \nabla u(t, x), & t > 0, x \in \mathbb{R}, \\ u(0, x) = f(x), & x \in \mathbb{R}. \end{cases}$$

admits a unique solution u in the sense of Definition 6. Moreover, according to Proposition 9,

$$\forall s \geq 0, dx \text{ a.e.}, u(s, x) = \mathbb{E}[f(Y_s^x)],$$

where $(Y_t^x)_{t \geq 0}$ solves (12). When $s > 0$, from Lemmas 2, 21 and 23 and Assumption **(min Spec)**, one can apply the dominated convergence theorem to differentiate $\mathbb{E}[f(Y_s^x)]$ with respect to x , obtaining $\nabla_x \mathbb{E}[f(Y_s^x)] = \mathbb{E}[R_{Y^x}^T(0, s) \nabla f(Y_s^x)]$. Since $u \in \bigcap_{T > 0} \mathbb{L}^2([0, T], \mathbb{H}^1(e^{-V(x)} dx))$, ds a.e., $u(s, \cdot)$ admits a distributional gradient denoted by $\nabla u(s, \cdot)$ and

$$ds \text{ a.e.}, dx \text{ a.e.}, \nabla u(s, x) = \mathbb{E}[R_{Y^x}^T(0, s) \nabla f(Y_s^x)].$$

When X_0 is distributed according to π_0 , from reversibility of the dynamics (2) and Lemma 22, the random vectors $(X_0, X_s^0, R_{X_0}^T(0, s))$ and $(X_s^0, X_0, R_{X_0}(0, s))$ have the same law. Hence

$$\text{ds a.e., a.s., } \mathbb{E}_{\pi_0} [f(X_0)|X_s^0] = u(s, X_s^0) \text{ and } \mathbb{E}_{\pi_0} [R_{X_0}(0, s)\nabla f(X_0)|X_s^0] = \nabla u(s, X_s^0). \quad (66)$$

For s such that Equation (66) holds, one deduces that

$$\begin{aligned} \mathbb{E}_{\pi_0} \left[\nabla f(X_0) \cdot R_{X_0}^T(0, s) \partial_\lambda^0 F_\lambda(X_s^0) \right] &= \mathbb{E}_{\pi_0} \left[\mathbb{E}_{\pi_0} [R_{X_0}(0, s) \nabla f(X_0) | X_s^0] \cdot \partial_\lambda^0 F_\lambda(X_s^0) \right] \\ &= \mathbb{E}_{\pi_0} \left[\nabla u(s, X_s^0) \cdot \partial_\lambda^0 F_\lambda(X_s^0) \right] \\ &= \int_{\mathbb{R}^d} \nabla u(s, x) \cdot \partial_\lambda^0 F_\lambda(x) e^{-V(x)} dx \\ &= \int_{\mathbb{R}^d} u(s, x) (\nabla V(x) \cdot \partial_\lambda^0 F_\lambda(x) - \nabla \cdot \partial_\lambda^0 F_\lambda(x)) e^{-V(x)} dx \\ &= \mathbb{E}_{\pi_0} \left[f(X_0) (\nabla V(X_s^0) \cdot \partial_\lambda^0 F_\lambda(X_s^0) - \nabla \cdot \partial_\lambda^0 F_\lambda(X_s^0)) \right], \end{aligned}$$

where we used Lemma 36 below with $v(\cdot) = u(s, \cdot)$ which is in $\mathbb{H}^1(e^{-V(x)} dx)$ for the last but one equality. \square

Lemma 36. *Let v be a function in $\mathbb{H}^1(e^{-V(x)} dx)$. Then*

$$\int_{\mathbb{R}^d} \nabla v(x) \cdot \partial_\lambda^0 F_\lambda(x) e^{-V(x)} dx = \int_{\mathbb{R}^d} v(x) (\nabla V(x) \cdot \partial_\lambda^0 F_\lambda(x) - \nabla \cdot \partial_\lambda^0 F_\lambda(x)) e^{-V(x)} dx.$$

Proof. Let $\chi_n(x) = \chi(x/n)$ where χ is a smooth, $[0, 1]$ -valued, cutoff function such that $\chi(x) = 1$ for $|x| < 1$ and $\chi(x) = 0$ for $|x| > 2$. By integration by parts, one gets

$$\begin{aligned} \int_{\mathbb{R}^d} \chi_n(x) \nabla v(x) \cdot \partial_\lambda^0 F_\lambda(x) e^{-V(x)} dx &= \int_{\mathbb{R}^d} \chi_n(x) v(x) (\nabla V(x) \cdot \partial_\lambda^0 F_\lambda(x) - \nabla \cdot \partial_\lambda^0 F_\lambda(x)) e^{-V(x)} dx \\ &\quad - \int_{\mathbb{R}^d} v(x) \nabla \chi_n(x) \cdot \partial_\lambda^0 F_\lambda(x) e^{-V(x)} dx. \end{aligned}$$

The result then follows from Lebesgue's theorem by taking the limit $n \rightarrow \infty$, using the fact that $\nabla V \in \mathbb{L}^2(e^{-V(x)} dx)$, $\partial_\lambda^0 F_\lambda \in \mathbb{L}^\infty$ and $\nabla \cdot \partial_\lambda^0 F_\lambda \in \mathbb{L}^2(e^{-V(x)} dx)$ from Assumptions **(Pot)**-(ii) and **(Drift)**-(i)-(ii). \square

By combining (62) and (65), one gets: for any $t \geq 0$,

$$\partial_\lambda^0 \mathbb{E}_{\pi_0} [f(X_t^\lambda)] = \int_0^t \mathbb{E}_{\pi_0} [f(X_0) (\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(X_s^0)] ds,$$

where, we recall, the process $(X_t^0)_{t \geq 0}$ satisfies (2) with an initial condition X_0 being distributed according to the equilibrium measure π_0 . Taking formally the limit $t \rightarrow \infty$, one obtains the classical Green-Kubo formula discussed in the next section.

4.2 Infinite time Green-Kubo formula

Theorem 37. *Consider the process $(X_t^0)_{t \geq 0}$ satisfying (2) with an initial condition X_0 being distributed according to the equilibrium measure π_0 . Assume that Assumption **(Poinc)**(η) holds for some positive η . Then, for any $f \in \mathbb{L}^2(e^{-V(x)} dx)$, $\lambda \mapsto \int_{\mathbb{R}^d} f d\pi_\lambda$ is differentiable at $\lambda = 0$ with derivative*

$$\partial_\lambda^0 \int_{\mathbb{R}^d} f d\pi_\lambda = \int_0^\infty \mathbb{E}_{\pi_0} [f(X_0) (\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(X_s^0)] ds. \quad (67)$$

Let us recall some results and notation from Section 2.4. The generator of the process $(X_t^0)_{t \geq 0}$ is $\mathcal{L}_0 = -\nabla V \cdot \nabla + \Delta$. The generator of the process $(X_t^\lambda)_{t \geq 0}$ is $\mathcal{L}_\lambda = F_\lambda \cdot \nabla + \Delta = \mathcal{L}_0 + \mathcal{T}_\lambda$ where $\mathcal{T}_\lambda = (F_\lambda + \nabla V) \cdot \nabla$. The domain of the operator \mathcal{L}_0 is

$$\mathcal{D}(\mathcal{L}_0) = \left\{ v \in \mathbb{L}_0^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx), \mathcal{L}_0 v \in \mathbb{L}_0^2(e^{-V(x)} dx) \right\}.$$

For any $f \in \mathbb{L}^2(e^{-V(x)} dx)$, there exists a unique function $g = -\mathcal{L}_0^{-1} f$ in $\mathbb{L}_0^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx)$ such that

$$\forall v \in \mathbb{L}_0^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx), \int_{\mathbb{R}^d} \nabla g(x) \cdot \nabla v(x) e^{-V(x)} dx = \int_{\mathbb{R}^d} f(x) v(x) e^{-V(x)} dx.$$

Let us start with a lemma which is a consequence of the results of Section 2.3 on the long-time behaviour of $\mathbb{E}(f(Y_t^x))$.

Lemma 38. *Let us assume that Assumption (Poinc(η)) holds for some positive η . Let us introduce the semigroup P_t associated to the Markovian evolution (2): for any $f \in \mathbb{L}_0^2(e^{-V(x)} dx)$,*

$$P_t f(x) = \mathbb{E}(f(Y_t^x))$$

where $(Y_t^x)_{t \geq 0}$ satisfies (12). We then have the following Laplace inversion formula for the operator \mathcal{L}_0^{-1} : for any f in $\mathbb{L}_0^2(e^{-V(x)} dx)$,

$$-\mathcal{L}_0^{-1} f = \int_0^\infty P_t f dt. \quad (68)$$

Proof. From Proposition 9, we know that $u(t, x) = P_t f(x) = \mathbb{E}[f(Y_t^x)]$ is well defined in $\mathbb{L}_0^2(e^{-V(x)} dx)$ and satisfies the partial differential equation (23) in the sense of Definition 6. From Proposition 11, (since $\int_{\mathbb{R}^d} f(x) e^{-V(x)} dx = 0$)

$$\forall t \geq 0, \|P_t f\|_{\mathbb{L}^2(e^{-V(x)} dx)} \leq e^{-\eta t} \|f\|_{\mathbb{L}^2(e^{-V(x)} dx)}. \quad (69)$$

This shows that $\int_0^\infty P_t f dt$ is well defined in $\mathbb{L}_0^2(e^{-V(x)} dx)$. Moreover, an adaptation with $\lambda = \varphi = 0$ (and thus $C_0 = C = 0$) of the first energy estimate in the proof of Proposition 7 shows that

$$\int_0^\infty \int_{\mathbb{R}^d} |\nabla P_t f(x)|^2 e^{-V(x)} dx dt < \infty. \quad (70)$$

Therefore, $\int_0^\infty P_t f dt \in \mathbb{H}^1(e^{-V(x)} dx)$.

From Definition 6, for any test function $v \in \mathbb{L}^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx)$,

$$\int_{\mathbb{R}^d} f(x) v(x) e^{-V(x)} dx = \int_{\mathbb{R}^d} P_t f(x) v(x) e^{-V(x)} dx + \int_0^t \int_{\mathbb{R}^d} \nabla P_s f(x) \cdot \nabla v(x) e^{-V(x)} dx ds.$$

From Equation (69), $\lim_{t \rightarrow \infty} \int_{\mathbb{R}^d} P_t f(x) v(x) e^{-V(x)} dx = 0$ and thus, from (70), for any test function $v \in \mathbb{L}^2(e^{-V(x)} dx) \cap \mathbb{H}^1(e^{-V(x)} dx)$,

$$\int_{\mathbb{R}^d} f(x) v(x) e^{-V(x)} dx = \int_{\mathbb{R}^d} \nabla \left(\int_0^\infty P_t f(x) dt \right) \cdot \nabla v(x) e^{-V(x)} dx.$$

This concludes the proof. \square

We recall that Π_0 the orthogonal projection from $\mathbb{L}^2(e^{-V(x)}dx)$ onto $\mathbb{L}_0^2(e^{-V(x)}dx)$ (see (47)). We can now give a different expression for the right-hand side of (67). From Lemma 36 applied to the constant 1, one has $\int_{\mathbb{R}^d} (\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(x) e^{-V(x)} dx = 0$. Then, using successively this equality, the self-adjointness of P_t in $\mathbb{L}^2(e^{-V(x)}dx)$ (which is a direct consequence of (14)), Equation (68) and Lemma 36, one has,

$$\begin{aligned}
& \int_0^\infty \mathbb{E}_{\pi_0} [f(X_0)(\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(X_t^0)] dt \\
&= \int_0^\infty \int_{\mathbb{R}^d} \mathbb{E} [f(x)(\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(Y_t^x)] e^{-V(x)} dx dt \\
&= \int_0^\infty \int_{\mathbb{R}^d} \mathbb{E} [\Pi_0 f(x)(\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(Y_t^x)] e^{-V(x)} dx dt \\
&= \int_0^\infty \int_{\mathbb{R}^d} \Pi_0 f(x) P_t (\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(x) e^{-V(x)} dx dt \\
&= \int_0^\infty \int_{\mathbb{R}^d} (P_t \Pi_0 f(x)) (\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(x) e^{-V(x)} dx dt \\
&= - \int_{\mathbb{R}^d} (\mathcal{L}_0^{-1} \Pi_0 f)(x) (\nabla V \cdot \partial_\lambda^0 F_\lambda - \nabla \cdot \partial_\lambda^0 F_\lambda)(x) e^{-V(x)} dx \\
&= - \int_{\mathbb{R}^d} \partial_\lambda^0 \mathcal{T}_\lambda [(\mathcal{L}_0^{-1} \Pi_0 f)](x) e^{-V(x)} dx,
\end{aligned}$$

where $\partial_\lambda^0 \mathcal{T}_\lambda$ stands for the operator $\partial_\lambda^0 F_\lambda \cdot \nabla$ (consistently with the definition (44) of \mathcal{T}_λ). As a consequence, proving Equation (67) boils down to proving: for any $f \in \mathbb{L}^2(e^{-V(x)}dx)$,

$$\partial_\lambda^0 \int_{\mathbb{R}^d} \Pi_0 f(x) d\pi_\lambda(x) = - \int_{\mathbb{R}^d} \partial_\lambda^0 \mathcal{T}_\lambda [(\mathcal{L}_0^{-1} \Pi_0 f)](x) e^{-V(x)} dx. \quad (71)$$

We are now in position to complete the proof of Theorem 37.

Proof of Theorem 37. Recall that for λ small enough, the operator $I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*$ is invertible from $\mathbb{L}^2(e^{-V(x)}dx)$ to itself with bounded inverse (see Lemma 17). For such a small λ , one has the equality

$$(I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*)^{-1} = I - (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^* + \mathcal{R}_\lambda, \quad (72)$$

where (by (49)) the remainder $\mathcal{R}_\lambda = (I + (\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*)^{-1} ((\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^*)^2$ has a norm from $\mathbb{L}^2(e^{-V(x)}dx)$ to itself of order $\mathcal{O}(\lambda^2)$. Thus, by the analytical formula for π_λ obtained in Lemma 17,

$$\begin{aligned}
\int_{\mathbb{R}^d} f(x) d\pi_\lambda(x) - \int_{\mathbb{R}^d} f(x) d\pi_0(x) &= - \int_{\mathbb{R}^d} [(\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0)^* \mathbf{1}](x) f(x) e^{-V(x)} dx + \int_{\mathbb{R}^d} [\mathcal{R}_\lambda \mathbf{1}](x) f(x) d\pi_0 \\
&= - \int_{\mathbb{R}^d} [(\mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0) f](x) e^{-V(x)} dx + \mathcal{O}(\lambda^2). \quad (73)
\end{aligned}$$

Since, according to **(Drift)-(i)**, $\frac{F_\lambda + \nabla V}{\lambda}$ is bounded by C for $\lambda \in (0, \lambda_0]$, one has, by Lebesgue's theorem,

$$\lim_{\lambda \rightarrow 0} \frac{1}{\lambda} \int_{\mathbb{R}^d} \mathcal{T}_\lambda \mathcal{L}_0^{-1} \Pi_0 f(x) e^{-V(x)} dx = \int_{\mathbb{R}^d} (\partial_\lambda^0 \mathcal{T}_\lambda) \mathcal{L}_0^{-1} \Pi_0 f(x) e^{-V(x)} dx.$$

Dividing (73) by λ and taking the limit $\lambda \rightarrow 0$, one concludes that $\lambda \mapsto \int_{\mathbb{R}^d} f d\pi_\lambda$ is differentiable at $\lambda = 0$ and (71) holds. \square

Combining the previous result with (65), we obtain the following corollary.

Corollary 39. Let $f \in \mathbb{L}^2(e^{-V(x)}dx)$ be a Lipschitz function. Also assume that the Assumptions **(Poinc(η))** (for some positive η) and **(min Spec)** are satisfied. Then, one has

$$\partial_\lambda^0 \int_{\mathbb{R}^d} f d\pi_\lambda = \int_0^\infty \mathbb{E}_{\pi_0} \left[\nabla f(X_0) \cdot R_{X_0^0}^T(0, s) \partial_\lambda^0 F_\lambda(X_s^0) \right] ds.$$

5 Long-time convergence of the estimators (10) and (11)

5.1 Statement of the main result

Let us study the long-time behavior of the two estimators (10) and (11).

Theorem 40. Let $f : \mathbb{R}^d \rightarrow \mathbb{R}$ be a C^1 function such that ∇f is bounded.

- Assume the existence of $\eta > 0$ such that either V is η -convex or Assumptions **(Poinc(η))** and **(Spec(η))** hold. Then $\lambda \mapsto \frac{1}{t} \int_0^t f(X_s^\lambda) ds$ is differentiable at $\lambda = 0$ with derivative $\frac{1}{t} \int_0^t \nabla f(X_s^0) \cdot T_s ds$ and

$$\lim_{t \rightarrow \infty} \partial_\lambda^0 \left(\frac{1}{t} \int_0^t f(X_s^\lambda) ds \right) = \partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right) \text{ a.s..} \quad (74)$$

- Assume either that V is η -convex for a positive constant $\eta > 0$ and $\mathbb{E}|X_0| < +\infty$, or that there exist $\eta > 0$ and $p \in (1, \infty]$ such that **(Poinc(η))** holds, X_0 is distributed according to a measure having a density in $\mathbb{L}^p(e^{-V(x)}dx)$ with respect to $e^{-V(x)}dx$ and **(Spec(ρ))** holds for some $\rho < \eta(p-1)/p$ (with the convention $\eta(\infty-1)/\infty = \eta$). Then $\forall \lambda \in [0, \lambda_0], \forall t \geq 0$, $\mathbb{E}|f(X_t^\lambda)| < +\infty$, $\lambda \mapsto \mathbb{E}[f(X_t^\lambda)]$ is differentiable at $\lambda = 0$ with derivative $\partial_\lambda^0 \mathbb{E}[f(X_t^\lambda)] = \mathbb{E}[\nabla f(X_t^0) \cdot T_t]$ and

$$\lim_{t \rightarrow \infty} \partial_\lambda^0 \mathbb{E}[f(X_t^\lambda)] = \partial_\lambda^0 \left(\int_{\mathbb{R}^d} f d\pi_\lambda \right). \quad (75)$$

Remark 41. When π_0 is assumed to satisfy a logarithmic Sobolev inequality with constant η , which is stronger than the Poincaré inequality **(Poinc(η))**, then the second statement still holds as soon as X_0 is distributed according to a measure having a density in $\mathbb{L}^p(e^{-V(x)}dx)$ with respect to $e^{-V(x)}dx$ for some $p > 1$ and **(Spec(ρ))** holds for some $\rho < \eta$, because of the hypercontractivity property of the semi-group associated with (2) ensured by the Gross theorem.

5.2 Long-time behaviour of $(X_t^0, T_t)_{t \geq 0}$

To prove Theorem 40, one first needs to know the long-time limit of the trajectory and its tangent vector. We more generally consider $(X_t^0, T_t^0)_{t \geq 0}$ solving

$$\begin{cases} dX_t^0 = -\nabla V(X_t^0) dt + \sqrt{2} dW_t \\ dT_t^0 = (\partial_\lambda^0 F_\lambda(X_t^0) - \nabla^2 V(X_t^0) T_t^0) dt \end{cases} \quad (76)$$

with (X_0^0, T_0^0) any initial condition independent from the Brownian motion $(W_t)_{t \geq 0}$. To write conveniently the long-time limit of (X_t^0, T_t^0) , we will run time backward and use Lemma 22 about the link between the forward resolvent and its backward counterpart.

Lemma 42. Under Assumptions **(Poinc(η))** (for some positive η), **(min Spec)** and **(Conv)**, the process $(X_t^0, T_t^0)_{t \geq 0}$ converges in law as t goes to infinity to the couple

$$\left(Y_0, \int_0^\infty R_Y^T(0, t) \partial_\lambda^0 F_\lambda(Y_t) dt \right),$$

where $(Y_t)_{t \geq 0}$ follows the dynamics (2) with Y_0 distributed according to $e^{-V(x)} dx$. Moreover, the law \mathcal{V} of this couple is invariant by the dynamics (76) and ergodic for this dynamics: for any test function $\varphi : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ in $\mathbb{L}^1(\mathcal{V})$, for \mathcal{V} -a.e. deterministic initial condition (X_0^0, T_0^0) ,

$$\lim_{t \rightarrow \infty} \frac{1}{t} \int_0^t \varphi(X_s^0, T_s^0) ds = \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi(x, \tau) d\mathcal{V}(x, \tau) \text{ a.s.}$$

Proof. The integral $\int_0^\infty R_Y^T(0, t) \partial_\lambda^0 F_\lambda(Y_t) dt$ is almost surely well defined, from Lemma 24 and the boundedness of $\partial_\lambda^0 F_\lambda$. To prove Lemma 42, we are going to use a time reversal argument.

For $t_0 > 0$, we construct a coupling of the trajectory $(X_t^0)_{t \geq t_0}$ with another process $(\chi_t^{t_0})_{t \geq t_0}$ following the dynamics (2), but being at equilibrium. Denote by q_{t_0} the density of the distribution of $X_{t_0}^0$ (which exists by Lemma 2), and define $\rho_{t_0} = \frac{q_{t_0} \wedge e^{-V}}{q_{t_0}}$. Let U and ζ_{t_0} be mutually independent random variables which are independent of X_0 and of the Brownian motion $(W_t)_{t \geq 0}$ driving $(X_t^0)_{t \geq 0}$, such that U is uniformly distributed over $[0, 1]$ and, when $q_{t_0} \neq e^{-V}$, ζ_{t_0} is distributed according to $C(e^{-V(x)} - q_{t_0}(x))^+ dx$, C being a normalization constant (ζ_{t_0} does not need to be defined when $q_{t_0} = e^{-V}$). We define the position of the process $(\chi_t^{t_0})_{t \geq t_0}$ at time t_0 by $\chi_{t_0}^{t_0} = X_{t_0}^0 \mathbf{1}_{U \leq \rho_{t_0}(X_{t_0}^0)} + \zeta_{t_0} \mathbf{1}_{U > \rho_{t_0}(X_{t_0}^0)}$, which is distributed according to π_0 . One has $\mathbb{P}(\chi_{t_0}^{t_0} \neq X_{t_0}^0) = \frac{1}{2} \|q_{t_0}(x) - e^{-V(x)}\|_{\mathbb{L}^1(dx)}$. For $t > t_0$, let $(\chi_t^{t_0})_{t \geq t_0}$ evolve according to the dynamics (2) with Brownian motion $(W_t)_{t \geq 0}$. Notice that $(\chi_{t+t_0}^{t_0})_{t \geq 0}$ has the same law as the process at equilibrium $(Y_t)_{t \geq 0}$ introduced in the statement of Lemma 42. Moreover, $(\chi_t^{t_0})_{t \geq t_0}$ is such that

$$\mathbb{P}(\forall t \geq t_0, \chi_t^{t_0} = X_t^0) = 1 - \frac{1}{2} \|q_{t_0}(x) - e^{-V(x)}\|_{\mathbb{L}^1(dx)}.$$

From an easy adaptation of Proposition 20, one has on the one hand

$$(X_t^0, T_t^0) = \left(X_{t_0}^0, R_{X^0}(0, t) T_{t_0}^0 + \int_{t_0}^t R_{X^0}(s, t) \partial_\lambda^0 F_\lambda(X_s^0) ds \right).$$

On the other hand, for $0 < t_0 \leq t$, we have the equalities, by using successively the time translation $s \rightarrow s - t_0$, the change of variable $u = t - t_0 - s$, Lemma 22 (using the notation, for $u \in [0, t - t_0]$, $Z_u = Y_{t-t_0-u}$) and the time reversibility of the dynamics (2):

$$\begin{aligned} \left(\chi_{t_0}^{t_0}, \int_{t_0}^t R_{\chi^{t_0}}(s, t) \partial_\lambda^0 F_\lambda(\chi_s^{t_0}) ds \right) &\stackrel{\mathcal{D}}{=} \left(Y_{t-t_0}, \int_0^{t-t_0} R_Y(s, t-t_0) \partial_\lambda^0 F_\lambda(Y_s) ds \right) \\ &= \left(Y_{t-t_0}, \int_0^{t-t_0} R_Y(t-t_0-u, t-t_0) \partial_\lambda^0 F_\lambda(Y_{t-t_0-u}) du \right) \\ &= \left(Z_0, \int_0^{t-t_0} R_Z^T(0, u) \partial_\lambda^0 F_\lambda(Z_u) du \right) \\ &\stackrel{\mathcal{D}}{=} \left(Y_0, \int_0^{t-t_0} R_Y^T(0, s) \partial_\lambda^0 F_\lambda(Y_s) ds \right), \end{aligned}$$

where $\stackrel{\mathcal{D}}{=}$ stands for the equality in distribution. As a consequence, for any bounded Lipschitz

function $\varphi : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ (with Lipschitz constant $\text{Lip}(\varphi)$), for $t \geq t_0 > 0$

$$\begin{aligned}
& \left| \mathbb{E} \left[\varphi \left(Y_0, \int_0^\infty R_Y^T(0, s) \partial_\lambda^0 F_\lambda(Y_s) ds \right) - \varphi(X_t^0, T_t^0) \right] \right| \\
& \leq \left| \mathbb{E} \left[\varphi \left(Y_0, \int_0^\infty R_Y^T(0, s) \partial_\lambda^0 F_\lambda(Y_s) ds \right) - \varphi \left(Y_0, \int_0^{t-t_0} R_Y^T(0, s) \partial_\lambda^0 F_\lambda(Y_s) ds \right) \right] \right| \\
& + \left| \mathbb{E} \left[\varphi \left(\chi_t^{t_0}, \int_{t_0}^t R_{\chi^{t_0}}(s, t) \partial_\lambda^0 F_\lambda(\chi_s^{t_0}) ds \right) \right. \right. \\
& \quad \left. \left. - \varphi \left(\chi_t^{t_0}, R_{X^0}(0, t) T_0^0 + \int_0^{t_0} R_{X^0}(s, t) \partial_\lambda^0 F_\lambda(X_s^0) ds + \int_{t_0}^t R_{\chi^{t_0}}(s, t) \partial_\lambda^0 F_\lambda(\chi_s^{t_0}) ds \right) \right] \right| \\
& + \left| \mathbb{E} \left[\varphi \left(\chi_t^{t_0}, R_{X^0}(0, t) T_0^0 + \int_0^{t_0} R_{X^0}(s, t) \partial_\lambda^0 F_\lambda(X_s^0) ds + \int_{t_0}^t R_{\chi^{t_0}}(s, t) \partial_\lambda^0 F_\lambda(\chi_s^{t_0}) ds \right) - \varphi(X_t^0, T_t^0) \right] \right| \\
& \leq \left| \mathbb{E} \left[\varphi \left(Y_0, \int_0^\infty R_Y^T(0, s) \partial_\lambda^0 F_\lambda(Y_s) ds \right) - \varphi \left(Y_0, \int_0^{t-t_0} R_Y^T(0, s) \partial_\lambda^0 F_\lambda(Y_s) ds \right) \right] \right| \\
& + \mathbb{E} \left[(2\|\varphi\|_{\mathbb{L}^\infty(\Omega)}) \wedge \left(\text{Lip}(\varphi) \left| R_{X^0}(t_0, t) \left(R_{X^0}(0, t_0) T_0^0 + \int_0^{t_0} R_{X^0}(s, t_0) \partial_\lambda^0 F_\lambda(X_s^0) ds \right) \right| \right) \right] \\
& + 2\|\varphi\|_\infty \mathbb{P}(X_{t_0}^0 \neq \chi_{t_0}^{t_0}). \tag{77}
\end{aligned}$$

Notice that we used the semi-group property of R_{X^0} to obtain the last but one inequality. The first term in the right-hand side converges to 0 as $t \rightarrow \infty$ by Lebesgue's theorem. A direct adaptation of Lemma 24 shows that $R_{X^0}(t_0, t)$ goes to 0 as t goes to infinity, yielding from Lebesgue's theorem that the second term in the right-hand side of (77) goes to 0 as t goes to infinity. The third term in the right-hand side of (77) can be rewritten as $2\|\varphi\|_\infty \mathbb{P}(X_{t_0}^0 \neq \chi_{t_0}^{t_0}) = \|\varphi\|_{\mathbb{L}^\infty(\Omega)} \|e^{-V(x)} - p_{t_0}(x)\|_{\mathbb{L}^1(dx)}$ and thus goes to 0 as t_0 goes to infinity, by Corollary 12. Letting $t \rightarrow \infty$ and then $t_0 \rightarrow \infty$ in (77), we conclude that the couple (X_t^0, T_t^0) converges in law to $(Y_0, \int_0^\infty R_Y^T(0, s) \partial_\lambda^0 F_\lambda(Y_s) ds)$ with law \mathcal{V} .

To check that \mathcal{V} is invariant by the dynamics (76), we denote by $(\mathcal{P}_s)_{s \geq 0}$ the Markov semi-group associated with this dynamics. One has $\mathbb{E}[\mathcal{P}_s \varphi(X_t^0, T_t^0)] = \mathbb{E}[\varphi(X_{t+s}^0, T_{t+s}^0)]$ where the right-hand side converges to $\int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi(x, \tau) d\mathcal{V}(x, \tau)$ as $t \rightarrow \infty$ and $\mathcal{P}_s \varphi(x, \tau) = \mathbb{E}[\varphi(Y_s^x, T_s^{x, \tau})]$ with

$$\begin{cases} Y_t^x = x - \int_0^t \nabla V(Y_s^x) ds + \sqrt{2} W_t, \\ T_t^{x, \tau} = \tau + \int_0^t (\partial_\lambda^0 F_\lambda(Y_s^x) - \nabla^2 V(Y_s^x) T_s^{x, \tau}) ds. \end{cases}$$

The continuity of $x \mapsto (Y_t^x)_{t \geq 0}$ for the topology of local uniform convergence on $\mathcal{C}(\mathbb{R}_+, \mathbb{R}^d)$ together with the continuity of $\nabla^2 V$ implies the continuity of $x \mapsto (R_{Y^x}(s, t))_{s, t \geq 0}$ for the topology of local uniform convergence on $\mathcal{C}(\mathbb{R}_+ \times \mathbb{R}_+, \mathbb{R}^{d \times d})$. With the continuity of $\partial_\lambda^0 F_\lambda$, one deduces the continuity of $(x, \tau) \mapsto T_s^{x, \tau} = R_{Y^x}(0, s) \tau + \int_0^s R_{Y^x}(r, s) \partial_\lambda^0 F_\lambda(Y_r^x) dr$. Hence, by Lebesgue's theorem, $\mathcal{P}_s \varphi(x, \tau)$ is continuous and bounded and $\mathbb{E}[\mathcal{P}_s \varphi(X_t^0, T_t^0)]$ converges to $\int_{\mathbb{R}^d \times \mathbb{R}^d} \mathcal{P}_s \varphi(x, \tau) d\mathcal{V}(x, \tau)$ as $t \rightarrow \infty$. Therefore $\int_{\mathbb{R}^d \times \mathbb{R}^d} \mathcal{P}_s \varphi(x, \tau) d\mathcal{V}(x, \tau) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi(x, \tau) d\mathcal{V}(x, \tau)$ and the probability measure \mathcal{V} is invariant.

Since \mathcal{V} is the unique invariant probability measure for the SDE (76), this measure is ergodic (see for example [27, Theorem 3.8 and Equation (52)]). \square

Let us deduce from the previous results the limit of $\frac{1}{t} \int_0^t \varphi(X_s^0) \cdot T_s^0 ds$ where $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is measurable and bounded.

Lemma 43. *Assume the existence of $\eta > 0$ such that either V is η -convex or Assumptions **(Poinc(η))** and **(Spec(η))** hold. Then $\int_{\mathbb{R}^d \times \mathbb{R}^d} |\tau| d\mathcal{V}(x, \tau) < \infty$ (where the probability distribution \mathcal{V} has been introduced in Lemma 42) and for any function $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}^d$ measurable and bounded, $\frac{1}{t} \int_0^t \varphi(X_s^0) \cdot T_s^0 ds$ converges a.s. to $\int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi(x) \cdot \tau d\mathcal{V}(x, \tau)$ as $t \rightarrow \infty$ whatever the choice of the initial condition (X_0^0, T_0^0) independent of the Brownian motion $(W_t)_{t \geq 0}$.*

Proof. Notice that if V is η -convex, Assumptions **(min Spec)**, **(Conv)** and **(Poinc(η))** hold. In addition, Assumption **(Spec(η))** implies Assumptions **(min Spec)** and **(Conv)**. Therefore, the conclusion of Lemma 42 holds under the two classes of hypotheses considered. Since $\partial_\lambda^0 F_\lambda$ is bounded, one has

$$\int_{\mathbb{R}^d \times \mathbb{R}^d} |\tau| d\mathcal{V}(x, \tau) \leq \int_0^\infty \mathbb{E} \left[|R_Y^T(0, t)| |\partial_\lambda^0 F_\lambda(Y_t)| \right] dt \leq C \int_0^\infty \mathbb{E} [|R_Y(0, t)|] dt,$$

where the right-hand side is finite by (58) when V is η -convex and by Proposition 27 otherwise.

In case the law of (X_0^0, T_0^0) is absolutely continuous with respect to \mathcal{V} , the result of Lemma 43 is then a direct consequence of the ergodic property of the process $(X_t^0, T_t^0)_{t \geq 0}$ stated in Lemma 42.

To extend this result to more general initial conditions, we proceed as follows. By Lemma 4, the law of X_1^0 is absolutely continuous with respect to π_0 which is the marginal law of the d first coordinates for the ergodic measure \mathcal{V} . Let $d\mathcal{V}_{T|X=x}(\tau)$ denote a regular conditional probability distribution of the d last coordinates given the d first ones under \mathcal{V} and \tilde{T}_1^0 be a random vector independent of $(W_t - W_1)_{t \geq 1}$ with conditional law given X_1^0 equal to $d\mathcal{V}_{T|X=X_1^0}(\tau)$. Let for $t \geq 1$, $\tilde{T}_t^0 = R_{X^0}(1, t)\tilde{T}_1^0 + \int_1^t R_{X^0}(s, t)\partial_\lambda^0 F_\lambda(X_s^0) ds$. Then $d\tilde{T}_t^0 = \left(\partial_\lambda^0 F_\lambda(X_t^0) - \nabla^2 V(X_t^0)\tilde{T}_t^0 \right) dt$ so that $(X_t^0, \tilde{T}_t^0)_{t \geq 1}$ solves (76) starting from (X_1^0, \tilde{T}_1^0) the law of which is absolutely continuous with respect to the measure \mathcal{V} ergodic for this stochastic differential equation (see Lemma 42). As a consequence $\frac{1}{t} \int_1^t \varphi(X_s^0) \cdot \tilde{T}_s^0 ds$ converges a.s. to $\int_{\mathbb{R}^d \times \mathbb{R}^d} \varphi(x) \cdot \tau d\mathcal{V}(x, \tau)$ as $t \rightarrow \infty$. Now, by an adaptation of Proposition 20, one can check that for $t \geq 1$, $\tilde{T}_t^0 - T_t^0 = R_{X^0}(1, t)(\tilde{T}_1^0 - T_1^0) = R_{X^0}(0, t)R_{X^0}(1, 0)(\tilde{T}_1^0 - T_1^0)$ so that

$$\begin{aligned} \frac{1}{t} \int_0^t \varphi(X_s^0) \cdot T_s^0 ds - \frac{1}{t} \int_1^t \varphi(X_s^0) \cdot \tilde{T}_s^0 ds &= \frac{1}{t} \int_0^1 \varphi(X_s^0) \cdot T_s^0 ds \\ &\quad + \frac{1}{t} \int_1^t \varphi(X_s^0) \cdot R_{X^0}(0, s) ds R_{X^0}(1, 0)(\tilde{T}_1^0 - T_1^0). \end{aligned}$$

The proof is completed by noticing that this quantity converges a.s. to 0 (for the second term in the right-hand side, this is a consequence of the boundedness of φ and of the almost sure estimate (60)). \square

5.3 Proof of Theorem 40

We are now in position to prove Theorem 40.

Proof of Theorem 40. Let us start by a preliminary result concerning the integrability of the random variable $\int_0^\infty |\nabla f(X_0)| |R_{X^0}^T(0, t)\partial_\lambda^0 F_\lambda(X_t^0)| dt$. By the boundedness of ∇f and $\partial_\lambda^0 F_\lambda$

$$\mathbb{E}_{\pi_0} \left[\int_0^\infty |\nabla f(X_0)| \left| R_{X^0}^T(0, t)\partial_\lambda^0 F_\lambda(X_t^0) \right| dt \right] \leq C \int_0^{+\infty} \mathbb{E}_{\pi_0} [|R_{X^0}(0, t)|] dt,$$

where, we recall, the subscript π_0 in \mathbb{E}_{π_0} indicates that X_0 is distributed according to π_0 . If V is η -convex, using (58), almost surely,

$$|R_{X^0}(0, t)| \leq e^{-\eta t}.$$

If Assumptions **(Poinc**(η)) and **(Spec**(η)) hold for some positive η (notice that **(Spec**(ρ)) for $\rho < \frac{\eta(p-1)}{p}$ with $p \in (1, +\infty]$ implies **(Spec**(η))), then, by Proposition 27 ,

$$\mathbb{E}_{\pi_0} [|R_{X^0}(0, t)|] \leq C e^{-t/C}$$

for some positive constant C . Hence, in all cases,

$$\mathbb{E}_{\pi_0} \left[\int_0^\infty |\nabla f(X_0)| \left| R_{X^0}^T(0, t) \partial_\lambda^0 F_\lambda(X_t^0) \right| dt \right] < +\infty. \quad (78)$$

Let us now prove the first statement of Theorem 40. By (63), the boundedness of ∇f and Proposition 19, Lebesgue's theorem implies that $\lambda \mapsto \frac{1}{t} \int_0^t f(X_s^\lambda) ds$ is differentiable at $\lambda = 0$ with derivative $\frac{1}{t} \int_0^t \nabla f(X_s^0) \cdot T_s ds$. By Lemma 43, $\frac{1}{t} \int_0^t \nabla f(X_s^0) \cdot T_s ds$ converges a.s. to $\int_{\mathbb{R}^d \times \mathbb{R}^d} \nabla f(x) \cdot \tau d\mathcal{V}(x, \tau) = \mathbb{E}_{\pi_0} [\nabla f(X_0) \cdot \int_0^\infty R_{X^0}^T(0, s) \partial_\lambda^0 F_\lambda(X_s^0) ds]$. The proof of (74) is then completed by the following computations:

$$\begin{aligned} \mathbb{E}_{\pi_0} \left[\nabla f(X_0) \cdot \int_0^\infty R_{X^0}^T(0, s) \partial_\lambda^0 F_\lambda(X_s^0) ds \right] &= \int_0^\infty \mathbb{E}_{\pi_0} \left[\nabla f(X_0) \cdot R_{X^0}^T(0, s) \partial_\lambda^0 F_\lambda(X_s^0) \right] ds \\ &= \partial_\lambda^0 \int_{\mathbb{R}^d} f(x) d\pi_\lambda(x) \end{aligned} \quad (79)$$

where we used Fubini's theorem and (78) for the first equality and Corollary 39 for the second one.

Let us finally deal with the second statement of Theorem 40. By (63), the boundedness of ∇f and Proposition 19, it is enough to check that $\mathbb{E}|f(X_t^0)| < +\infty$ to deduce that $\forall \lambda \in [0, \lambda_0]$, $\mathbb{E}|f(X_t^\lambda)| < +\infty$ and $\lambda \mapsto \mathbb{E}[f(X_t^\lambda)]$ is differentiable at $\lambda = 0$ with derivative $\partial_\lambda^0 \mathbb{E}[f(X_t^\lambda)] = \mathbb{E}[\nabla f(X_t^0) \cdot T_t]$. When $e^{-V(x)} dx$ satisfies a Poincaré inequality, then according to [4] and the references therein, since f is a Lipschitz function, there exists a positive ε such that $\int_{\mathbb{R}^d} e^{\varepsilon|f(x)|} e^{-V(x)} dx < +\infty$. Therefore, when the law μ_0 of X_0 has a density with respect to $e^{-V(x)} dx$ in $\mathbb{L}^p(e^{-V(x)} dx)$, by Lemma 4,

$$\sup_{t \geq 0} \mathbb{E}|f(X_t^0)| \leq \|f\|_{\mathbb{L}^{\frac{p}{p-1}}(e^{-V(x)} dx)} \left\| \frac{d\mu_0}{e^{-V(x)} dx} \right\|_{\mathbb{L}^p(e^{-V(x)} dx)} < +\infty.$$

When V is η -convex, then computing $|Y_t^x|^2$ by Itô's formula, remarking that

$$-2\nabla V(Y_t^x) \cdot Y_t^x = -2(\nabla V(Y_t^x) - \nabla V(0)) \cdot Y_t^x - 2\nabla V(0) \cdot Y_t^x \leq -\eta|Y_t^x|^2 + \frac{|\nabla V(0)|^2}{\eta},$$

applying a localization procedure to get rid of the expectation of the stochastic integral, one obtains $\forall t \geq 0$, $\mathbb{E}[|Y_t^x|^2] \leq e^{-\eta t} |x|^2 + \frac{1-e^{-\eta t}}{\eta} \left(\frac{|\nabla V(0)|^2}{\eta} + 2d \right)$. Hence, when the initial random variable X_0 with law μ_0 is integrable,

$$\begin{aligned} \mathbb{E}|X_t^0| &\leq \int_{\mathbb{R}^d} \mathbb{E}|Y_t^x| d\mu_0(x) \leq \int_{\mathbb{R}^d} \sqrt{\mathbb{E}[|Y_t^x|^2]} d\mu_0(x) \\ &\leq \mathbb{E} \left[\sqrt{e^{-\eta t} |X_0|^2 + \frac{1-e^{-\eta t}}{\eta} \left(\frac{|\nabla V(0)|^2}{\eta} + 2d \right)} \right] < +\infty, \end{aligned}$$

and $\mathbb{E}|f(X_t^0)| < +\infty$ by the Lipschitz continuity of f .

Notice that if V is η -convex, Assumptions **(min Spec)**, **(Conv)** and **(Poinc**(η)) hold. Moreover, Assumption **(Spec**(ρ)) implies Assumptions **(min Spec)** and **(Conv)**. Therefore, the conclusion of Lemma 42 holds under the two classes of hypotheses considered. The function $(x, \tau) \mapsto \nabla f(x) \cdot \tau$

is continuous and the family $(\nabla f(X_t^0) \cdot T_t)_{t \geq 0}$ is uniformly integrable by Proposition 29 when V is η -convex and since $\sup_{t \geq 0} \mathbb{E} \left(|\nabla f(X_t^0) \cdot T_t|^{\frac{\eta(\rho-1)}{\rho p}} \right) < \infty$, by Proposition 30, in the second framework. Therefore the convergence in distribution in Lemma 42 yields

$$\lim_{t \rightarrow \infty} \mathbb{E} (\nabla f(X_t^0) \cdot T_t) = \mathbb{E}_{\pi_0} \left[\nabla f(X_0) \cdot \int_0^\infty R_{X^0}^T(0, s) \partial_\lambda^0 F_\lambda(X_s^0) ds \right],$$

where the right-hand side is equal to $\partial_\lambda^0 \int_{\mathbb{R}^d} f(x) d\pi_\lambda(x)$ according to (79). \square

6 Numerical illustrations

In this section, we illustrate through various numerical experiments the theoretical results obtained above. In Section 6.1, we study numerically on a one-dimensional toy model the integrability of the tangent vector T_t and the sharpness of the integrability exponent obtained in Proposition 30. In Section 6.2, we illustrate the interest of the estimator (11) on a more realistic test case proposed in [34]. Finally, we investigate in Section 6.3 on the one-dimensional toy model a variance reduction method for the estimator (11).

6.1 A one-dimensional toy model

In this section, we would like to study on a simple test case the integrability of the tangent vector T_t , and to compare the theoretical bounds obtained in Proposition 30, with a numerical estimation of the integrability exponent. Let us consider the potential

$$\forall x \in \mathbb{R}, V_\lambda(x) = x^4 - \frac{c}{2}x^2 + \lambda x,$$

where c is some fixed constant, and $\lambda \in \mathbb{R}$ is the parameter. For $\lambda = 0$, V_0 has curvature $-c$ at the origin, and for $c > 0$, V_0 is a double-well potential, with wells located at $\pm\sqrt{c}/2$ and separated by a barrier with height $c^2/16$. In particular, as c gets larger, the dynamics (2) of $(X_t^0)_{t \geq 0}$ becomes more and more metastable.

Let us start with some explicit computation on T_t . When $\lambda \geq 0$, the perturbative force pushes the system to the left. Therefore, one expects the tangent vector T_t to be negative in the mean. In fact, one can prove that T_t is in that case almost surely negative for $t > 0$. Indeed, $(T_t)_{t \geq 0}$ satisfies the equation

$$\begin{cases} \partial_t T_t = -1 + (c - 12(X_t^0)^2)T_t, \\ T_0 = 0, \end{cases}$$

which can be solved explicitly, since in dimension 1, the resolvent $R_{X^0}(s, t)$ is given by the exponential $R_{X^0}(s, t) = \exp\left(c(t-s) - 12 \int_s^t (X_u^0)^2 du\right)$. Equation (56) then becomes

$$T_t = - \int_0^t \exp\left(c(t-s) - 12 \int_s^t (X_u^0)^2 du\right) ds < 0.$$

Concerning the upper bound on the integrability exponent obtained in Proposition 30, if the initial condition X_0 has a bounded density, then the tangent vector is bounded in \mathbb{L}^α uniformly in time for all α strictly smaller than η/ρ . Here, η is the Poincaré constant of the potential V_0 and ρ is the quantity

$$\rho = -(\inf \min \text{Spec}(\nabla^2 V(x))) \frac{\int_{\mathbb{R}^d} (\min \text{Spec}(\nabla^2 V(x)))^2 e^{-V(x)} dx}{\left(\int_{\mathbb{R}^d} \min \text{Spec}(\nabla^2 V(x)) e^{-V(x)} dx\right)^2} = c \frac{\int_{\mathbb{R}} (12x^2 - c)^2 e^{-V(x)} dx}{\left(\int_{\mathbb{R}} (12x^2 - c) e^{-V(x)} dx\right)^2} \quad (80)$$

appearing in Assumption **(Spec**(η/α)). The real number ρ can easily be approximated by one-dimensional numerical integration. Concerning the Poincaré constant η of V_0 , let us first notice that the potential V_0 can be written as the sum of a convex potential and a bounded perturbation and thus satisfies a Poincaré inequality thanks to the Holley-Stroock perturbation lemma (see [1, Theorem 3.4.1]). The corresponding Poincaré constant can be computed numerically, since it is the second eigenvalue of the operator $L = \partial_x^2 - V_0'(x)\partial_x = e^{V_0}\partial_x(e^{-V_0}\partial_x)$, whose first eigenvalue and eigenvector are 0 and the constant function $\mathbf{1}$. The numerical method we use to approximate η is the following. First, notice that the spectrum of the operator L is identical to the one of $\tilde{L} = e^{-V_0/2}Le^{V_0/2} = e^{V_0/2}\partial_x(e^{-V_0}\partial_x(e^{V_0/2}\cdot))$ which is self-adjoint in the space $\mathbb{L}^2(dx)$. The operator \tilde{L} is then discretized using a regular mesh with constant space step δx by the infinite tridiagonal matrix $(M_{i,j})_{i,j \in \mathbb{Z}}$ defined by

$$M_{i,i} = -\frac{1}{\delta x^2} \left(e^{V(i\delta x) - V((i+1/2)\delta x)} + e^{V(i\delta x) - V((i-1/2)\delta x)} \right)$$

and

$$M_{i,i+1} = M_{i+1,i} = \frac{1}{\delta x^2} e^{\frac{1}{2}V(i\delta x) + \frac{1}{2}V((i+1)\delta x) - V((i+1/2)\delta x)},$$

(with $M_{i,j} = 0$ whenever $|i-j| > 1$). We consider the restriction to a finite set of indices $(M_{i,j})_{-N \leq i,j \leq N}$, which is equivalent to imposing homogeneous Dirichlet boundary conditions at $x = -N\delta x$ and $x = N\delta x$. These artificial boundary conditions are justified (in the limit $N \rightarrow \infty$) by the fact that the eigenvectors of \tilde{L} go to 0 at infinity. Since the matrix $(M_{i,j})_{-N \leq i,j \leq N}$ is a nonpositive symmetric matrix, one can successively compute its first eigenvalues by the inverse power method, using at each step a projection on the orthogonal of the eigenvector which have already been computed. We checked that the numerical approximation obtained for the second eigenvalue is converged when $\delta x \rightarrow 0$ and $N \rightarrow \infty$. The graphs of numerical approximations of both ρ and the Poincaré constant are plotted on Figure 1. In particular, for a curvature constant c located left to the intersection of the two curves (approximately $c \leq 0.86$), Proposition 30 ensures that T_t is bounded in \mathbb{L}^1 , uniformly in time. Also, for curvature constants such that ρ is less than half the Poincaré constant (corresponding approximately to $c \leq 0.50$), T_t is bounded in \mathbb{L}^2 , and thus has a bounded variance uniformly in time. On Figure 2, we plot the critical exponent η/ρ such that, according to Proposition 30, T_t is in \mathbb{L}^α for $\alpha < \eta/\rho$.

Let us now explain how we estimate numerically the integrability exponent α such that T_t actually is in \mathbb{L}^α . This is done by computing the tail of the empirical cumulative distribution function of T_t . We simulate 10^6 independent realizations of the process (T_t, X_t) , starting from $\sqrt{c}/2$ (that is, at the bottom of the right well), up to the time $t = 40$, at which the systems seems to be at equilibrium. On Figure 3, we plot in logarithmic scale the tail of the empirical cumulative distribution function of those $N = 10^6$ independent realizations $(T_t^i)_{i=1, \dots, N}$, namely

$$[0, \infty) \ni x \mapsto \frac{1}{N} \sum_{i=1}^N \mathbf{1}_{|T_t^i| \geq x} = \frac{1}{N} \sum_{i=1}^N \mathbf{1}_{T_t^i \leq -x}$$

with curvature c being respectively 2, 3, 4 and 5, from bottom to top. Linear regression in those four cases gives the following slopes:

c	2	3	4	5
slope	-3.09	-1.95	-1.29	-1.12

We have checked that the results are the same for $t = 40$ and for $t = 80$. Note that an integrable random variable corresponds roughly to a slope less than -1 , and a square integrable variable corresponds to a slope less than -2 . We also plot on Figure 2 the empirical integrability exponent for

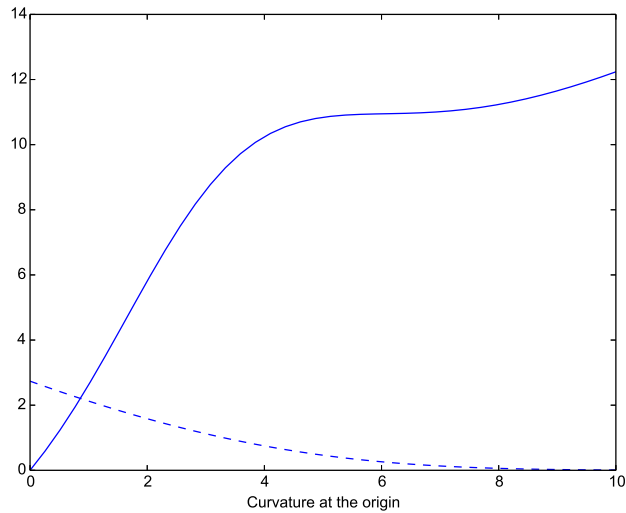


Figure 1: Poincaré constant of the measure e^{-V_0} (dashed line), and parameter ρ defined in (80) (solid line), as a function of the curvature c .

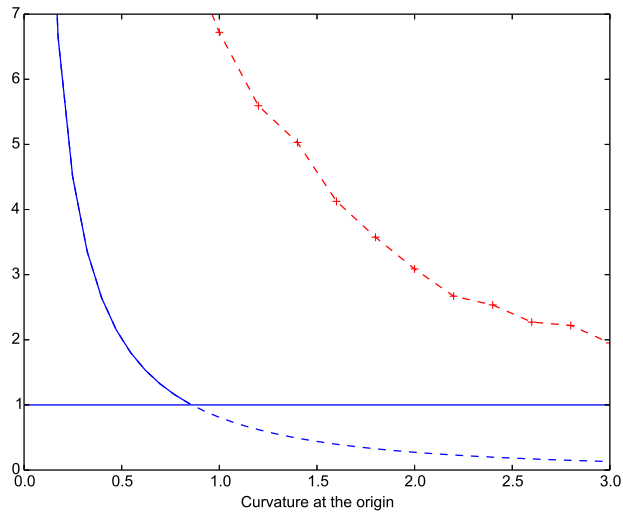


Figure 2: Blue: theoretical lower bound of integrability for T_t , according to Proposition 30 as a function of the curvature c (In fact, Proposition 30 yields boundedness in L^α only for $\alpha \geq 1$, corresponding to $c \lesssim 0.86$) ; Red : Numerical estimation of the integrability exponent α (for $t = 40$).

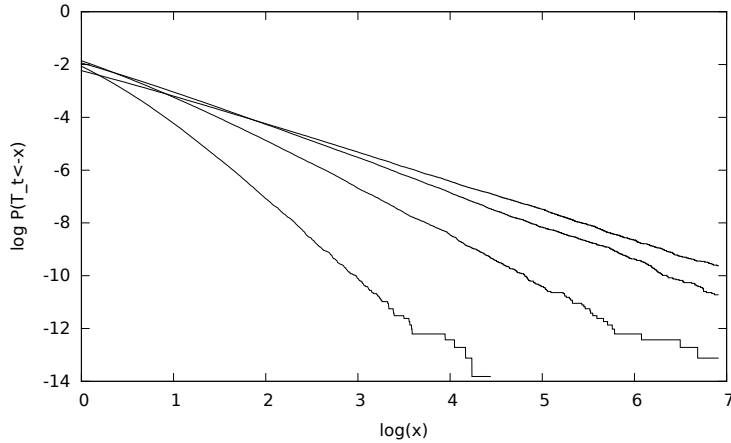


Figure 3: Logarithmic plot of the empirical cumulative distribution function of 10^6 independent realizations of T_t (for $t = 40$), with parameter (from bottom to top) $c = 2$, $c = 3$, $c = 4$, $c = 5$.

different curvatures between 0 and 3. We observe that the results are in accordance with Proposition 30: the theoretical lower bound is indeed smaller than the effective integrability exponent.

For a curvature larger than 3, the tangent vector T_t at time $t = 40$ does not seem to be of finite variance. This raises the question of appropriate variance reduction technique to be used in order to use the estimators (10) or (11). We will investigate in Section 6.3 a first idea that could be used in this one-dimensional situation. Further studies related to this problem will be the subject of future works.

6.2 A many particle system

In this section, we consider a more complex problem introduced in [34], and motivated by experimental studies of colloidal particles in optical traps. Let us consider $X_t^\lambda = (Y_t^1, \dots, Y_t^N)$ where $(Y_t^i)_{i=1, \dots, N} \in (\mathbb{R}^2)^N$ are the positions of N two-dimensional particles evolving according to

$$dY_t^i = -\kappa Y_t^i dt + \sum_{j=1}^N \nabla U(Y_t^i - Y_t^j) dt + \lambda e_1 dt + dW_t^i, \quad 1 \leq i \leq N \quad (81)$$

with $\kappa > 0$, $\lambda \in \mathbb{R}$, e_1 the normed vector directed along the first coordinate, and $U(x) = \Gamma e^{-|x|}/|x|$. The particles undergo a quadratic confining potential near the origin with strength κ , a repulsive interaction given by U , a shear in the x -direction with strength λ and a thermal noise.

We study the case of $N = 10$ particles with repulsion range $\Gamma = 25$ and attraction intensity $\kappa = 10$ corresponding to the parameters studied in [34]. For those parameters, at equilibrium, particles are gathered around the origin. At $\lambda = 0$, no particular direction appears in the dynamics, and the equilibrium measure is invariant with respect to rotations around the origin.

One wants to study the effect of shearing on the symmetry of the invariant measure. This symmetry can be measured by the empirical covariance Φ of the particle system, defined by

$$\Phi(X_t^\lambda) = \frac{1}{N} \sum_{i=1}^N (Y_t^{i,1} - \bar{Y}_t^1)(Y_t^{i,2} - \bar{Y}_t^2),$$

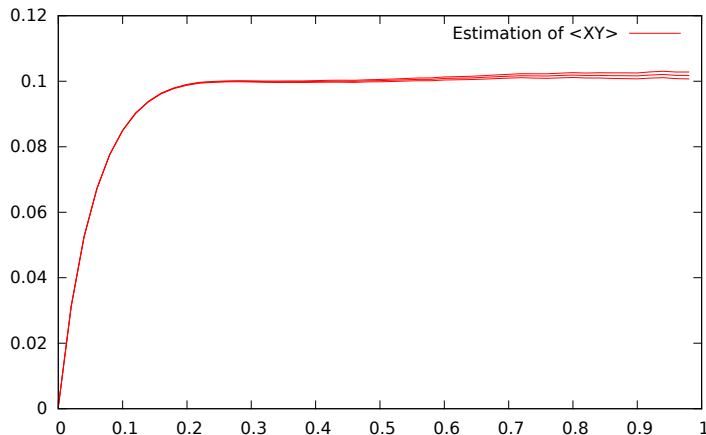


Figure 4: Sensitivity of the covariance with respect to the shear.

where $Y_t^i = (Y_t^{i,1}, Y_t^{i,2})$ and for $k \in \{1, 2\}$, $\bar{Y}_t^k = \frac{1}{N} \sum_{i=1}^N Y_t^{i,k}$. One is interested in computing the derivative $\partial_\lambda^0 \int_{(\mathbb{R}^2)^N} \Phi d\pi_\lambda$.

On Figure 4, we plot the confidence interval obtained for the expectation $\mathbb{E}[\partial_\lambda^0 \Phi(X_t^\lambda)]$, with $N = 10^5$ independent simulations, as a function of the time t . The dynamics (81) has been simulated using an explicit Euler-Maruyama scheme with time step $\delta t = 10^{-5}$, and the expectation has been calculated through the Monte Carlo approximation

$$\mathbb{E}[\partial_\lambda^0 \Phi(X_t^\lambda)] = \mathbb{E}[T_t \cdot \nabla \Phi(X_t^0)] \simeq \frac{1}{N} \sum_{i=1}^N T_t^i \cdot \nabla \Phi(X_t^{0,i})$$

where the $(X_t^{0,i}, T_t^i)_{1 \leq i \leq N}$ are independent simulations of the Euler-Maruyama discretization of the dynamics (7) ruling the evolution of (X_t^0, T_t) . As in [34], we observe that the correlation function $\mathbb{E}[\partial_\lambda^0 \Phi(X_t^\lambda)]$ increases as a function of time, before reaching a plateau. We have checked that similar results are obtained using a finite differentiation instead of the simulation of the couple (X_t^0, T_t) .

6.3 Particle merging

As mentioned in Section 6.1, in some situations, the variance of the tangent vector may become very large (or even infinite) which means that the estimators (10) and (11) become ineffective. Therefore, it is desirable to introduce variance reduction mechanisms. We explore in this section a first idea in the simple one-dimensional test case of Section 6.1. Extensions and further variance reduction techniques will be the subject of forthcoming works.

A first simple idea to reduce the variance is to replace the tangent vector T_s in the estimator of $\mathbb{E}[\nabla f(X_s^0) \cdot T_s]$ by its conditional expectation given X_s^0 . This corresponds in practice to replacing the tangent vector of particles which are at the same position at a given time s by the average of their tangent vectors. Then, the particles evolve again following the dynamics (7). We refer to this procedure as “particle merging”. In practice, with this naive procedure the probability to observe two particles at the same position is zero, in dimension larger than one. A first simple practical way to implement this technique is to introduce small subsets of the configuration space, and to merge particles which are in the same subset, which of course reduces the variance but introduce

some bias. The merging can be performed in a much efficient way and in larger dimensions, by correlating the particles, see e.g. [20]. This will be the scope of future work. Before studying the interest of particle merging on the simple case of Section 6.1, let us first state the theoretical result which justifies the use of this approach.

Lemma 44. *Assume (min Spec). For $s \geq 0$, let $(\tilde{T}_t)_{t \geq s}$ be the solution to*

$$\begin{cases} \frac{d\tilde{T}_t}{dt} = \partial_\lambda^0 F_\lambda(X_t^0) - \nabla^2(X_t^0)\tilde{T}_t, \text{ for all } t \geq s, \\ \tilde{T}_s = \mathbb{E}[T_s | X_s^0]. \end{cases}$$

Then $\forall t \geq s$, $\tilde{T}_t = \mathbb{E}[T_t | X_s^0, (W_r - W_s)_{r \in [s, t]}]$. Assume moreover that $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a Lipschitz function belonging to $\mathbb{L}^p(e^{-V(x)} dx)$ for some $p \in [1, \infty]$ and that the initial condition X_0 to (1) admits a density with respect to π_0 belonging to $\mathbb{L}^{\frac{p}{p-1}}(e^{-V(x)} dx)$ (where, by convention, $\frac{p}{p-1} = \infty$ if $p = 1$). Then, for each $t \geq 0$, $f(X_t^\lambda)$ is integrable for $\lambda \in [0, \lambda_0]$, $\lambda \mapsto \mathbb{E}[f(X_t^\lambda)]$ is differentiable at $\lambda = 0$ and

$$\partial_\lambda^0 \left(\mathbb{E}[f(X_t^\lambda)] \right) = \mathbb{E}[\nabla f(X_t^0) \cdot T_t] = \mathbb{E}[\nabla f(X_t^0) \cdot \tilde{T}_t], \text{ for each } t \geq s.$$

This Lemma shows that if, at a given time s , the particles at position X_s^0 replace their current tangent vectors by an average of these tangent vectors, and then follow the dynamics (7) for $t \geq s$, the estimator (11) is still consistent.

Proof. By Lemma 23, Assumption (min Spec) ensures that T_t is integrable for each $t \geq 0$. In view of the equality (56) and using the semigroup property (55) of R_{X^0} , one gets that for $t \geq s \geq 0$,

$$T_t = R_{X^0}(s, t)T_s + \int_s^t R_{X^0}(r, t)\partial_\lambda^0 F_\lambda(X_r^0)dr.$$

Since $(X_r^0)_{r \in [s, t]}$ and therefore $(R_{X^0}(r, t))_{r \in [s, t]}$ are measurable with respect to the sigma-field generated by X_s^0 and $(W_r - W_s)_{r \in [s, t]}$, one deduces that

$$\mathbb{E}[T_t | X_s^0, (W_r - W_s)_{r \in [s, t]}] = R_{X^0}(s, t)\mathbb{E}[T_s | X_s^0, (W_r - W_s)_{r \in [s, t]}] + \int_s^t R_{X^0}(r, t)\partial_\lambda^0 F_\lambda(X_r^0)dr.$$

The independence of (X_s^0, T_s) and $(W_r - W_s)_{r \in [s, t]}$ implies that $\mathbb{E}[T_s | X_s^0, (W_r - W_s)_{r \in [s, t]}] = \mathbb{E}[T_s | X_s^0]$. Since, by an adaptation of Proposition 20,

$$\tilde{T}_t = R_{X^0}(s, t)\mathbb{E}[T_s | X_s^0] + \int_s^t R_{X^0}(r, t)\partial_\lambda^0 F_\lambda(X_r^0)dr,$$

one concludes that $\tilde{T}_t = \mathbb{E}[T_t | X_s^0, (W_r - W_s)_{r \in [s, t]}]$.

If the initial condition X_0 to (1) admits a density with respect to π_0 belonging to $\mathbb{L}^{\frac{p}{p-1}}(e^{-V(x)} dx)$, then so does X_t^0 for each $t \geq 0$ by Lemma 4. When $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a Lipschitz function belonging to $\mathbb{L}^p(e^{-V(x)} dx)$, the integrability of $\mathbb{E}[f(X_t^\lambda)]$, the differentiability of $\lambda \mapsto \mathbb{E}[f(X_t^\lambda)]$ at $\lambda = 0$ and the equality $\partial_\lambda^0 (\mathbb{E}[f(X_t^\lambda)]) = \mathbb{E}[\nabla f(X_t^0) \cdot T_t]$ are deduced from an adaptation of the beginning of the proof of Theorem 33. Now, for $t \geq s$,

$$\begin{aligned} \mathbb{E}[\nabla f(X_t^0) \cdot T_t] &= \mathbb{E}[\mathbb{E}[\nabla f(X_t^0) \cdot T_t | X_s^0, (W_r - W_s)_{r \in [s, t]}]] \\ &= \mathbb{E}[\nabla f(X_t^0) \cdot \mathbb{E}[T_t | X_s^0, (W_r - W_s)_{r \in [s, t]}]] = \mathbb{E}[\nabla f(X_t^0) \cdot \tilde{T}_t]. \end{aligned}$$

□

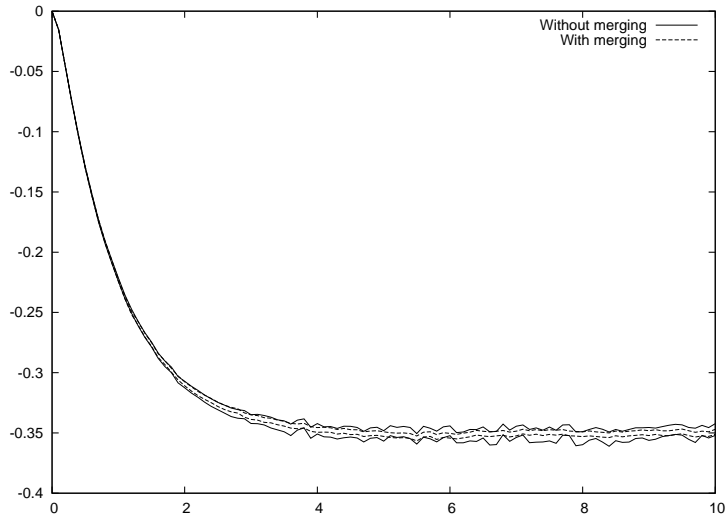


Figure 5: Empirical average and 95%-confidence interval for the Monte Carlo estimator of $\partial_\lambda \mathbb{E}[f(X_t^\lambda)]$ as a function of time, f being a smooth approximation of the indicator function of \mathbb{R}_+ : $f(x) = \frac{1}{2} + \frac{1}{\pi} \arctan(10x)$. The estimator is built with 10^6 realizations. Green: with merging (10^3 independent realizations of 10^3 interacting particles); Red: without merging (10^6 independent realizations).

To test the interest of this approach, we consider again the setting of Section 6.1 with $c = 2.9$ (which corresponds to case where the variance of tangent vector T_t , at $t = 40$, is very large, see Figure 2). The merging procedure is done as follows: a uniform mesh with step size 0.04 is introduced, and, every ten timesteps, the tangent vectors of particles which are in the same bin are replaced by an average of these tangent vectors. On Figure 5, we observe that this procedure divides approximately the variance by 4, while introducing a bias which is sufficiently small so that the confidence interval of the simulation with merging is included in the confidence interval of the simulation without merging. Figure 6 then gives more quantitative estimates of the variances of these two simulations (with and without merging), as a function of time. We have observed numerically that large values of T_t become very unlikely with the merging procedure: using 10^3 independent realizations of 10^3 interacting particles over the time interval $(0, 10)$, we did not observe any realization of T_t with absolute value larger than 3 (compare with what is reported on Figure 3).

A Alternative bounds on the density of X_t^0

In this section, we would like to present a few results which can be obtained under the assumption

Assumption (V). *The function V is of class \mathcal{C}^2 and satisfies*

$$C_V = \sup_{x \in \mathbb{R}^d} (2\Delta V(x) - |\nabla V(x)|^2) < +\infty.$$

Note that simple assumptions on the quantity $a_V(x) = 2\Delta V(x) - |\nabla V(x)|^2$ can give strong results on the equilibrium measure $e^{-V(x)} dx$. For instance, if $a_V(x)$ goes to $-\infty$ at infinity, then the equilibrium measure satisfies a Poincaré inequality (see for example the appendix in [32]).

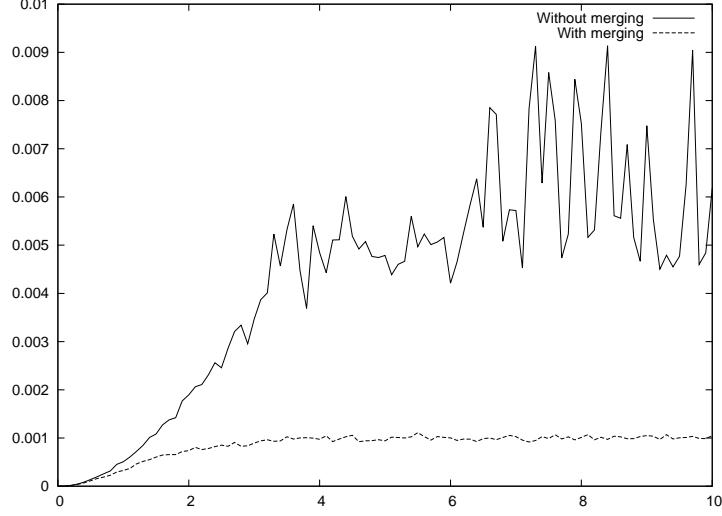


Figure 6: Empirical variance for the Monte Carlo estimator of $\partial_\lambda \mathbb{E}[f(X_t^\lambda)]$ as a function of time, f being the indicator function of \mathbb{R}_+ . Green: with merging ; Red: without merging.

A.1 Bounds on the density of X_t^0

Proposition 45. Consider the setting and the notation of Lemma 4 and let Assumption (V) hold. Assume that the measure $e^{\frac{1}{2}V} d\mu_0$ can be written as

$$e^{\frac{1}{2}V(x)} d\mu_0 = f(x) dx + d\nu,$$

where f is some function in $\mathbb{L}^p(dx)$ with $p \in [1, 2]$ and ν is some finite measure on \mathbb{R}^d . Then, for any $t > 0$, μ_t is absolutely continuous with respect to $e^{-\frac{1}{2}V(x)} dx$ with

$$\left\| \frac{d\mu_t}{e^{-\frac{1}{2}V(x)} dx} \right\|_{\mathbb{L}^2(dx)} \leq C e^{Ct} \left(\frac{C_p}{t^{(1/p-1/2)d/2}} + \frac{\nu(\mathbb{R}^d)}{t^{d/4}} \right). \quad (82)$$

Proof. Let $\psi : \mathbb{R}^d \rightarrow \mathbb{R}$ be a bounded measurable function and recall the formula

$$\mathbb{E}[\psi(X_t^0)] = \mathbb{E} \left[\psi(X_0 + \sqrt{2}W_t) e^{-\frac{1}{2}V(X_0 + \sqrt{2}W_t)} e^{\frac{1}{2}V(X_0)} e^{\frac{1}{4} \int_0^t (2\Delta V - |\nabla V|^2)(X_0 + \sqrt{2}W_s) ds} \right]$$

obtained by the Girsanov theorem, see Equation (15).

If C is an upper bound for $\frac{1}{4}(2\Delta V - |\nabla V|^2)$, and if one assumes $\psi \geq 0$, one obtains

$$\begin{aligned} \int_{\mathbb{R}^d} \psi d\mu_t &\leq e^{Ct} \mathbb{E} \left[\psi(X_0 + \sqrt{2}W_t) e^{-\frac{1}{2}V(X_0 + \sqrt{2}W_t)} e^{\frac{1}{2}V(X_0)} \right] \\ &= \frac{e^{Ct}}{(4\pi t)^{d/2}} \int_{\mathbb{R}^d} \psi(y) e^{-\frac{1}{2}V(y)} \left(\int_{\mathbb{R}^d} e^{\frac{1}{2}V(x)} e^{-\frac{|y-x|^2}{4t}} d\mu_0(x) \right) dy. \end{aligned}$$

so that $\mu_t \ll e^{-\frac{1}{2}V(x)} dx$ with a Radon-Nikodym derivative $\frac{d\mu_t}{e^{-\frac{1}{2}V(x)} dx}$ satisfying

$$\frac{d\mu_t}{e^{-\frac{1}{2}V(x)} dx} \leq e^{Ct} \left(e^{\frac{1}{2}V} \mu_0 \right) * \gamma_t = e^{Ct} (f * \gamma_t + \nu * \gamma_t),$$

where $*$ stands for the convolution product, and $\gamma_t(x) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{|x|^2}{4t}}$ denotes the centered Gaussian density with covariance matrix $2tI_d$. One concludes that (82) holds by:

- the Young inequality $\|f * \gamma_t\|_{\mathbb{L}^2(\mathrm{d}x)} \leq \|f\|_{\mathbb{L}^p(\mathrm{d}x)} \|\gamma_t\|_{\mathbb{L}^q(\mathrm{d}x)}$ where $1/p + 1/q = 3/2$ ($p, q \in [1, \infty]$) and the heat kernel estimate $\|\gamma_t\|_{\mathbb{L}^q(\mathrm{d}x)} \leq C_q t^{-\left(1 - \frac{1}{q}\right) \frac{d}{2}}$;
- the estimate $\|\nu * \gamma_t\|_{\mathbb{L}^2(\mathrm{d}x)}^2 \leq \|\nu * \gamma_t\|_{\mathbb{L}^1(\mathrm{d}x)} \|\nu * \gamma_t\|_{\mathbb{L}^\infty(\mathrm{d}x)} \leq \frac{(\nu(\mathbb{R}^d))^2}{(4\pi t)^{d/2}}$.

□

A.2 An additional result

Assumption **(V)** can also be useful to prove the second point in Assumption **(Pot)**-(ii) on the potential V .

Lemma 46. *Under Assumption **(V)**, the function ∇V is in $\mathbb{L}^2(e^{-V(x)} \mathrm{d}x)$:*

$$\int_{\mathbb{R}^d} |\nabla V|^2(x) e^{-V(x)} \mathrm{d}x \leq C_V.$$

Proof. Let $\chi_n(x) = \chi(x/n)$ where χ is a smooth, $[0, 1]$ -valued, cutoff function such that $\chi(x) = 1$ for $|x| < 1$ and $\chi(x) = 0$ for $|x| > 2$.

$$\begin{aligned} \int_{\mathbb{R}^d} |\nabla V|^2(x) \chi_n(x) e^{-V(x)} \mathrm{d}x &= - \int_{\mathbb{R}^d} (\chi_n(x) \nabla V(x)) \cdot \nabla e^{-V(x)} \mathrm{d}x \\ &= \int_{\mathbb{R}^d} \nabla \chi_n(x) \cdot \nabla V(x) e^{-V(x)} \mathrm{d}x + \int_{\mathbb{R}^d} \chi_n(x) \Delta V(x) e^{-V(x)} \mathrm{d}x \\ &\leq \int_{\mathbb{R}^d} \Delta \chi_n(x) e^{-V(x)} \mathrm{d}x + \frac{1}{2} \int_{\mathbb{R}^d} \chi_n(x) |\nabla V|^2(x) e^{-V(x)} \mathrm{d}x + \frac{1}{2} C_V. \end{aligned}$$

As a consequence,

$$\int_{\mathbb{R}^d} |\nabla V|^2(x) \chi_n(x) e^{-V(x)} \mathrm{d}x \leq 2 \int_{\mathbb{R}^d} \Delta \chi_n(x) e^{-V(x)} \mathrm{d}x + C_V$$

and the result follows from taking $n \rightarrow \infty$ by Fatou's lemma for the left-hand side and Lebesgue's theorem for the right-hand side. □

B About the Assumption **(Conv)**

In this section, we show that Assumption **(Conv)** is a natural one, since it appears as a sufficient condition in another related problem.

We recall that $(Y_t^x)_{t \geq 0}$ is defined in (12) as the solution to

$$\forall t \geq 0, Y_t^x = x - \int_0^t \nabla V(Y_s^x) \mathrm{d}s + \sqrt{2} W_t. \quad (83)$$

Since $(R_{Y^x}(0, t))_{t \geq 0}$ is the differential of the trajectory $(Y_t^x)_{t \geq 0}$ with respect to x , we expect that a condition yielding long-time decay for R_{Y^x} will imply that trajectories with same noise and close initial conditions will eventually converge toward each other. More precisely, we are interested in the joint long-time behavior of the so-called duplicated dynamics $(Y_t^x, Y_t^y)_{t \geq 0}$, where x and y are two different initial conditions. Note here that the two processes $(Y_t^x)_{t \geq 0}$ and $(Y_t^y)_{t \geq 0}$ are driven by the same Brownian motion.

In [23], the same problem is considered for a diffusion whose diffusion matrix may not be constant. In that case, an example is provided, where the process $Y_t^x - Y_t^y$ does not converge to 0.

A similar problem is considered in [5]: the process is a Brownian motion reflected on the boundary of a domain Ω . Such a dynamics can be formally seen as a singular case of the problem we consider, with $V = \infty \times \mathbf{1}_{\Omega^c}$. Equation (83) then has to be written with a local time on the boundary in place of ∇V . In that case, the difference $Y_t^x - Y_t^y$ will converge to 0 if the domain Ω is smooth enough and has at most one hole. However, it is conjectured that the same result holds for much more general domains.

We will use the fact that V is such that the dynamics (83) is ergodic with respect to the invariant measure $e^{-V(x)}dx$.

B.1 The one-dimensional case

In the one-dimensional case, this question is especially simple, because of the order structure on the state space. In particular (see [23]), it can be checked that if for any $x \in \mathbb{R}$, Y_t^x converge weakly to π_0 as $t \rightarrow \infty$, then the only invariant distribution of the duplicated dynamics is the image of $e^{-V(x)}dx$ by $x \mapsto (x, x)$. Actually, under additional assumption, one can show that $Y_t^x - Y_t^y$ converges in mean to 0 in the long-time limit.

Proposition 47. *Assume that the dimension is $d = 1$. If for any $x \in \mathbb{R}$ the time marginals of the process $(Y_t^x)_{t \geq 0}$ converge weakly to π_0 as $t \rightarrow \infty$ and the random variables $(Y_t^x)_{t \geq 0}$ are uniformly integrable, then, for any $x, y \in \mathbb{R}$, the process $(Y_t^x - Y_t^y)_{t \geq 0}$ converges to 0 in $\mathbb{L}^1(\Omega)$.*

According to Corollary 12, the long-time convergence of the marginals holds for instance if the potential V satisfies a Poincaré inequality (see Assumption **(Poinc(η))**).

Proof. First, from the uniform integrability of $(X_t^x)_{t \geq 0}$ and the weak convergence of the time marginals, both $\mathbb{E}[Y_t^x]$ and $\mathbb{E}[Y_t^y]$ converge to $\int_{\mathbb{R}} x e^{-V(x)} dx$ as $t \rightarrow \infty$.

Now assume, without loss of generality that $x \leq y$. Then, from a comparison theorem, $Y_t^x \leq Y_t^y$ holds for all positive times, and one obtains

$$\mathbb{E}[|Y_t^x - Y_t^y|] = \mathbb{E}[Y_t^y - Y_t^x] = \mathbb{E}[Y_t^x] - \mathbb{E}[Y_t^y] \rightarrow 0.$$

□

B.2 A general criterion

Proposition 48. *The following facts hold true:*

1. *Assume that*

$$\forall x, y \in \mathbb{R}^d, (x - y) \cdot (\nabla V(x) - \nabla V(y)) \geq \frac{v(x) + v(y)}{2} |x - y|^2 \quad (84)$$

with $v : \mathbb{R}^d \rightarrow \mathbb{R}$ such that $\int_{\mathbb{R}^d} \max(0, -v(x)) e^{-V(x)} dx < \infty$ and $\int_{\mathbb{R}^d} v(x) e^{-V(x)} dx > 0$. Then for all $x, y \in \mathbb{R}^d$, $|Y_t^x - Y_t^y|$ converges a.s. to 0, exponentially fast at any rate between 0 and $\int_{\mathbb{R}^d} v(x) e^{-V(x)} dx$ as $t \rightarrow \infty$.

2. *The exponential convergence to 0 still holds if V is convex and there exist $x_0 \in \mathbb{R}^d$ and $\varepsilon > 0$ such that the inequality $\inf_{x \in B(x_0, \varepsilon)} \min \text{Spec}(\nabla^2 V(x)) > 0$ holds.*
3. *If V is convex, then the only invariant measure of the duplicated dynamics is the image of $e^{-V(x)} dx$ by $x \mapsto (x, x)$.*

Let us start with a few remarks:

Remark 49. • The first point can be applied to the so-called Mexican hat potential $V(x) = \beta(|x|^4 - \gamma|x|^2)$, with $\beta > 0$ and $\gamma > 0$, in dimension $d \geq 2$. For this potential, one has

$$\begin{aligned} (x-y) \cdot (\nabla V(x) - \nabla V(y)) &= 2\beta|x-y|^2(|x|^2 + |y|^2 - \gamma) + 2\beta(|x|^2 - |y|^2)^2 \\ &\geq \frac{v(x) + v(y)}{2}|x-y|^2, \end{aligned}$$

for $v(x) = \beta(4|x|^2 - 2\gamma)$. In addition, one has $\int_{\mathbb{R}^d} v(x)e^{-V(x)}dx > 0$ since

$$\begin{aligned} \frac{\int_{\mathbb{R}^d} |x|^2 e^{\beta(\gamma|x|^2 - |x|^4)} dx}{\int_{\mathbb{R}^d} e^{\beta(\gamma|x|^2 - |x|^4)} dx} &= \frac{\int_0^{+\infty} r^{\frac{d}{2}} e^{\beta(\gamma r - r^2)} dr}{\int_0^{+\infty} r^{\frac{d}{2}-1} e^{\beta(\gamma r - r^2)} dr} \\ &= \frac{\gamma}{2} + \frac{\int_0^{+\infty} r^{\frac{d}{2}-1} (r - \frac{\gamma}{2}) e^{\beta(\gamma r - r^2)} dr}{\int_0^{+\infty} r^{\frac{d}{2}-1} e^{\beta(\gamma r - r^2)} dr} \\ &= \frac{\gamma}{2} + \frac{1_{\{d=2\}}}{2\beta \int_0^{+\infty} e^{\beta(\gamma r - r^2)} dr} + 1_{\{d>2\}} \frac{(d-2) \int_0^{+\infty} r^{\frac{d}{2}-2} e^{\beta(\gamma r - r^2)} dr}{4\beta \int_0^{+\infty} r^{\frac{d}{2}-1} e^{\beta(\gamma r - r^2)} dr} \\ &> \frac{\gamma}{2}. \end{aligned}$$

- Letting $y \rightarrow x$ in (84), one obtains that $\forall x \in \mathbb{R}^d$, $v(x) \leq \min \text{Spec}(\nabla^2 V(x))$. When $x \mapsto \min \text{Spec}(\nabla^2 V(x))$ is concave,

$$\begin{aligned} (x-y) \cdot (\nabla V(x) - \nabla V(y)) &= \int_0^1 (x-y) \cdot \nabla^2 V(\theta x + (1-\theta)y)(x-y) d\theta \\ &\geq |x-y|^2 \int_0^1 \min \text{Spec}(\nabla^2 V(\theta x + (1-\theta)y)) d\theta \\ &\geq |x-y|^2 \int_0^1 \theta \min \text{Spec}(\nabla^2 V(x)) + (1-\theta) \min \text{Spec}(\nabla^2 V(y)) d\theta \\ &\geq \frac{1}{2} (\min \text{Spec}(\nabla^2 V(x)) + \min \text{Spec}(\nabla^2 V(y))) |x-y|^2 \end{aligned}$$

and one may choose $v(x) = \min \text{Spec}(\nabla^2 V(x))$ in (84).

- When $V = \bar{V} + \hat{V}$ with \bar{V} such that $x \mapsto \min \text{Spec}(\nabla^2 \bar{V}(x))$ is concave and \hat{V} such that $x \mapsto \nabla \hat{V}(x)$ is Lipschitz with constant δ and constant outside some Borel subset A of \mathbb{R}^d , then one may choose $v(x) = \min \text{Spec}(\nabla^2 \bar{V}(x)) - 2\delta 1_A(x)$ in (84).

Proof. 1. One has

$$\begin{aligned} d|Y_t^x - Y_t^y|^2 &= -2(Y_t^x - Y_t^y) \cdot (\nabla V(Y_t^x) - \nabla V(Y_t^y)) dt \\ &\leq -(v(Y_t^x) + v(Y_t^y)) |Y_t^x - Y_t^y|^2 dt, \end{aligned} \tag{85}$$

under (84). Hence

$$|Y_t^x - Y_t^y|^2 \leq |x-y|^2 e^{-\int_0^t (v(Y_s^x) + v(Y_s^y)) ds}.$$

Since, by (51), $\frac{1}{t} \int_0^t (v(Y_s^x) + v(Y_s^y)) ds$ converges a.s. to $2 \int_{\mathbb{R}^d} v(x) e^{-V(x)} dx > 0$, one easily deduces the first assertion.

2. When V is convex, then $t \mapsto |Y_t^x - Y_t^y|$ is nonincreasing by (85). Now, for $z \in B(x_0, \frac{\varepsilon}{2})$ and $w \in \mathbb{R}^d$, one has

$$(z-w) \cdot (\nabla V(z) - \nabla V(w)) \geq |z-w| \inf_{B(x_0, \varepsilon)} \min \text{Spec}(\nabla^2 V(\cdot)) \left(\frac{\varepsilon}{2} 1_{B(x_0, \varepsilon)^c}(w) + |z-w| 1_{B(x_0, \varepsilon)}(w) \right).$$

As a consequence,

$$(Y_t^x - Y_t^y) \cdot (\nabla V(Y_t^x) - \nabla V(Y_t^y)) \geq 1_{B(x_0, \frac{\varepsilon}{2})}(Y_t^x) \inf_{B(x_0, \varepsilon)} \min \text{Spec}(\nabla^2 V(\cdot)) \left(\frac{\varepsilon}{2|x-y|} \wedge 1 \right) |Y_t^x - Y_t^y|^2.$$

One concludes by arguments similar to the ones used for the first assertion.

3. Let V be convex and differentiable and let $x \neq y$ be such that $(x - y) \cdot (\nabla V(x) - \nabla V(y)) = 0$. Then V is affine on the segment $[x, y]$ and $V\left(\frac{x+y}{2}\right) = \frac{V(x)+V(y)}{2}$. For $z \in \mathbb{R}^d \setminus \{0\}$ and $\varepsilon \in \mathbb{R}$,

$$\begin{aligned} \frac{V(x) + V(y)}{2} = V\left(\frac{x+y}{2}\right) &\leq \frac{V(x + \varepsilon z) + V(y - \varepsilon z)}{2} \\ &= \frac{V(x) + V(y)}{2} + \frac{\varepsilon z}{2} \cdot (\nabla V(x) - \nabla V(y)) + o(\varepsilon) \end{aligned}$$

as $|\varepsilon| \rightarrow 0$. As a consequence $z \cdot (\nabla V(x) - \nabla V(y)) = 0$ and $\nabla V(x) = \nabla V(y)$.

Let $(X_t)_{t \geq 0}$ and $(Y_t)_{t \geq 0}$ be two solutions to the stochastic differential equation (2), such that (X_0, Y_0) is distributed according to some invariant probability measure of the duplicated dynamics. Since $|X_t - Y_t|^2$ is *a.s.* non-increasing with t and constant in distribution, *a.s.* $t \mapsto |X_t - Y_t|^2$ is constant and therefore *dt-a.e.* $(X_t - Y_t) \cdot (\nabla V(X_t) - \nabla V(Y_t)) = 0$ which implies $\nabla V(X_t) = \nabla V(Y_t)$. One deduces that *a.s.*, $t \mapsto X_t - Y_t$ is constant.

Now, since $x \mapsto e^{-V(x)}$ is integrable, then V cannot be affine in some direction and for any $z \in \mathbb{R}^d \setminus \{0\}$, $x \mapsto z \cdot (\nabla V(x) - \nabla V(x - z))$ is not constant equal to zero. By continuity of ∇V , one deduces the existence of $y \in \mathbb{R}^d$ and $\varepsilon > 0$ such that $\forall x \in B(y, \varepsilon)$, $z \cdot (\nabla V(x) - \nabla V(x - z)) > 0$. With the ergodicity of $(X_t)_{t \geq 0}$ and the fact that *dt-a.e.* $(X_0 - Y_0) \cdot (\nabla V(X_t) - \nabla V(X_t - X_0 + Y_0)) = 0$, one concludes that *a.s.* $X_0 = Y_0$. □

Acknowledgements

This work is supported by the European Research Council under the European Union's Seventh Framework Programme (FP/2007-2013) / ERC Grant Agreement number 614492 and by the French National Research Agency under the grant ANR-12-BS01-0019 (STAB). The authors would like to thank fruitful discussions with G. Stoltz on nonequilibrium methods and Green-Kubo formulae.

References

- [1] C. Ané, S. Blachère, D. Chafaï, P. Fougères, I. Gentil, F. Malrieu, C. Roberto, and G. Scheffer. *Sur les inégalités de Sobolev logarithmiques*. Société Mathématique de France, 2000. In French.
- [2] R. Assaraf, M. Caffarel, and A.C. Kollias. Chaotic versus nonchaotic stochastic dynamics in monte carlo simulations: A route for accurate energy differences in n -body systems. *Phys. Rev. Lett.*, 106:150601, 2011.
- [3] V. Bally, M.P. Bavouzet, and M. Messaoud. Integration by parts formula for locally smooth laws and applications to sensitivity computations. *Ann. Appl. Probab.*, 17:33–66, 2007.
- [4] S. Bobkov and M. Ledoux. Poincaré's inequalities and Talagrand's concentration phenomenon for the exponential distribution. *Probab. Theory Related Fields*, 107(3):383–400, 1997.
- [5] K. Burdzy, Z.-Q. Chen, and P. Jones. Synchronous couplings of reflected brownian motions in smooth domains. *Illinois Journal of Mathematics*, 50(1-4):189–268, 2006.
- [6] D. Chandler. *Introduction to Modern Statistical Mechanics*. Oxford University Press, 1987.

- [7] J. Chen, G. Zhang, and B. Li. How to improve the accuracy of equilibrium molecular dynamics for computation of thermal conductivity? *Physics Letters A*, 374(23):2392 – 2396, 2010.
- [8] G. Ciccotti and G. Jacucci. Direct computation of dynamical response by molecular-dynamics - mobility of a charged Lennard-Jones particle. *Physical Review Letters*, 35(12):789–792, 1975.
- [9] G. Ciccotti, R. Kapral, and A. Sergi. Non-equilibrium molecular dynamics. In S. Yip, editor, *Handbook of Materials Modeling*, pages 745–761. Springer Netherlands, 2005.
- [10] M. Cwikel. Weak type estimates for singular values and the number of bound states of Schrödinger operators. *Ann. of Math. (2)*, 106(1):93–100, 1977.
- [11] F. den Hollander. *Large deviations*, volume 14 of *Fields Institute Monographs*. American Mathematical Society, Providence, RI, 2000.
- [12] M. Dufflo. *Random iterative models*. Springer, 1997.
- [13] K.D. Elworthy and X.M. Li. Formulae for the derivatives of heat semigroups. *J. Func. Anal.*, 125:252–286, 1994.
- [14] D.J. Evans and G. Morriss. *Statistical mechanics of nonequilibrium liquids*. Cambridge University Press, 2008.
- [15] J. Fontbona and B. Jourdain. On the long time behaviour of stochastic vortices systems. *Markov Process. Related Fields*, 20(4):675–704, 2014.
- [16] Ī.Ī. Gihman and A.V. Skorohod. *Stochastic differential equations*. Springer-Verlag, New York-Heidelberg, 1972. Translated from the Russian by Kenneth Wickwire, *Ergebnisse der Mathematik und ihrer Grenzgebiete, Band 72*.
- [17] D. Gilbarg and N.S. Trudinger. *Elliptic partial differential equations of second order*. Classics in Mathematics. Springer-Verlag, Berlin, 2001.
- [18] M. Hairer and A.J. Majda. A simple framework to justify linear response theory. *Nonlinearity*, 23(4):909–922, 2010.
- [19] Bismut J.M. *Large deviations and the Malliavin calculus*. Birkhäuser, 1984.
- [20] M. H. Kalos and F. Pederiva. Exact monte carlo method for continuum fermion systems. *Physical review letters*, 85(17):3547, 2000.
- [21] I. Karatzas and S.E. Shreve. *Brownian motion and stochastic calculus*. Springer-Verlag, 1988.
- [22] N. V. Krylov. *Lectures on elliptic and parabolic equations in Hölder spaces*, volume 12 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 1996.
- [23] V. Lemaire, G. Pagès, and F. Panloup. Invariant measure of duplicated diffusions and application to Richardson-Romberg extrapolation, 2013. <http://arxiv.org/abs/1302.1651>.
- [24] E. Lieb. Bounds on the eigenvalues of the Laplace and Schroedinger operators. *Bull. Amer. Math. Soc.*, 82(5):751–753, 1976.
- [25] P. Malliavin. *Integration and probability*, volume 157 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, 1995.
- [26] A. Quarteroni and A. Valli. *Numerical Approximation of Partial Differential Equations*. Springer, 1997.
- [27] L. Rey-Bellet. Ergodic properties of Markov processes. In *Open quantum systems. II*, volume 1881 of *Lecture Notes in Math.*, pages 1–39. Springer, Berlin, 2006.
- [28] G. V. Rozenbljum. Distribution of the discrete spectrum of singular differential operators. *Dokl. Akad. Nauk SSSR*, 202:1012–1015, 1972.

- [29] T.H. Rydberg. A note on the existence of unique equivalent martingale measures in a markovian setting. *Finance and Stochastics*, 1(3):251–257, 1997.
- [30] J. Tailleur and J. Kurchan. Probing rare physical trajectories with Lyapunov weighted dynamics. *Nature Physics*, 3:203–207, 2007.
- [31] R. Temam. *Navier-Stokes equations*, volume 2 of *Studies in Mathematics and its Applications*. North-Holland Publishing Co., Amsterdam-New York, 1979.
- [32] C. Villani. Hypocoercivity. *Memoirs Amer. Math. Soc.*, 202, 2009.
- [33] W. von Wahl. The equation $u' + A(t)u = f$ in a Hilbert space and L^p -estimates for parabolic equations. *J. London Math. Soc. (2)*, 25(3):483–497, 1982.
- [34] P.B. Warren and R.J. Allen. Malliavin weight sampling for computing sensitivity coefficients in brownian dynamics simulations. *Physical Review Letters*, 109(25):250601, 2012.