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Long-time convergence of an Adaptive Biasing Force method

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Abstract

We propose a proof of convergence of an adaptive method used in molecular dynamics to compute free energy profiles (see [7, 9, 13]). Mathematically, it amounts to studying the long-time behavior of a stochastic process which satisfies a non-linear stochastic differential equation, where the drift depends on conditional expectations of some functionals of the process. We use entropy techniques to prove exponential convergence to the stationary state.

1 Introduction

In Section 1.1, we introduce the physical context of this work, namely molecular dynamics and the computation of free energy differences in the canonical statistical ensemble. In Section 1.2, we introduce the adaptive dynamics we study and the main results we prove are presented in Section 1.3.

1.1 Computations of free energy differences and metastability

Let us consider the Gibbs-Boltzmann measure

$$d\mu(q) = Z^{-1} \exp(-\beta V(q)) dq, \tag{1}$$

where $q \in \mathcal{D}$, $V : \mathcal{D} \to \mathbb{R}$, $Z = \int_{\mathcal{D}} \exp(-\beta V(q))\, dq$ and $\mathcal{D} = \{q,\, V(q) < \infty\}$ is the configuration space. In the applications we consider, q represents the position of N particles so that, in the following, $\mathcal{D}$ is an open subset (possibly the whole) of $\mathbb{R}^n$, with $n = 3N$. All the results we prove are also satisfied if $\mathcal{D}$ is an open subset of $\mathbb{T}^n$ (where $\mathbb{T} = \mathbb{R}/\mathbb{Z}$ denotes the one-dimensional torus). The function V is the energy associated with the positions of the particles and β is proportional to the inverse of the temperature. The probability measure μ represents the equilibrium measure sampled by the particles in the canonical statistical ensemble. A typical dynamics that can be used to sample this measure is

$$dQ_t = -\nabla V(Q_t)\, dt + \sqrt{2\beta^{-1}} dB_t, \tag{2}$$

where B_t is a n-dimensional standard Brownian motion. More generally, for any smooth positive function $\gamma : \mathcal{D} \to \mathbb{R}_+^*$, the stochastic process Q_t which satisfies

$$dQ_t = -\nabla(V - \beta^{-1} \ln \gamma)(Q_t)\gamma(Q_t)\, dt + \sqrt{2\beta^{-1}\gamma(Q_t)} dB_t \tag{3}$$

samples the measure μ.

Let us introduce a so-called *reaction coordinate* $\xi : \mathcal{D} \to \mathcal{M}$, with $\mathcal{M} = \mathbb{R}$ or $\mathcal{M} = \mathbb{T}$. For a given configuration q, $\xi(q)$ represents a coarse-grained information, which is valuable from a physical point of view. For instance, $\xi(q)$ may be a dihedral angle, for example to characterize the conformation of a molecule, in which case $\mathcal{M} = \mathbb{T}$, or the signed distance to an hypersurface of $\mathcal{D}$ (characterizing a transition state), for example to measure the evolution of a chemical reaction, in which case $\mathcal{M} = \mathbb{R}$. The function ξ is therefore related to some macroscopic information of the system. Usually, in (2), the time-scale for the dynamics on $\xi(Q_t)$ is larger than the time-scale for the dynamics on Q_t (due to metastable states), so that ξ can also be understood as a function such that $\xi(Q_t)$ is a slow variable compared to Q_t.

In the following, we suppose that

[H1] ξ is a smooth function such that $|\nabla\xi| > 0$ on $\mathcal{D}$.

Thus, the subsets $\Sigma_z = \{x \in \mathcal{D}, \, \xi(x) = z\}$ of $\mathcal{D}$ are smooth submanifolds of co-dimension one which define a partition of $\mathcal{D}$:

$$\mathcal{D} = \bigcup_{z \in \mathcal{M}} \Sigma_z \text{ and } \Sigma_z \cap \Sigma_{z'} = \emptyset \text{ for } z \neq z'.$$

We denote by σ_{Σ_z} the surface measure on Σ_z, *i.e.* the Lebesgue measure on Σ_z induced by the Lebesgue measure in the ambient space $\mathcal{D} \supset \Sigma_z$. The submanifold Σ_z naturally has a (complete and locally compact) Riemannian structure induced by the Euclidean structure of the ambient space $\mathcal{D}$.

The image of the measure μ by ξ is $\frac{\exp(-\beta A(z))\, dz}{\int_{\mathcal{M}} \exp(-\beta A(z))\, dz}$ where A is the so-called *free energy* defined by:

$$A(z) = -\beta^{-1} \ln(Z_{\Sigma_z}) \tag{4}$$

where

$$Z_{\Sigma_z} = \int_{\Sigma_z} |\nabla\xi|^{-1} \exp(-\beta V) d\sigma_{\Sigma_z}.$$

We assume henceforth that ξ and V are such that $Z_{\Sigma_z} < \infty$. The free energy is actually defined up to an additive constant, the quantity $\exp(-\beta A)$ being then defined up to a multiplicative constant, which disappears in the normalization of the probability measure $\frac{\exp(-\beta A(z))\, dz}{\int_{\mathcal{M}} \exp(-\beta A(z))\, dz}$. Many algorithms in molecular dynamics [5] aim to compute the image of the measure μ by ξ, which amounts to compute free energy differences, namely quantities of the form $A(z) - A(z_0)$. This is typically obtained by computing (and then integrating) the derivative $A'(z)$, called the *mean force*. Using the co-area formula (see Appendix A), the following expression for $A'(z)$ can be obtained (see [6], or the proof of Lemma 7 below):

$$\boxed{A'(z) = Z_{\Sigma_z}^{-1} \int_{\Sigma_z} F \, |\nabla\xi|^{-1} \exp(-\beta V) d\sigma_{\Sigma_z},} \tag{5}$$

where F is the so-called *local mean force* defined by

$$\boxed{F = \left(\frac{\nabla V \cdot \nabla\xi}{|\nabla\xi|^2} - \beta^{-1} \mathrm{div} \left(\frac{\nabla\xi}{|\nabla\xi|^2} \right) \right).} \tag{6}$$

This can be rewritten in terms of conditional expectation as: For a random variable X with law μ,

$$A'(z) = \mathbb{E}\left(F(X) \middle| \xi(X) = z \right). \tag{7}$$

In practice, free energy profiles are used for example to compare the likelihood of various conformations of a molecule, or to compute the rate of a chemical reaction. Free energy can also be useful to compute ensemble averages in the canonical ensemble using the following formula (which is a conditioning formula): For any function $\phi : \mathcal{D} \to \mathbb{R}$,

$$\int_{\mathcal{D}} \phi \, d\mu = \frac{\displaystyle\int_{\mathcal{M}} \int_{\Sigma_z} \phi \, d\mu_{\Sigma_z} \exp(-\beta A(z))\, dz}{\displaystyle\int_{\mathcal{M}} \exp(-\beta A(z))\, dz}, \tag{8}$$

where μ_{Σ_z} is the probability measure μ conditioned to a fixed value z of the reaction coordinate:

$$d\mu_{\Sigma_z} = Z_{\Sigma_z}^{-1} |\nabla \xi|^{-1} \exp(-\beta V) d\sigma_{\Sigma_z}. \tag{9}$$

Notice that (5) also writes $A'(z) = \int_{\Sigma_z} F \, d\mu_{\Sigma_z}$. Equation (8) may be interesting to compute averages in the canonical ensemble since, if the reaction coordinate is well chosen, it is expected that the sampling of the conditioned probability measure μ_{Σ_z} is easier than the sampling of μ (the metastable features of the measure μ being mostly in the direction of the reaction coordinate ξ). The sampling of μ_{Σ_z} can be done for example by projection of the gradient dynamics on Σ_z (see [6]). The quantity $\int_{\Sigma_z} \phi \, d\mu_{\Sigma_z}$ can thus be evaluated by an efficient Monte Carlo procedure, and the computation of $\int_{\mathcal{D}} \phi \, d\mu$ through (8) then only requires a one-dimensional integration, and the computation of the free energy (up to an additive constant).

Due to the high dimensionality of the problem (the number of particles N is usually very large), methods to compute mean forces or free energy differences are Monte Carlo methods. They typically rely on the simulation of a diffusion Markov process. The most recent methods use non-homogeneous or non-linear Markov processes. Classical examples are exponential reweighting of non-equilibrium paths (based upon the so-called Jarzynski equality, see [11, 12]) or adaptive methods (see [7, 9, 10, 18]).

We are interested here in adaptive methods to compute free energy differences, and more precisely Adaptive Biasing Force techniques (see [7, 9]). The principle of adaptive methods is to modify the potential V during the simulation, in order to remove the metastable features of the simple dynamics (2), while approximating the free energy A. Many methods have been proposed and we refer to [13] for a unified presentation of these techniques, as well as a discussion of efficient parallel implementations. The aim of this paper is to propose a mathematical study of the Adaptive Biasing Force method to give a rigorous formulation and proofs of the following statements (which are the main arguments of practitioners of the field to advocate the use of adaptive methods):

[S1] The adaptive biasing force technique helps to remove the metastable features of the simple dynamics (2), and thus enables efficient exploration of the configuration space.

[S2] With the adaptive biasing force technique, the free energy A is obtained in the longtime limit, and the convergence is exponentially fast in time.

1.2 An Adaptive Biasing Force technique

The Adaptive Biasing Force (ABF) method was introduced in [7, 9] and is recast in a general mathematical framework in [13]. We propose to study here one version of this method, applied to the context of Brownian (or overdamped Langevin) dynamics[1].

The ABF dynamics we propose to study is the following non-linear stochastic differential equation:

$$\boxed{\begin{aligned} dX_t = & -\nabla\Big(V - A_t \circ \xi + W \circ \xi - \beta^{-1} \ln(|\nabla \xi|^{-2})\Big)(X_t)\, |\nabla \xi|^{-2}(X_t)\, dt \\ & + \sqrt{2\beta^{-1}} |\nabla \xi|^{-1}(X_t) dB_t, \end{aligned}} \tag{10}$$

where W is an additional well-chosen potential that we will define below and A_t is the "free energy observed at time t". More precisely, the derivative of A_t with respect to the reaction coordinate is defined as (compare with (7)): $\forall z \in \mathcal{M}$,

$$\boxed{A'_t(z) = \mathbb{E}\left(F(X_t) \,\Big|\, \xi(X_t) = z \right),} \tag{11}$$

---

[1] Such methods can also be applied for other dynamics, like Langevin dynamics. We only consider Brownian dynamics in this paper.

where F is defined by (6). With a slight abuse of terminology, the function A_t' is called the *biasing force*. Notice that here and in the following, the notation $'$ denotes a derivative with respect to the reaction coordinate values, while the notation $\circ$ denotes the composition operator. Equation (11) defines A_t up to an additive (time-dependent) constant, which does not modify (10).

Compared to the simple dynamics (2), three modifications have been made to obtain (10)–(11):

1. First and foremost, the potential V has been changed to the biasing potential $V - A_t \circ \xi$. This is the bottom line of the adaptive strategy. The algorithm we study here is prototypical of many adaptive methods used in molecular dynamics (see [13]). In the original Adaptive Biasing Force technique as presented in [7, 9], the conditional expectation (11) is actually "approximated" by some conditional averages over one single trajectory. The dynamics we study here is not clearly related with such a discretization, but rather with a discretization of (11) using an interacting particle system, where many replicas of the system contribute to the free energy profile (see [13]).
2. Second, a potential $W \circ \xi$ has been added. This is actually needed only in the case when $\mathcal{M}$ is an unbounded domain (we recall that $\mathcal{M}$ is the domain where the reaction coordinate lives). In theses cases, W is chosen so that the law of $\xi(X_t)$ converges exponentially fast to its longtime limit (more precisely, the Fisher information associated with this law converges exponentially fast to zero, see [H4] below for a more detailed statement). Besides, from a numerical point of view, such a potential is sometimes used in practice in order to separately sample some parts of the reaction coordinate space $\mathcal{M}$ (as in stratified sampling strategies).
3. Third, some terms depending on $|\nabla\xi|$ have been introduced. This modification is made in order to obtain a simple diffusive behavior for the law of $\xi(X_t)$ (see Proposition 1 below). It is expected that the longtime convergence of A_t' towards A' still holds without this modification, by simply considering the gradient dynamics
$$dX_t = -\nabla(V - A_t \circ \xi + W \circ \xi)(X_t)\, dt + \sqrt{2\beta^{-1}} dB_t, \tag{12}$$
with the same definition (11) for A_t'. However, we are only able to prove a weaker convergence result in this case. This is the matter of Sections 2.3 and 3.4. Notice that if $|\nabla\xi|$ is constant (for example if ξ is a length), a simple change of time relates (12) with (10). Notice also that if we take $A_t = W = 0$ in (10), then X_t samples the original Gibbs measure μ defined by (1) (see Equation (3) above).

Remark 1 (On the computation of $A_t'(z)$) *From a practical point of view, with the additional terms mentioned in item 3 above, it is possible to compute the biasing force $A_t'(z)$ without explicitly evaluating F since (by Itô's calculus on X_t that satisfies (10), and assuming $W = 0$ for simplicity)*

$$F(X_t)\, dt = d\xi(X_t) + A_t'(\xi(X_t))\, dt - \sqrt{2\beta^{-1}} \frac{\nabla\xi}{|\nabla\xi|}(X_t) \cdot dB_t. \tag{13}$$

By a simple finite difference scheme, we thus have the following approximation

$$F(X_{t_{n+1}}) \simeq A_{t_n}'(\xi(X_{t_n})) + \frac{\xi(X_{t_{n+1}}) - \xi(X_{t_n}) - \sqrt{2\beta^{-1}} \frac{\nabla\xi}{|\nabla\xi|}(X_{t_n}) \cdot (B_{t_{n+1}} - B_{t_n})}{\Delta t}.$$

1.3 A PDE formulation and presentation of the main result

We would like to emphasize that our arguments are partially *formal*: we assume that we are given a process X_t and a function A_t' which satisfy (10)–(11), and such that X_t has a smooth density $\psi(t, \cdot)$ with respect to the Lebesgue measure on $\mathcal{D}$. We suppose that this density is sufficiently regular so that the computations are valid. In particular, we assume that the potential V is such that either the stochastic process

X_t lives in $\mathcal{D}$ and thus that its density $\psi(t,\cdot)$ decays sufficiently fast on $\partial\mathcal{D}$ or the stochastic process X_t has some reflecting behavior on $\partial\mathcal{D}$ and thus that its density $\psi(t,\cdot)$ has zero normal derivatives on $\partial\mathcal{D}$. In both cases, no boundary terms appear in the integrations by parts we perform to derive the entropy estimates. We refer for example to [3] for an appropriate functional framework in which such entropy estimates hold.

Since only the law of the process X_t at a fixed time t is used in (11), it is possible to recast the dynamics in the following nonlinear partial differential equation (PDE) on the density $\psi(t,\cdot)$ of X_t:

$$\boxed{\left\{\begin{aligned} &\partial_t\psi = \operatorname{div}\left(|\nabla\xi|^{-2}\left(\nabla(V - A_t\circ\xi + W\circ\xi)\psi + \beta^{-1}\nabla\psi\right)\right),\\ &A_t'(z) = \frac{\displaystyle\int_{\Sigma_z} F|\nabla\xi|^{-1}\psi(t,\cdot)d\sigma_{\Sigma_z}}{\displaystyle\int_{\Sigma_z}|\nabla\xi|^{-1}\psi(t,\cdot)d\sigma_{\Sigma_z}}, \end{aligned}\right.} \tag{14}$$

where F is defined by (6). This is obtained by using the fact that if X_t has law $\psi(t,x)\,dx$, then the law of $\xi(X_t)$ is $\psi^\xi(t,z)\,dz$ with

$$\psi^\xi(t,z) = \int_{\Sigma_z}|\nabla\xi|^{-1}\psi(t,\cdot)d\sigma_{\Sigma_z}, \tag{15}$$

and the conditional law of X_t with respect to $\xi(X_t)=z$ is $\mu_{t,z}$ defined by

$$d\mu_{t,z} = \frac{\psi(t,\cdot)|\nabla\xi|^{-1}d\sigma_{\Sigma_z}}{\psi^\xi(t,z)}. \tag{16}$$

The probability measure $\psi^\xi(t,z)\,dz$ is the image of the probability measure $\psi(t,x)\,dx$ by ξ. These expressions can be obtained using the co-area formula (see Appendix A).

Before presenting the results, we would like to motivate the introduction of this dynamics by the following formal observation. If the potential A_t and the law of X_t reach a stationary state, then, from the dynamics (10) on X_t (or from the partial differential equation (14) satisfied by the distribution of X_t), we observe that this stationary law is proportional to $\exp(-\beta(V(x) - A_\infty\circ\xi(x) + W\circ\xi(x)))\,dx$, where A_∞ denotes the stationary state for A_t (this requires a uniqueness result for the law of X_t, which holds for example if $|\nabla\xi|$ is uniformly bounded from below by a positive constant). Then, from the definition (11) of the biasing force, we obtain that, necessarily, $A'_\infty = A'$ (where A' is the mean force defined by (5)). This proves the uniqueness of the stationary state for this dynamics. We can thus expect that A'_t converges to the mean force A' in the longtime limit.

The interest of the dynamics (10)–(11) is actually twofold. First, as expected from the formal argument above, in the longtime limit, A'_t converges to the mean force A' defined by (5) (see Equation (24) below). Second, using the ABF method, the law of $\xi(X_t)$ has a simple diffusive behavior (see Equation (20) below). The metastable feature of the simple dynamics (2) along ξ is thus corrected by the addition of the adaptive potential A_t. The aim of this paper is to give a precise statement for these two assertions, which are mathematical formalizations of the two main characteristics [S1] and [S2] of adaptive techniques mentioned in Section 1.1. The proof of the longtime convergence relies on entropy techniques, and requires appropriate assumptions on the potentials V, W and the reaction coordinate ξ. We prove that under suitable assumptions, the convergence of A'_t to A' is exponentially fast, with a rate of convergence limited, at the macroscopic level, by the rate of convergence of the law of $\xi(X_t)$ to its longtime limit, and, at the microscopic level, by the rate of convergence to the equilibrium conditioned probability measures μ_{Σ_z}, for all values z of the reaction coordinate.

All these results are more precisely stated in Section 2, and the proofs are given in Section 3. We would like to mention that the main arguments of the proof are given in a very simple case in Section 3.1 and that we also present a result of convergence for the dynamics (12)–(11) in Section 2.3.

2 Precise statements of the results

In Section 2.1, we recall some well-known results on entropy and introduce the main notation used in the following to state the convergence result. Section 2.2 is devoted to the presentation of the convergence result for the dynamics (10)–(11). Finally, we give in Section 2.3 a (weaker) convergence result for the dynamics (12)–(11).

2.1 Entropy and Fisher information

Let us consider ψ and A'_t which satisfy (14) and let introduce the long-time limit of ψ, ψ^ξ (defined by (15)) and $\mu_{t,z}$ (defined by (16)):

$$\psi_\infty = (ZZ^\xi)^{-1}\exp(-\beta(V - A\circ\xi + W\circ\xi)),$$

$$\psi^\xi_\infty(z) = (Z^\xi)^{-1}\exp(-\beta W(z)),$$

$$d\mu_{\infty,z} = d\mu_{\Sigma_z} = Z_{\Sigma_z}^{-1}\exp(-\beta V)|\nabla\xi|^{-1}d\sigma_{\Sigma_z},$$

where

$$Z^\xi = \int_{\mathcal{M}} \exp(-\beta W(z))\,dz.$$

We recall that

$$Z_{\Sigma_z} = \int_{\Sigma_z} |\nabla\xi|^{-1}\exp(-\beta V)d\sigma_{\Sigma_z},\ Z = \int_{\mathcal{D}} \exp(-\beta V(x))\,dx.$$

Notice that $\int_{\mathcal{D}}\psi_\infty = 1$, and that the probability measure $\psi^\xi_\infty(z)\,dz$ is the image of the probability measure $\psi_\infty(x)\,dx$ by ξ.

In order to state the results, we also need to introduce the following projection operators. For any $x\in\mathcal{D}$, we denote by

$$P(x) = \mathrm{Id} - \frac{\nabla\xi\otimes\nabla\xi}{|\nabla\xi|^2}(x)$$

the orthogonal projection operator onto the tangent space $T_x\Sigma_{\xi(x)}$ to $\Sigma_{\xi(x)}$ at point x, and by

$$Q(x) = \frac{\nabla\xi\otimes\nabla\xi}{|\nabla\xi|^2}(x)$$

the orthogonal projection operator onto the normal space $N_x\Sigma_{\xi(x)}$ to $\Sigma_{\xi(x)}$ at point x. We denote by $\otimes$ the tensor product: For two vectors $u, v\in\mathcal{D}$, $u\otimes v$ is a $n\times n$ matrix with components $(u\otimes v)_{i,j} = u_i v_j$.

We measure the "distance" between ψ (respectively ψ^ξ) and ψ_∞ (respectively ψ^ξ_∞) using the relative entropy $H(\psi|\psi_\infty)$ (respectively $H(\psi^\xi|\psi^\xi_\infty)$), where, for any two probability measures μ and ν such that μ is absolutely continuous with respect to ν (this property being denoted $\mu \ll \nu$ in the following),

$$H(\mu|\nu) = \int \ln\left(\frac{d\mu}{d\nu}\right)d\mu.$$

We recall the Csiszar-Kullback inequality:

$$\|\mu-\nu\|_{TV} \le \sqrt{2H(\mu|\nu)} \tag{17}$$

where $\|\mu-\nu\|_{TV} = \sup_{f,\,\|f\|_{L^\infty}\le 1}\{\int f d(\mu-\nu)\}$ denotes the total variation norm of the signed measure $\mu-\nu$. When μ and ν both have densities with respect to the Lebesgue measure, $\|\mu-\nu\|_{TV}$ is simply the L^1 norm of the difference between the two densities.

We denote the *total entropy* by

$$E(t) = H(\psi(t,\cdot)|\psi_\infty),$$

the *macroscopic entropy* by

$$E_M(t) = H(\psi^\xi(t,\cdot)|\psi^\xi_\infty),$$

the "local entropy" at a fixed value z of the reaction coordinate by

$$e_m(t,z) = H(\mu_{t,z}|\mu_{\infty,z}) = \int_{\Sigma_z} \ln\left(\frac{\psi(t,\cdot)}{\psi^\xi(t,z)} \Big/ \frac{\psi_\infty}{\psi^\xi_\infty(z)}\right) \frac{\psi(t,\cdot)|\nabla\xi|^{-1} d\sigma_{\Sigma_z}}{\psi^\xi(t,z)},$$

and the *microscopic entropy* by

$$E_m(t) = \int_{\mathcal{M}} e_m(t,z)\psi^\xi(t,z)\,dz.$$

It is straightforward to obtain the following result which can be seen as the extensivity of the entropy:

Lemma 1 *It holds*

$$E(t) = E_M(t) + E_m(t).$$

Let us now introduce the Fisher information: For any two probability measures μ and ν such that $\mu \ll \nu$,

$$I(\mu|\nu) = \int \left|\nabla \ln\left(\frac{d\mu}{d\nu}\right)\right|^2 d\mu. \tag{18}$$

In the case ν is a probability measure on the (Riemannian) submanifold Σ_z, ∇ actually denotes the gradient on Σ_z in (18), namely

$$\nabla_{\Sigma_z} = P\nabla. \tag{19}$$

Therefore, for the conditional probability measures $\mu_{t,z}$ and $\mu_{\infty,z}$, the Fisher information writes

$$I(\mu_{t,z}|\mu_{\infty,z}) = \int_{\Sigma_z} \left|\nabla_{\Sigma_z} \ln\left(\frac{\psi(t,\cdot)}{\psi_\infty}\right)\right|^2 \frac{\psi(t,\cdot)|\nabla\xi|^{-1} d\sigma_{\Sigma_z}}{\psi^\xi(t,z)}.$$

Let us finally introduce another way to compare two probability measures, namely the Wasserstein distance with quadratic cost: for two probability measures μ and ν defined on a Riemannian manifold Σ,

$$W(\mu,\nu) = \sqrt{\inf_{\pi \in \Pi(\mu,\nu)} \int_{\Sigma\times\Sigma} d_\Sigma(x,y)^2\, d\pi(x,y)}.$$

In this expression, d_Σ denotes the geodesic distance on Σ: $\forall x,y \in \Sigma$,

$$d_\Sigma(x,y) = \inf\left\{ \sqrt{\int_0^1 |\dot{w}(t)|^2\,dt} \,\middle|\, w \in \mathcal{C}^1([0,1],\Sigma),\, w(0)=x,\, w(1)=y \right\},$$

where $\Pi(\mu,\nu)$ denotes the set of coupling probability measures, namely probability measures on $\Sigma \times \Sigma$ such that their marginals are μ and ν. We need the following definitions:

Definition 1 *The probability measure ν is said to satisfy a logarithmic Sobolev inequality with constant $\rho > 0$ (in short: LSI(ρ)) if for all probability measures μ such that $\mu \ll \nu$,*

$$H(\mu|\nu) \le \frac{1}{2\rho} I(\mu|\nu).$$

Definition 2 *The probability measure ν is said to satisfy a Talagrand inequality with constant $\rho > 0$ (in short: T(ρ)) if for all probability measures μ such that $\mu \ll \nu$,*

$$W(\mu, \nu) \leq \sqrt{\frac{2}{\rho} H(\mu|\nu)}.$$

In the latter definition, we implicitly assume that the probability measures have finite moments of order 2. This will always be the case for all the probability measures we consider. We will need the following important result (see [15, Theorem 1]).

Lemma 2 *If ν satisfies LSI(ρ), then ν satisfies T(ρ).*

For an introduction to logarithmic Sobolev inequalities, their properties and their relation to longtime behavior of solutions to PDEs, we refer to [2, 3, 16].

2.2 Convergence of the adaptive dynamics (10)–(11)

We are now in position to state our main results. Concerning the dynamics on the law of $\xi(X_t)$, we have:

Proposition 1 (Equation satisfied by the marginal density ψ^ξ) *Let (ψ, A'_t) be a smooth solution to (14) and let us assume [H1]. Then ψ^ξ satisfies the following equation:*

$$\partial_t \psi^\xi = \partial_z \left(W' \psi^\xi + \beta^{-1} \partial_z \psi^\xi \right) \text{ on } \mathcal{M}. \tag{20}$$

Remark 2 *Notice that even if ψ^ξ satisfies a closed PDE, $\xi(X_t)$ does not satisfy a closed SDE (see Equation (13) above).*

The fundamental assumptions we need to prove longtime convergence are the following (we recall that the local mean force F is defined by (6)):

$$\textbf{[H2]} \quad \left\{ \begin{array}{c} V \text{ and } \xi \text{ are sufficiently differentiable functions such that} \\ \|\nabla \xi\|_{L^\infty} \leq m < \infty \text{ and } \|\nabla_{\Sigma_z} F\|_{L^\infty} \leq M < \infty, \end{array} \right.$$

$$\textbf{[H3]} \quad \left\{ \begin{array}{l} V \text{ and } \xi \text{ are such that } \exists \rho > 0, \text{ for all } z \in \mathcal{M}, \\ \text{the conditional measure } \mu_{\infty,z} \text{ satisfies LSI}(\rho). \end{array} \right.$$

In Assumption [H2], the requirement on F can be seen as a boundedness condition on the coupling between the conditional measures $\mu_{\infty,z}$ and the corresponding marginal ψ^ξ_∞, since it involves the mixed derivatives (along the tangential space and the normal space of the submanifold Σ_z) $P\nabla(Q\nabla V)$ (see [14] and Remark 11 below).

Assumption [H3] ensures that if, for a fixed value z of the reaction coordinate, the conditioned probability measure $\mu_{\infty,z}$ were to be sampled by a simple constrained gradient dynamics (see [6]), the convergence to equilibrium would be exponential with rate ρ. We refer to ρ as the *microscopic rate of convergence* in the sequel.

We refer to Section 3.1 for an explicit framework where [H2] and [H3] are satisfied, and to Remark 3 below for alternative assumptions on V and ξ.

Let us now introduce the assumption we need on W.

$$\textbf{[H4]} \quad W \text{ is such that } \exists I_0 > 0, r > 0, \forall t \geq 0,\ I(\psi^\xi(t, \cdot)|\psi^\xi_\infty) \leq I_0 \exp(-2\beta^{-1} r\, t).$$

Assumption [H4] is indeed an assumption on W because ψ^ξ satisfies the PDE (20) where only W appears. Assumption [H4] ensures that the law of $\xi(X_t)$ converges to equilibrium exponentially fast with rate r, which we refer to as the *macroscopic rate of convergence* in the sequel.

We will see below (see [H4']) some sufficient explicit conditions on W for [H4] to be satisfied.

Theorem 1 (Exponential convergence of the entropy to zero) *Let us assume [H1], [H2], [H3] and [H4]. Then the microscopic entropy E_m satisfies:*

$$\sqrt{E_m(t)} \le C \exp(-\lambda t) \tag{21}$$

where $C = 2 \max\left(\sqrt{E_m(0)}, \frac{M}{\beta^{-1}|\rho m^{-2} - r|}\sqrt{\frac{I_0}{2\rho}}\right)$ *and*

$$\lambda = \beta^{-1} \min(\rho m^{-2}, r). \tag{22}$$

In the special case $\rho m^{-2} = r$, E_m *satisfies* $\sqrt{E_m(t)} \le \left(\sqrt{E_m(0)} + M\sqrt{\frac{I_0}{2\rho}}\, t\right)\exp(-\beta^{-1} r\, t)$.

This implies that the total entropy E and thus $\|\psi(t,\cdot) - \psi_\infty\|_{L^1(\mathcal{D})}$ both converge exponentially fast to zero with rate λ.

We thus obtain that the biasing force A'_t converges to the mean force A' in the following sense: $\forall t \ge 0$,

$$\int_{\mathcal{M}} |A'_t - A'|^2(z)\psi^\xi(t,z)\,dz \le \frac{2M^2}{\rho} E_m(t). \tag{23}$$

Notice that the fact that E and $\|\psi(t,\cdot) - \psi_\infty\|_{L^1(\mathcal{D})}$ converge exponentially fast to zero with rate λ is an immediate consequence of (21), [H4], Lemma 1 and the Csiszar-Kullback inequality (17).

We will actually consider the two following cases for which [H4] is satisfied:

$$\textbf{[H4']} \quad \left\{ \begin{array}{ll} \text{If } \mathcal{M} = \mathbb{T}, & \text{then } W = 0. \\ \text{If } \mathcal{M} = \mathbb{R}, & \text{then } W \text{ is a potential such that } W'' \text{ is bounded from below} \\ & \text{and there exists } \overline{r} > 0 \text{ such that } \frac{\exp(-\beta W)}{\int_{\mathcal{M}} \exp(-\beta W)} \text{ satisfies LSI}(\overline{r}). \end{array} \right.$$

Notice that in the case $\mathcal{M} = \mathbb{R}$, the assumptions stated in [H4'] on W are satisfied for an α-convex potential (namely if $W'' \ge \alpha$ for a positive α), and then it is possible to choose $r = \alpha$ in [H4] (see Lemma 13 below). We refer to Remark 4 below for alternative assumptions on W.

Corollary 1 (Convergence of the biasing force) *If [H4'] is satisfied and ψ^ξ satisfies (20) then [H4] holds.*

More precisely, if $\mathcal{M} = \mathbb{T}$ and $W = 0$, then [H4] is satisfied with $I_0 = I(\psi^\xi(0,\cdot)|\psi^\xi_\infty)$ and $r = 4\pi^2$. If $\mathcal{M} = \mathbb{R}$, W'' is bounded from below and $\frac{\exp(-\beta W)}{\int_{\mathcal{M}} \exp(-\beta W)}$ satisfies LSI($\overline{r}$), then [H4] is satisfied with $r = \overline{r} - \varepsilon$ for any $\varepsilon \in (0, \overline{r})$.

Let us now assume [H1], [H2], [H3] and [H4']. From (23), we deduce that for all compact $K \subset \mathcal{M}$, $\exists \overline{C}, t^* > 0$, $\forall t \ge t^*$,

$$\int_K |A'_t - A'|(z)\psi^\xi_\infty(z)\,dz \le \overline{C}\exp(-\lambda t), \tag{24}$$

where λ is the rate of convergence defined by (22) in Theorem 1.

These results therefore show that A'_t converges exponentially fast to A' (in $L^1(\psi^\xi_\infty(z)\,dz)$-norm) at a rate $\lambda = \beta^{-1}\min(\rho m^{-2}, r)$. The limitations on the rate λ are related to the rate of convergence r at the macroscopic level, for the equation (20) satisfied by ψ^ξ, and the rate of convergence at the microscopic level, which depends on the constant ρ of the logarithmic Sobolev inequalities satisfied by the conditional measures $\mu_{\infty,z}$. This constant of course depends on the choice of the reaction coordinate. In our framework, we could state that a "good reaction coordinate" is such that ρ is as large as possible.

The proof of these results is given in Sections 3.1, 3.2 and 3.3 below.

Remark 3 (Other possible assumptions on V and ξ) *We would like to mention other possible assumptions on V and ξ than [H2]–[H3] for which the results of Theorem 1 still hold.*

- *First, in [H2], it is possible to change the assumption* $\|\nabla_{\Sigma_z} F\|_{L^\infty} \leq M < \infty$ *to*

$$\|F\|_{L^\infty} \leq M < \infty.$$

Indeed, this simply changes the estimate (35) in Lemma 10 below to the following

$$\begin{aligned} |A'_t(z) - A'(z)| &\leq \|F\|_{L^\infty} \|\mu_{t,z} - \mu_{\infty,z}\|_{TV}, \\ &\leq M\sqrt{2H(\mu_{t,z}|\mu_{\infty,z})}, \end{aligned}$$

by the Csiszar-Kullback inequality (17). The rest of the proof remains exactly the same.

- *Second, it is possible to obtain a similar result of convergence under slightly different assumptions than [H2]–[H3] by introducing another Riemannian structure on the submanifolds* Σ_z*. This is made precise in Appendix B (see assumptions [H2']–[H3']).*

Remark 4 (Other possible assumptions on W) *From Lemma 12 and 13 below (used to prove Corollary 1), it will become clear that [H4] is actually satisfied with* $W = 0$ *as soon as* $\mathcal{M}$ *is a bounded domain. If* $\mathcal{M}$ *is an unbounded domain, then a potential* W *with properties such as those stated in [H4'] is needed. We discuss in this remark other properties on* W *to satisfy [H4] than those proposed in [H4'], in the case* $\mathcal{M} = \mathbb{R}$ *(or* $\mathcal{M}$ *is an unbounded domain).*

In this case, it is actually also possible to satisfy [H4] by choosing W *such that the dynamics is confined in a domain* $\bigcup_{z\in\mathcal{N}} \Sigma_z$*, where* $\mathcal{N}$ *is a bounded subset of* $\mathcal{M}$*. This can be done by using a sufficiently confining potential* W *and adapting Lemma 13 below, or by adding reflexion terms to restrict* ξ *to* $\mathcal{N}$ *(which loosely speaking corresponds to take* W *zero on* $\mathcal{N}$ *and infinite on* $\mathcal{M} \setminus \mathcal{N}$*) and adapting Lemma 12 below.*

Let us make precise this latter case. Suppose for example we are interested in the values of $A'(z)$ *for* $z \in \mathcal{N} = (0,1)$*. The dynamics is confined in the domain* $\mathcal{O} = \bigcup_{0<z<1} \Sigma_z$*. The ABF dynamics is*

$$\begin{cases} \partial_t \psi = \operatorname{div}\left(|\nabla\xi|^{-2}\left(\nabla(V - A_t\circ\xi)\psi + \beta^{-1}\nabla\psi\right)\right), & \text{on } \mathcal{O}, \\ \left(\nabla(V - A_t\circ\xi)\psi + \beta^{-1}\nabla\psi\right)\cdot\nabla\xi = 0, & \text{on } \Sigma_0 \cup \Sigma_1, \\ A'_t(z) = \dfrac{\displaystyle\int_{\Sigma_z} F|\nabla\xi|^{-1}\psi(t,\cdot)\,d\sigma_{\Sigma_z}}{\displaystyle\int_{\Sigma_z} |\nabla\xi|^{-1}\psi(t,\cdot)\,d\sigma_{\Sigma_z}}, & \text{for } z \in (0,1), \end{cases}$$

where F *is defined by (6). From the point of view of the stochastic process* X_t*, the boundary condition translates to a normal reflexion on the two submanifolds* Σ_0 *and* Σ_1*. Moreover, it can be checked (using Lemma 7) that the boundary condition on* ψ *translates to a zero Neumann boundary condition on* ψ^ξ*:* $\partial_z\psi^\xi(0) = \partial_z\psi^\xi(1) = 0$*. A proof similar to that of Lemma 12 then shows that* $I(\psi^\xi|\psi^\xi_\infty)$ *converges exponentially fast to* 0*, so that [H4] holds. The arguments we use to prove Theorem 1 and Corollary 1 then show that* $\|A'_t - A'\|_{L^2(0,1)}$ *goes to* 0 *exponentially fast.*

Remark 5 (Vectorial reaction coordinate) *In this work, we assume that the reaction coordinate* ξ *has values in* $\mathbb{T}$ *or* $\mathbb{R}$*. The dynamics (10)–(11) and the results of convergence presented in this section can be straightforwardly extended to the case when* $\xi = (\xi_1, \ldots, \xi_m)$ *has values in* $\mathbb{T}^m$ *or* $\mathbb{R}^m$*, with* $2 \leq m < n$*, under the orthogonality condition:*

$$\forall i \neq j,\ \nabla\xi_i \cdot \nabla\xi_j = 0. \tag{25}$$

The generalization of this dynamics to non orthogonal reaction coordinates is unclear. In this case, it is possible to resort to metadynamics (see Remark 6 below). Alternatively, the dynamics (12)–(11) (and the result of convergence of Section 2.3 for this dynamics) can straightforwardly be generalized to a vectorial reaction coordinate.

Remark 6 (Metadynamics) *The adaptive biasing force technique can also be used in the context of metadynamics [10, 4, 13]. The principle of metadynamics is to introduce an additional variable* z *with dimension the dimension of* ξ *(say* $z \in \mathbb{R}^m$*, with* $1 \leq m < n$*), and an extended potential* $V_\zeta(q,z) = V(q) + \frac{\zeta}{2}|z - \xi(q)|^2$*. The reaction coordinate is then chosen to be* $\xi_{\text{meta}}(q,z) = z$ *so that the associated free energy is*

$$A_\zeta(z) = -\beta^{-1} \ln \int_{\mathcal{D}} \exp(-\beta V_\zeta(q,z))\, dq,$$

which converges to $A(z)$ *when* ζ *goes to infinity. In our framework, the ABF method applied to this extended system writes:*

$$\begin{cases} dX_t = (-\nabla V(X_t) + \zeta(Z_t - \xi(X_t))\nabla\xi(X_t))\, dt + \sqrt{2\beta^{-1}} dB_t, \\ dZ_t = \zeta\Big(\xi(X_t) - \mathbb{E}(\xi(X_t)|Z_t)\Big)\, dt + \sqrt{2\beta^{-1}} d\overline{B}_t, \end{cases}$$

where $\overline{B}_t$ *is a* m*-dimensional Brownian motion, independent of* B_t*. Notice that by construction, the orthogonality condition* (25) *is satisfied by* ξ_{meta}*, so that the convergence results of this section apply to these kinds of models.*

Remark 7 (On the initial condition) *If* $\psi^\xi(0,\cdot)$ *is zero at some points or is not sufficiently smooth, then* A'_0 *may be not well defined or* $I(\psi^\xi(0,\cdot)|\psi^\xi_\infty)$ *may be infinite (which is in contradiction with [H4]). But since we show that* ψ^ξ *satisfies a simple diffusion equation (see Proposition 1), these difficulties disappear as soon as* $t > 0$*. Therefore, up to considering the problem for* $t \geq t_* > 0$*, we can suppose that* $\psi^\xi(0,\cdot) > 0$*.*

Remark 8 (On the choice of the entropy) *In the case of linear Fokker Planck equations, it is well known that one can obtain exponential convergence to equilibrium by considering various entropies of the form* $\int h\left(\frac{d\mu}{d\nu}\right) d\mu$*, where* h *is typically a strictly convex function such that* $h(1) = 0$ *(see [3] for more assumptions required on* h*). For example, the classical choice* $h(x) = \frac{1}{2}(x-1)^2$ *is linked to Poincaré type inequalities and leads to* L^2*-convergence, while the function* $h(x) = x\ln x - x + 1$ *we have used here to build the entropy is linked to logarithmic Sobolev inequalities and leads to* $L^1 \ln L^1$*-convergence. However, for the study of the non-linear Fokker Planck equation (14), it seems that the choice* $h(x) = x\ln x - x + 1$ *is necessary to derive the estimates, for example to have the extensivity property of Lemma 1.*

Remark 9 (Smoother evolution in time of A'_t**)** *In practice, it may be useful to update the adaptive potential* A'_t *in a smoother way in time, for example by replacing (11) by*

$$dA'_t(z) = \frac{1}{\tau}\left(\mathbb{E}\left(F(X_t)\,\Big|\xi(X_t) = z\right) - A'_t(z)\right) dt,$$

where F *is defined by (6) and* $\tau > 0$ *denotes a characteristic time (possibly depending on* (t,z)*), to be fixed. This amounts to replace* A'_t *by* $\kappa_\tau * A'_t$ *in (10), where* κ_τ *is an exponential convolution kernel. Formally, we here consider the limit case* $\tau = 0$*. To prove the convergence of* A'_t *towards* A' *for* $\tau \neq 0$ *is an open problem.*

Remark 10 (Enhancing the macroscopic rate of convergence) *Let us consider the case* $\mathcal{M} = \mathbb{R}$*. For an* α*-convex potential* W*, Corollary 1 states that* A'_t *converges towards* A' *exponentially fast, with a rate* $\lambda = \beta^{-1}\min(\rho m^{-2}, \alpha)$*. This may seem surprising since for large enough* α*, the rate of convergence is no more limited by* α*. However, it is typically expected that the constant* I_0 *in assumption [H4] increases with growing* α*, which means that the constant* C *increases in the convergence estimate (21). Moreover, in practice, if* α *is very large,* ψ^ξ_∞ *is very peaked and some parts of* $\mathcal{M}$ *are poorly sampled, so that the variance of the result is large in these areas (which can not be seen in our convergence result). Actually, a good method to enhance the rate of convergence at the macroscopic level while keeping a good sampling and thus low variance, is to use a particle systems with many replicas and a selection mechanism. We refer to [13] for more details.*

2.3 A convergence result for the adaptive dynamics (12)–(11)

In this section, we present a weaker convergence result for another adaptive overdamped Langevin dynamics, namely (12)–(11). For simplicity, we only consider the case

$$\mathcal{M} = \mathbb{T} \text{ and } W = 0,$$

but the results can be extended to the case $\mathcal{M} = \mathbb{R}$ with a suitable $W \neq 0$, as in Section 2.2 (see [H4] and [H4']). One interest of this dynamics and this result of convergence is that they can be straightforwardly extended to the case of a multi-dimensional reaction coordinate (see Remark 5 above). For the sake of conciseness, we do not provide the details of the result in this case which follows exactly the same lines (see [6] and Appendix A for formulas in the case of a multi-dimensional reaction coordinate). Let us recall the dynamics (12)–(11) we consider here:

$$\boxed{dX_t = -\nabla\Big(V - A_t \circ \xi\Big)(X_t)\, dt + \sqrt{2\beta^{-1}}dB_t,} \tag{26}$$

with the same definition as before for A_t: $\forall z \in \mathbb{T}$,

$$\boxed{A_t'(z) = \mathbb{E}\left(F(X_t)\,\Big|\xi(X_t) = z\right),} \tag{27}$$

where F is defined by (6). The associated non-linear Fokker Planck equation is now:

$$\boxed{\left\{\begin{aligned} &\partial_t\psi = \operatorname{div}\,\left(\nabla(V - A_t\circ\xi)\psi + \beta^{-1}\nabla\psi\right), \\ &A_t'(z) = \frac{\displaystyle\int_{\Sigma_z} F\,|\nabla\xi|^{-1}\psi(t,\cdot)d\sigma_{\Sigma_z}}{\displaystyle\int_{\Sigma_z} |\nabla\xi|^{-1}\psi(t,\cdot)d\sigma_{\Sigma_z}}. \end{aligned}\right.} \tag{28}$$

The main difference with the dynamics (10)–(11) considered in Theorem 1 is that the marginal distribution ψ^ξ does not satisfy a closed partial differential equation. Therefore, we do not know *a priori* that the Fisher information $I(\psi^\xi|\psi^\xi_\infty)$ converges to 0. The strategy here is to directly estimate the derivative of the total entropy E. We obtain a convergence result under two additional assumptions (see [H5]–[H6]).

Theorem 2 (Longtime convergence for the dynamics (12)–(11)) *Let (ψ, A_t') be a smooth solution to (28) and let us assume [H1], [H2], [H3]. Moreover, we suppose*

$$\textbf{[H5]} \quad V \textit{ and } \xi \textit{ are such that } \exists R > 0,\ \psi_\infty \textit{ satisfies LSI(R)}, \tag{29}$$

and

$$\textbf{[H6]} \quad \frac{mM\beta}{2\sqrt{\rho}} < 1.$$

Then the total entropy E satisfies:

$$\sqrt{E(t)} \leq \sqrt{E(0)}\exp(-\lambda t)$$

where $\lambda = \beta^{-1}\left(-1 + \frac{mM\beta}{2\sqrt{\rho}}\right) R$ is positive using [H6]. In particular, as in Theorem 1, the biasing force A_t' converges exponentially fast to the mean force A'.

The proof of this result is given in Section 3.4 below.

Remark 11 (On assumption [H5]) *In [14, Theorem 2], it is shown that if* $\mu = \exp(-H(x_1,x_2))dx_1dx_2$ *is a probability measure on a product space $X = X_1 \times X_2$ (where X_i are Euclidean spaces), if the conditional probabilities $\mu(dx_2|x_1)$ satisfy LSI(ρ_2) (with ρ_2 independent of x_1) and the marginal $\overline{\mu}(dx_1)$ satisfies LSI($\overline{\rho_1}$), then μ*

satisfies LSI(ρ) provided the coupling between the two directions is bounded: $\exists \kappa_{1,2} > 0$, $\forall (x_1, x_2) \in X_1 \times X_2$,

$$\left|\partial^2_{x_1,x_2} H(x_1,x_2)\right| \leq \kappa_{1,2}.$$

Thus, in the simple framework of Section 3.1 for example, where the configuration space is $\mathbb{T}\times\mathbb{R}$ *and the reaction coordinate is* $\xi(x,y) = x$*, the fact that* ψ_∞ *satisfies a LSI (assumption [H5]) can be deduced from the fact that the conditioned distributions* $\mu_{\infty,z}$ *satisfy a LSI (which is [H3]), the marginal* ψ^ξ_∞ *satisfy a LSI (which is related to [H4]) and the coupling is bounded (which is [H2]). Thus [H5] is not needed as an additional assumption compared to the framework of Theorem 1. The generalization of this result to the case when* X *is not a product does not seem to be straightforward.*

3 Proofs

One remark to simplify the presentation of the proofs is that we can suppose $\beta = 1$ up to the following change of variable: $\tilde{t} = \beta^{-1} t$, $\tilde{\psi}(\tilde{t}, x) = \psi(t, x)$, $\tilde{V}(x) = \beta V(x)$ and $\tilde{W}(x) = \beta W(x)$. Therefore, we suppose in the following that

$$\beta = 1. \tag{30}$$

3.1 Proof of Proposition 1 and Theorem 1 in a simple case

In this section, we propose to prove Proposition 1 and Theorem 1 in the simple case $n = 2$, $\xi(x,y) = x$ (so that we use in this section the notation x instead of z for the reaction coordinate variable) and the configuration space is $\mathcal{D} = \mathbb{T}\times\mathbb{R}$ (which means that all the data are periodic with respect to the first coordinate x). In this case, we thus have $\xi \in \mathbb{T}$ ($\mathcal{M} = \mathbb{T}$) so that we choose $W = 0$ (see [H4']). Notice also that the local mean force F is simply given by $F = \partial_x V$ (see (6)). Our aim is to introduce the main arguments in this simple case before presenting the general proof in Section 3.2.

In this simple setting, the system (14) writes (recall $\beta = 1$):

$$\left\{\begin{array}{l} \partial_t \psi = \operatorname{div}\,(\nabla V \psi + \nabla \psi) - \partial_x (A'_t \psi), \\ A'_t(x) = \dfrac{\displaystyle\int_{\mathbb{R}} \partial_x V(x,y)\psi(t,x,y)dy}{\psi^\xi(t,x)}, \end{array}\right. \tag{31}$$

where $\psi^\xi(t,x) = \int_{\mathbb{R}} \psi(t,x,y)dy$. Notice that in this case $\psi^\xi_\infty \equiv 1$.

It can be checked that the assumptions [H2] and [H3] are satisfied in this context for a potential V of the following form:

$$V(x,y) = V_0(x,y) + V_1(x,y)$$

where $\inf_{\mathbb{T}\times\mathbb{R}} \partial_{y,y} V_0 > 0$, $\|V_1\|_{L^\infty} < \infty$, $\|\partial_{x,y}(V_0 + V_1)\|_{L^\infty} < \infty$. The potential V is thus a bounded perturbation of an α-convex potential, with a bounded mixed derivative $\partial_{x,y} V$. Then, assumptions [H2]–[H3] are satisfied with $m = 1$, $M = \|\partial_{x,y} V\|_{L^\infty}$ and $\rho = (\inf_{\mathbb{T}\times\mathbb{R}} \partial_{y,y} V_0) \exp(-\mathrm{osc}\; V_1)$, where $\mathrm{osc}\; V_1 = \sup_{\mathbb{T}\times\mathbb{R}} V_1 - \inf_{\mathbb{T}\times\mathbb{R}} V_1$ (see [2]).

Proposition 1 is simply obtained by integration of (31) with respect to $y \in \mathbb{R}$:

Lemma 3 *The density* ψ^ξ *satisfies the following equation on* $\mathbb{T}$*:*

$$\partial_t \psi^\xi = \partial_{x,x} \psi^\xi. \tag{32}$$

As stated in Corollary 1, this result already yields the exponential convergence to zero of the macroscopic Fisher information $I(\psi^\xi | \psi^\xi_\infty)$ (this is the matter of Lemma 12 below), and thus [H4] is indeed satisfied with $I_0 = I(\psi^\xi(0,\cdot)|\psi^\xi_\infty)$ and $r = 4\pi^2$.

A fundamental lemma needed in the sequel is

Lemma 4 *The difference between the biasing force A'_t and the mean force A' can be expressed in term of the densities as*

$$A'_t - A' = \int_{\mathbb{R}} \partial_x \ln\left(\frac{\psi}{\psi_\infty}\right) \frac{\psi}{\psi^\xi}\, dy - \partial_x \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right).$$

Proof : This is a simple computation (using the fact that $\psi^\xi_\infty \equiv 1$):

$$\begin{aligned}\int_{\mathbb{R}} \partial_x \ln\left(\frac{\psi}{\psi_\infty}\right) \frac{\psi}{\psi^\xi}\, dy - \partial_x \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right) &= \int_{\mathbb{R}} \partial_x \ln\psi \frac{\psi}{\psi^\xi}\, dy - \int_{\mathbb{R}} \partial_x \ln\psi_\infty \frac{\psi}{\psi^\xi}\, dy - \partial_x \ln\psi^\xi,\\ &= \int_{\mathbb{R}} \frac{\partial_x\psi}{\psi^\xi}\, dy + \int_{\mathbb{R}} \partial_x(V-A)\frac{\psi}{\psi^\xi}\, dy - \partial_x \ln\psi^\xi,\\ &= A'_t - A'.\end{aligned}$$

♢

We will also use the following two estimates:

Lemma 5 *Let us assume [H2]–[H3]. Then, for all $t \geq 0$, for all $x \in \mathbb{T}$,*

$$|A'_t(x) - A'(x)| \leq \|\partial_{x,y}V\|_{L^\infty}\sqrt{\frac{2}{\rho}e_m(t,x)}.$$

Proof : For any coupling measure $\pi \in \Pi(\mu_{t,x}, \mu_{\infty,x})$, it holds:

$$\begin{aligned}|A'_t(x) - A'(x)| &= \left|\int_{\mathbb{R}\times\mathbb{R}} (\partial_x V(x,y) - \partial_x V(x,y'))\, \pi(dy,dy')\right|,\\ &\leq \|\partial_{x,y}V\|_{L^\infty} \int_{\mathbb{R}\times\mathbb{R}} |y-y'|\pi(dy,dy'),\\ &\leq \|\partial_{x,y}V\|_{L^\infty} \sqrt{\int_{\mathbb{R}\times\mathbb{R}} |y-y'|^2\pi(dy,dy')}.\end{aligned}$$

Taking now the infimum over all $\pi \in \Pi(\mu_{t,x}, \mu_{\infty,x})$ and using [H3] together with Lemma 2, we obtain

$$|A'_t(x) - A'(x)| \leq \|\partial_{x,y}V\|_{L^\infty} W(\mu_{t,x}, \mu_{\infty,x}) \leq \|\partial_{x,y}V\|_{L^\infty}\sqrt{\frac{2}{\rho}H(\mu_{t,x}|\mu_{\infty,x})},$$

which concludes the proof. ♢

Lemma 6 *Let us assume [H3]. Then for all $t \geq 0$,*

$$E_m(t) \leq \frac{1}{2\rho}\int_{\mathbb{T}\times\mathbb{R}} \left|\partial_y \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 \psi.$$

Proof : Using [H3], it holds:

$$\begin{aligned}E_m &= \int_{\mathbb{T}} e_m \psi^\xi\, dx,\\ &\leq \int_{\mathbb{T}} \frac{1}{2\rho}\int_{\mathbb{R}} \left|\partial_y \ln\left(\frac{\psi}{\psi^\xi}\Big/\frac{\psi_\infty}{\psi^\xi_\infty}\right)\right|^2 \frac{\psi}{\psi^\xi}\, dy\, \psi^\xi\, dx,\end{aligned}$$

which yields the result since ψ^ξ/ψ^ξ_∞ does not depend on y. ♢

We are now in position to prove the exponential convergence of $E_m(t)$ to zero stated in Theorem 1 (see Equation (21)).

Equation (31) on ψ can be rewritten as:

$$\partial_t\psi = \mathrm{div}\,(\psi_\infty\nabla(\psi/\psi_\infty)) + \partial_x((A' - A'_t)\psi).$$

Notice that the derivative $\frac{dE}{dt}$ can be obtained by multiplying this equation by $\ln\left(\frac{\psi}{\psi_\infty}\right)$ and integrating over $\mathbb{T}\times\mathbb{R}$. Thus, one obtains after some integrations by parts, using a Cauchy-Schwarz inequality (to prove that (33) is non positive) and Lemma 4 (used twice):

$$\begin{aligned}
\frac{dE_m}{dt} &= \frac{dE}{dt} - \frac{dE_M}{dt},\\
&= -\int_{\mathbb{T}}\int_{\mathbb{R}} \left|\nabla \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 \psi + \int_{\mathbb{T}}\int_{\mathbb{R}} (A'_t - A')\partial_x \ln\left(\frac{\psi}{\psi_\infty}\right)\psi + \int_{\mathbb{T}} \left|\partial_x \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\right|^2 \psi^\xi,\\
&= -\int_{\mathbb{T}}\int_{\mathbb{R}} \left|\partial_y \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 \psi\\
&\quad - \int_{\mathbb{T}}\int_{\mathbb{R}} \left|\partial_x \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 \psi + \int_{\mathbb{T}} \left(\int_{\mathbb{R}} \partial_x \ln\left(\frac{\psi}{\psi_\infty}\right)\psi\,dy\right)^2 \frac{1}{\psi^\xi}\,dx \qquad (33)\\
&\quad - \int_{\mathbb{T}}\int_{\mathbb{R}} \partial_x \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\partial_x \ln\left(\frac{\psi}{\psi_\infty}\right)\psi + \int_{\mathbb{T}} \left|\partial_x \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\right|^2 \psi^\xi,\\
&\le -\int_{\mathbb{T}}\int_{\mathbb{R}} \left|\partial_y \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 \psi - \int_{\mathbb{T}} \partial_x \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\psi^\xi (A'_t - A').
\end{aligned}$$

We now use Lemmas 5 and 6:

$$\begin{aligned}
\frac{dE_m}{dt} &\le -2\rho E_m + \sqrt{\int_{\mathbb{T}} |A'_t - A'|^2\,\psi^\xi}\sqrt{\int_{\mathbb{T}} \left|\partial_x \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\right|^2 \psi^\xi},\\
&\le -2\rho E_m + \|\partial_{x,y}V\|_{L^\infty}\sqrt{\frac{2}{\rho}E_m}\sqrt{I(\psi^\xi|\psi^\xi_\infty)}.
\end{aligned}$$

Using [H4], we thus have:

$$\frac{d\sqrt{E_m}}{dt} \le -\rho\sqrt{E_m} + \|\partial_{x,y}V\|_{L^\infty}\sqrt{\frac{I_0}{2\rho}}\exp(-rt),$$

from which we deduce (21).

Equation (23) is then easily obtained using Lemma 5.

3.2 Proof of Proposition 1 and Theorem 1 in the general case

We now present the proof of Proposition 1 and Theorem 1 in the more general setting of Section 2.2. The proof follows the same lines as in the simple case presented in Section 3.1, but with additional difficulties related to the geometry of the submanifolds Σ_z.

We need the following result

Lemma 7 *The derivative of ψ^ξ with respect to the reaction coordinate value reads:*

$$\partial_z \psi^\xi(t,z) = \int_{\Sigma_z} \left(\frac{\nabla\xi\cdot\nabla\psi(t,\cdot)}{|\nabla\xi|^2} + \operatorname{div}\left(\frac{\nabla\xi}{|\nabla\xi|^2}\right)\psi(t,\cdot)\right)|\nabla\xi|^{-1} d\sigma_{\Sigma_z}.$$

Proof : For any smooth test function $g:\mathcal{M}\to\mathbb{R}$, we obtain (using the co-area formula (39) and an integration by parts):

$$\begin{aligned}
\int_{\mathcal{M}} \psi^\xi(t,z) g'(z)\,dz &= \int_{\mathcal{D}} \psi(t,x) g'\circ\xi(x)\,dx,\\
&= \int_{\mathcal{D}} \psi(t,x)\nabla(g\circ\xi)\cdot\nabla\xi|\nabla\xi|^{-2}(x)\,dx,\\
&= -\int_{\mathcal{D}} \operatorname{div}\left(\frac{\psi(t,\cdot)\nabla\xi}{|\nabla\xi|^2}\right) g\circ\xi\,dx,\\
&= -\int_{\mathcal{M}} g(z)\int_{\Sigma_z}\left(\frac{\nabla\xi\cdot\nabla\psi(t,\cdot)}{|\nabla\xi|^2} + \operatorname{div}\left(\frac{\nabla\xi}{|\nabla\xi|^2}\right)\psi(t,\cdot)\right)|\nabla\xi|^{-1} d\sigma_{\Sigma_z}\,dz,
\end{aligned}$$

which yields the result. ♢

Using this lemma, it can be shown that ψ^ξ satisfies a simple diffusion equation, which is Proposition 1.

Lemma 8 *The density ψ^ξ satisfies the following diffusion equation on $\mathcal{M}$:*

$$\partial_t \psi^\xi = \partial_z \left(W' \psi^\xi + \partial_z \psi^\xi \right). \tag{34}$$

Proof : For any smooth test function $g : \mathcal{M} \to \mathbb{R}$, we have (using the co-area formula (39), (14), an integration by parts and finally Lemma 7):

$$\begin{aligned}
\frac{d}{dt} \int_{\mathcal{M}} \psi^\xi(t,\cdot) g \, dz &= \frac{d}{dt} \int_{\mathcal{D}} \psi(t,\cdot) g \circ \xi \, dx, \\
&= \int_{\mathcal{D}} \mathrm{div} \, \left(|\nabla \xi|^{-2} \left(\nabla (V - A_t \circ \xi + W \circ \xi) \psi + \nabla \psi \right) \right) g \circ \xi \, dx, \\
&= - \int_{\mathcal{D}} |\nabla \xi|^{-2} \left(\nabla (V - A_t \circ \xi + W \circ \xi) \psi + \nabla \psi \right) \cdot \nabla \xi \, g' \circ \xi \, dx, \\
&= - \int_{\mathcal{D}} |\nabla \xi|^{-2} \left(\nabla V \cdot \nabla \xi \psi + \nabla \psi \cdot \nabla \xi \right) \, g' \circ \xi \, dx \\
&\quad + \int_{\mathcal{D}} A'_t \circ \xi g' \circ \xi \psi \, dx - \int_{\mathcal{D}} W' \circ \xi g' \circ \xi \psi \, dx, \\
&= - \int_{\mathcal{M}} \int_{\Sigma_z} |\nabla \xi|^{-3} \left(\nabla V \cdot \nabla \xi \psi + \nabla \psi \cdot \nabla \xi \right) \, d\sigma_{\Sigma_z} g'(z) \, dz \\
&\quad + \int_{\mathcal{M}} A'_t(z) g'(z) \psi^\xi(z) \, dz - \int_{\mathcal{M}} W'(z) g'(z) \psi^\xi(z) \, dz, \\
&= - \int_{\mathcal{M}} \int_{\Sigma_z} \left(|\nabla \xi|^{-3} \nabla \psi \cdot \nabla \xi + \mathrm{div} \, (\nabla \xi |\nabla \xi|^{-2}) |\nabla \xi|^{-1} \psi \right) \, d\sigma_{\Sigma_z} g'(z) \, dz \\
&\quad - \int_{\mathcal{M}} W'(z) \psi^\xi(z) g'(z) \, dz, \\
&= - \int_{\mathcal{M}} \left(\partial_z \psi^\xi(t,z) + W'(z) \psi^\xi(z) \right) g'(z) \, dz,
\end{aligned}$$

which is a weak formulation of (34). ♢

As stated in Corollary 1, this result already yields the exponential convergence to zero of the macroscopic Fisher information $I(\psi^\xi | \psi^\xi_\infty)$ under adequate assumption on W (this is the matter of [H4'] and Lemma 13 below). We suppose in the following that [H4] is indeed satisfied.

The equivalent of Lemma 4 writes

Lemma 9 *The difference between the biasing force A'_t and the mean force A' can be expressed in term of the densities as*

$$A'_t(z) - A'(z) = \int_{\Sigma_z} \frac{\nabla \xi}{|\nabla \xi|} \cdot \nabla \ln \left(\frac{\psi}{\psi_\infty} \right) \frac{\psi}{\psi^\xi} |\nabla \xi|^{-2} \, d\sigma_{\Sigma_z} - \partial_z \ln \left(\frac{\psi^\xi}{\psi^\xi_\infty} \right).$$

Proof : Using Lemma 7 and the definition of A'_t, it holds:

$$\begin{aligned}
&\int_{\Sigma_z} \frac{\nabla\xi}{|\nabla\xi|} \cdot \nabla \ln\left(\frac{\psi}{\psi_\infty}\right) \frac{\psi}{\psi^\xi} |\nabla\xi|^{-2}\, d\sigma_{\Sigma_z} - \partial_z \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right) \\
&\quad = \int_{\Sigma_z} \frac{\nabla\xi}{|\nabla\xi|} \cdot \nabla \ln\psi \frac{\psi}{\psi^\xi} |\nabla\xi|^{-2}\, d\sigma_{\Sigma_z} - \int_{\Sigma_z} \frac{\nabla\xi}{|\nabla\xi|} \cdot \nabla \ln\psi_\infty \frac{\psi}{\psi^\xi} |\nabla\xi|^{-2}\, d\sigma_{\Sigma_z} \\
&\qquad - \partial_z \ln\psi^\xi + \partial_z \ln\psi^\xi_\infty, \\
&\quad = \frac{1}{\psi^\xi} \int_{\Sigma_z} \frac{\nabla\xi \cdot \nabla\psi}{|\nabla\xi|} |\nabla\xi|^{-2}\, d\sigma_{\Sigma_z} \\
&\qquad + \int_{\Sigma_z} \frac{\nabla\xi}{|\nabla\xi|} \cdot \nabla \left(V - A\circ\xi + W\circ\xi\right) \frac{\psi}{\psi^\xi} |\nabla\xi|^{-2}\, d\sigma_{\Sigma_z} - \partial_z \ln\psi^\xi - W'(z), \\
&\quad = \frac{\partial_z \psi^\xi}{\psi^\xi} - \frac{1}{\psi^\xi} \int_{\Sigma_z} \mathrm{div}\,\left(\frac{\nabla\xi}{|\nabla\xi|^2}\right) |\nabla\xi|^{-1} \psi\, d\sigma_{\Sigma_z} + \int_{\Sigma_z} \frac{\nabla\xi \cdot \nabla V}{|\nabla\xi|^3} \frac{\psi}{\psi^\xi}\, d\sigma_{\Sigma_z} \\
&\qquad - A'(z) - \partial_z \ln\psi^\xi, \\
&\quad = A'_t(z) - A'(z).
\end{aligned}$$

♢

The equivalent of Lemmas 5 and 6 write:

Lemma 10 *Let us assume [H2]–[H3]. Then for all $t \geq 0$, for all $z \in \mathcal{M}$,*

$$|A'_t(z) - A'(z)| \leq M \sqrt{\frac{2}{\rho} e_m(t,z)}.$$

Proof : For any coupling measure $\pi \in \Pi(\mu_{t,z}, \mu_{\infty,z})$ defined on $\Sigma_z \times \Sigma_z$, it holds:

$$\begin{aligned}
|A'_t(z) - A'(z)| &= \left| \int_{\Sigma_z \times \Sigma_z} (F(x) - F(x'))\pi(dx, dx') \right|, \\
&\leq \|\nabla_{\Sigma_z} F\|_{L^\infty} \sqrt{\int_{\Sigma_z \times \Sigma_z} d_{\Sigma_z}(x, x')^2 \pi(dx, dx')}.
\end{aligned}$$

Taking now the infimum over all $\pi \in \Pi(\mu_{t,z}, \mu_{\infty,z})$ and using [H2]–[H3] together with Lemma 2, we thus obtain

$$|A'_t(z) - A'(z)| \leq M W(\mu_{t,z}, \mu_{\infty,z}) \leq M \sqrt{\frac{2}{\rho} H(\mu_{t,z}|\mu_{\infty,z})}, \tag{35}$$

which concludes the proof. ♢

Lemma 11 *Let us assume [H3]. Then for all $t \geq 0$,*

$$E_m(t) \leq \frac{1}{2\rho} \int_{\mathcal{D}} \left| \nabla_{\Sigma_z} \ln\left(\frac{\psi(t,\cdot)}{\psi_\infty}\right) \right|^2 \psi.$$

Proof : Using [H3], it follows:

$$\begin{aligned}
E_m &= \int_{\mathcal{M}} e_m \psi^\xi\, dz, \\
&\leq \int_{\mathcal{M}} \frac{1}{2\rho} \int_{\Sigma_z} \left| \nabla_{\Sigma_z} \ln\left(\frac{\psi(t,\cdot)}{\psi_\infty}\right) \right|^2 \frac{\psi(t,\cdot)|\nabla\xi|^{-1} d\sigma_{\Sigma_z}}{\psi^\xi(t,z)} \psi^\xi\, dz,
\end{aligned}$$

which yields the result, using the co-area formula (39). ♢

We are now in position to prove the exponential convergence of $E_m(t)$ to zero stated in Theorem 1 (see Equation (21)). Equation (14) on ψ can be rewritten as:

$$\partial_t \psi = \mathrm{div}\,(|\nabla\xi|^{-2} \psi_\infty \nabla(\psi/\psi_\infty)) + \mathrm{div}\,(|\nabla\xi|^{-2} \nabla\left((A - A_t)\circ\xi\right)\, \psi).$$

Notice that the derivative $\frac{dE}{dt}$ can be obtained by multiplying this equation by $\ln\left(\frac{\psi}{\psi_\infty}\right)$ and integrating over $\mathcal{D}$. Thus, one obtains after some integrations by parts, using the co-area formula (39) and Lemma 9:

$$\begin{aligned}
\frac{dE_m}{dt} &= \frac{dE}{dt} - \frac{dE_M}{dt},\\
&= -\int_{\mathcal{D}} \left|\nabla \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 |\nabla\xi|^{-2}\psi + \int_{\mathcal{D}} (A'_t - A')\circ\xi\,\nabla\xi\cdot\nabla\ln\left(\frac{\psi}{\psi_\infty}\right)|\nabla\xi|^{-2}\psi\\
&\quad + \int_{\mathcal{M}} \left|\partial_z \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\right|^2 \psi^\xi,\\
&= -\int_{\mathcal{D}} \left|\nabla_{\Sigma_z} \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 |\nabla\xi|^{-2}\psi - \int_{\mathcal{D}} \left(\frac{\nabla\xi}{|\nabla\xi|}\cdot\nabla\ln\left(\frac{\psi}{\psi_\infty}\right)\right)^2 |\nabla\xi|^{-2}\psi\\
&\quad + \int_{\mathcal{M}} (A'_t - A')(z) \int_{\Sigma_z} \frac{\nabla\xi}{|\nabla\xi|}\cdot\nabla\ln\left(\frac{\psi}{\psi_\infty}\right)|\nabla\xi|^{-2}\psi d\sigma_{\Sigma_z}\,dz\\
&\quad + \int_{\mathcal{M}} \left|\partial_z \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\right|^2 \psi^\xi,\\
&= -\int_{\mathcal{D}} \left|\nabla_{\Sigma_z} \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 |\nabla\xi|^{-2}\psi - \int_{\mathcal{D}} \left(\frac{\nabla\xi}{|\nabla\xi|}\cdot\nabla\ln\left(\frac{\psi}{\psi_\infty}\right)\right)^2 |\nabla\xi|^{-2}\psi\\
&\quad + \int_{\mathcal{M}} \left(\int_{\Sigma_z} \frac{\nabla\xi}{|\nabla\xi|}\cdot\nabla\ln\left(\frac{\psi}{\psi_\infty}\right)|\nabla\xi|^{-2}\psi d\sigma_{\Sigma_z}\right)^2 (\psi^\xi)^{-1} dz\\
&\quad - \int_{\mathcal{M}} \int_{\Sigma_z} \frac{\nabla\xi}{|\nabla\xi|}\cdot\nabla\ln\left(\frac{\psi}{\psi_\infty}\right)|\nabla\xi|^{-2}\psi d\sigma_{\Sigma_z}\,\partial_z\ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)dz\\
&\quad + \int_{\mathcal{M}} \left|\partial_z \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\right|^2 \psi^\xi.
\end{aligned}$$

Using the Cauchy-Schwarz inequality:

$$\begin{aligned}
&\left(\int_{\Sigma_z} \frac{\nabla\xi}{|\nabla\xi|}\cdot\nabla\ln\left(\frac{\psi}{\psi_\infty}\right)|\nabla\xi|^{-1}\frac{|\nabla\xi|^{-1}\psi d\sigma_{\Sigma_z}}{\psi^\xi(z)}\right)^2\\
&\qquad \le \int_{\Sigma_z} \left(\frac{\nabla\xi}{|\nabla\xi|}\cdot\nabla\ln\left(\frac{\psi}{\psi_\infty}\right)|\nabla\xi|^{-1}\right)^2 \frac{|\nabla\xi|^{-1}\psi d\sigma_{\Sigma_z}}{\psi^\xi(z)}
\end{aligned}$$

and Lemma 9 again, we thus obtain

$$\frac{dE_m}{dt} \le -\int_{\mathcal{D}} \left|\nabla_{\Sigma_z} \ln\left(\frac{\psi}{\psi_\infty}\right)\right|^2 |\nabla\xi|^{-2}\psi - \int_{\mathcal{M}} \partial_z \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\psi^\xi (A'_t - A').$$

We now use [H2], Lemmas 10 and 11:

$$\begin{aligned}
\frac{dE_m}{dt} &\le -2\rho m^{-2} E_m + \sqrt{\int_{\mathcal{M}} |A'_t - A'|^2 \psi^\xi}\sqrt{\int_{\mathcal{M}} \left|\partial_z \ln\left(\frac{\psi^\xi}{\psi^\xi_\infty}\right)\right|^2 \psi^\xi},\\
&\le -2\rho m^{-2} E_m + M\sqrt{\frac{2}{\rho}E_m}\sqrt{I(\psi^\xi|\psi^\xi_\infty)}.
\end{aligned}$$

Using [H4], we thus have:

$$\frac{d\sqrt{E_m}}{dt} \le -\rho m^{-2}\sqrt{E_m} + M\sqrt{\frac{I_0}{2\rho}}\exp(-rt),$$

from which we deduce (21).

Equation (23) is then easily obtained using Lemma 10.

3.3 Proof of Corollary 1

3.3.1 Convergence of the macroscopic Fisher information

Let us first show that in both cases considered in [H4'], the exponential convergence [H4] of the macroscopic Fisher information indeed holds.

Let us first consider the case $\mathcal{M} = \mathbb{T}$ and $W = 0$. We know from (20) that ψ^ξ satisfies $\partial_t \psi^\xi = \partial_{z,z}\psi^\xi$ on $\mathbb{T}$, and we would like to show exponential convergence of the Fisher information $I(\psi^\xi(t,\cdot)|\psi^\xi_\infty)$.

Lemma 12 (Convergence of the Fisher information when $\mathcal{M} = \mathbb{T}$ and $W = 0$) *Let ϕ be a function defined for $t \geq 0$ and $x \in \mathbb{T}$ which satisfies*

$$\partial_t \phi = \partial_{x,x}\phi \text{ on } \mathbb{T}$$

and such that $\int_{\mathbb{T}} \phi(0,\cdot) = 1$, $\phi(0,\cdot)$ is non negative, and $I(\phi(0,\cdot)|\phi_\infty) < \infty$, where $\phi_\infty \equiv 1$ is the longtime limit of ϕ. Then, $\forall t \geq 0$,

$$I(\phi(t,\cdot)|\phi_\infty) \leq I(\phi(0,\cdot)|\phi_\infty)\exp(-8\pi^2 t).$$

Proof : Let us denote $u = \sqrt{\phi}$. We notice that $I(\phi|\phi_\infty) = \int_{\mathbb{T}} |\partial_x \ln \phi|^2 \phi = 4\int_{\mathbb{T}} |\partial_x u|^2$. Moreover, we have from (32)

$$\partial_t u = \partial_{x,x} u + \frac{(\partial_x u)^2}{u}.$$

Therefore,

$$\begin{aligned}
\frac{d}{dt}\int_{\mathbb{T}} (\partial_x u)^2 &= 2\int_{\mathbb{T}} \partial_{x,x,x} u\, \partial_x u + 2\int_{\mathbb{T}} \partial_x \left(\frac{(\partial_x u)^2}{u}\right)\partial_x u,\\
&= -2\int_{\mathbb{T}} (\partial_{x,x} u)^2 - 2\int_{\mathbb{T}} \frac{(\partial_x u)^2}{u}\partial_{x,x} u,\\
&= -2\int_{\mathbb{T}} (\partial_{x,x} u)^2 - 2\int_{\mathbb{T}} \frac{\partial_x((\partial_x u)^3)}{3u},\\
&= -2\int_{\mathbb{T}} (\partial_{x,x} u)^2 - \frac{2}{3}\int_{\mathbb{T}} \frac{(\partial_x u)^4}{u^2},\\
&\leq -8\pi^2 \int_{\mathbb{T}} (\partial_x u)^2,
\end{aligned}$$

where we have used the Poincaré-Wirtinger inequality on $\mathbb{T}$, applied to $\partial_x u$: For any function $f \in H^1(\mathbb{T})$,

$$\int_{\mathbb{T}} \left(f - \int_{\mathbb{T}} f\right)^2 \leq \frac{1}{4\pi^2}\int_{\mathbb{T}} (\partial_x f)^2.$$

$\diamondsuit$

Let us now consider the case $\mathcal{M} = \mathbb{R}$ and $W \neq 0$ which is such that W'' is bounded from below and $\frac{\exp(-\beta W)}{\int_{\mathcal{M}} \exp(-\beta W)}$ satisfies a logarithmic Sobolev inequality (as stated in [H4']). We know from (20) that ψ^ξ satisfies $\partial_t \psi^\xi = \partial_z \left(W'\psi^\xi + \partial_z \psi^\xi\right)$ on $\mathbb{R}$, and we would like to show exponential convergence of the Fisher information $I(\psi^\xi(t,\cdot)|\psi^\xi_\infty)$.

Lemma 13 (Convergence of the Fisher information when $\mathcal{M} = \mathbb{R}$ and $W \neq 0$) *Let ϕ be a function defined for $t \geq 0$ and $x \in \mathbb{R}$ which satisfies*

$$\partial_t \phi = \partial_x \left(W'\phi + \partial_x \phi\right) \text{ on } \mathbb{R},$$

and such that $\int_{\mathbb{R}} \phi(0,\cdot) = 1$, $\phi(0,\cdot)$ is non negative, and $I(\phi(0,\cdot)|\phi_\infty) < \infty$, where $\phi_\infty \equiv \frac{\exp(-W)}{\int_{\mathbb{R}} \exp(-W)}$ is the longtime limit of ϕ. Let us assume that W'' is bounded from *below by a constant α and ϕ_∞ satisfies LSI($\overline{r}$), with $\overline{r} > 0$. We can suppose without loss of generality that*

$$\overline{r} \geq \alpha.$$

Then there exists $I_0 > 0$ and $r > 0$ such that $\forall t \geq 0$,

$$I(\phi(t,\cdot)|\phi_\infty) \leq I_0 \exp(-2rt).$$

More precisely, when $\alpha = \overline{r} > 0$, it is possible to take $I_0 = I(\phi(0,\cdot)|\phi_\infty)$ and $r = \alpha$. When $\alpha < \overline{r}$, for any $\varepsilon \in (0, \overline{r})$, it is possible to choose $r = \overline{r} - \varepsilon$ for a well-chosen constant $I_0 > 0$.

Proof : The fact that $\overline{r} \geq \alpha$ is clear since either $\alpha \leq 0$, or $\alpha > 0$ in which case it is well-known that ϕ_∞ satisfies LSI(α) (see for example [2]), so that one can choose at least $\overline{r} = \alpha$.

Let us recall the expression for the entropy $H(\phi(t,\cdot)|\phi_\infty) = \int_{\mathbb{R}} \ln(\phi/\phi_\infty)\phi$ and the Fisher information $I(\phi(t,\cdot)|\phi_\infty) = \int_{\mathbb{R}} |\partial_x \ln(\phi/\phi_\infty)|^2 \phi$. Since ϕ_∞ satisfies LSI($\overline{r}$), we have

$$H(\phi(t,\cdot)|\phi_\infty) \leq \frac{1}{2\overline{r}} I(\phi(t,\cdot)|\phi_\infty).$$

Moreover, by standard computations (see for example [3]), we have

$$\frac{d}{dt} H(\phi(t,\cdot)|\phi_\infty) = -I(\phi(t,\cdot)|\phi_\infty)$$

and

$$\frac{d}{dt} I(\phi(t,\cdot)|\phi_\infty) = -2\int_{\mathbb{R}} \frac{\phi}{\phi_\infty} \left| \partial_{x,x} \ln\left(\frac{\phi}{\phi_\infty}\right) \right|^2 \phi_\infty - 2\int_{\mathbb{R}} \frac{\phi}{\phi_\infty} \left| \partial_x \ln\left(\frac{\phi}{\phi_\infty}\right) \right|^2 W'' \phi_\infty. \tag{36}$$

If $\alpha = \overline{r}$, we thus obtain from (36) that $\frac{d}{dt} I(\phi(t,\cdot)|\phi_\infty) \leq -2\alpha I(\phi(t,\cdot)|\phi_\infty)$ which concludes the proof in this case.

Let us now suppose that $\alpha < \overline{r}$. The technique of proof we propose is taken from [17]. For any $\lambda > 0$, we have

$$\begin{aligned}
&\frac{d}{dt} \left(H(\phi(t,\cdot)|\phi_\infty) + \lambda I(\phi(t,\cdot)|\phi_\infty) \right) \\
&\quad = -\int_{\mathbb{R}} \frac{\phi}{\phi_\infty} \left| \partial_x \ln\left(\frac{\phi}{\phi_\infty}\right) \right|^2 \phi_\infty - 2\lambda \int_{\mathbb{R}} \frac{\phi}{\phi_\infty} \left| \partial_{x,x} \ln\left(\frac{\phi}{\phi_\infty}\right) \right|^2 \phi_\infty \\
&\qquad - 2\lambda \int_{\mathbb{R}} \frac{\phi}{\phi_\infty} \left| \partial_x \ln\left(\frac{\phi}{\phi_\infty}\right) \right|^2 W'' \phi_\infty, \\
&\quad \leq -\int_{\mathbb{R}} (1 + 2\lambda W'') \frac{\phi}{\phi_\infty} \left| \partial_x \ln\left(\frac{\phi}{\phi_\infty}\right) \right|^2 \phi_\infty, \\
&\quad \leq -(1 + 2\lambda \inf W'') I(\phi(t,\cdot)|\phi_\infty), \\
&\quad \leq -\frac{1 + 2\alpha\lambda}{\lambda + 1/(2\overline{r})} \left(H(\phi(t,\cdot)|\phi_\infty) + \lambda I(\phi(t,\cdot)|\phi_\infty) \right).
\end{aligned}$$

We thus obtain that, for any $\lambda > 0$,

$$H(\phi(t,\cdot)|\phi_\infty) + \lambda I(\phi(t,\cdot)|\phi_\infty) \leq \left(H(\phi(0,\cdot)|\phi_\infty) + \lambda I(\phi(0,\cdot)|\phi_\infty) \right) \exp\left(-\frac{1 + 2\alpha\lambda}{\lambda + 1/(2\overline{r})} t \right),$$

and therefore

$$I(\phi(t,\cdot)|\phi_\infty) \leq \left(\frac{1}{\lambda} H(\phi(0,\cdot)|\phi_\infty) + I(\phi(0,\cdot)|\phi_\infty) \right) \exp\left(-\frac{1 + 2\alpha\lambda}{\lambda + 1/(2\overline{r})} t \right).$$

Since $\frac{1+2\alpha\lambda}{\lambda+1/(2\overline{r})}$ goes to $2\overline{r}$ when λ goes to 0, for any $\varepsilon \in (0, \overline{r})$, one can find a $\lambda > 0$ such that $\frac{1+2\alpha\lambda}{\lambda+1/(2\overline{r})} = 2(\overline{r} - \varepsilon)$, which concludes the proof. ♢

3.3.2 Convergence of the biasing force

Let us now prove the convergence result (24) for the biasing force.

In the case $\mathcal{M} = \mathbb{T}$ (and thus $W = 0$), we can prove the convergence of $\|A'_t - A'\|_{L^2(\mathbb{T})}$ to zero in the following sense (which implies (24), using (21)): for any $\varepsilon \in (0,1)$, $\forall t \geq t_\varepsilon$,

$$\|A'_t - A'\|^2_{L^2(\mathbb{T})} \leq \frac{2}{1-\varepsilon} \frac{M^2}{\rho} E_m(t), \tag{37}$$

where $t_\varepsilon = \min\left(0, (4\pi^2)^{-1} \ln\left(\varepsilon^{-1}\sqrt{\int_{\mathbb{T}} (\partial_z \psi^\xi(0,\cdot))^2}\right)\right)$. This is obtained using the fact that $\int_{\mathbb{T}} (\partial_x \psi^\xi(t,\cdot))^2 \leq \int_{\mathbb{T}} (\partial_x \psi^\xi(0,\cdot))^2 \exp(-8\pi^2 t)$ (the proof of this estimate is similar to the one of Lemma 12) and the fact that for any function $f \in H^1(\mathbb{T})$,

$$\left\| f - \int_{\mathbb{T}} f \right\|^2_{L^\infty} \leq \int_{\mathbb{T}} (\partial_x f)^2,$$

applied to $f = \psi^\xi$. Thus we have $\left\|\psi^\xi - 1\right\|^2_{L^\infty} \leq \int_{\mathbb{T}} (\partial_x \psi^\xi(0,\cdot))^2 \exp(-8\pi^2 t)$ which implies that for $t \geq t_\varepsilon$, $\psi^\xi(t,\cdot) \geq 1 - \varepsilon$ which yields (37) from (23).

Let us now prove (24) in the case $\mathcal{M} = \mathbb{R}$, under assumption [H4'] on W. Let us introduce a compact $K \subset \mathcal{M}$. Since $L^\infty(K) \subset H^1(K)$ (with continuous injection), there exists $c > 0$ such that

$$\begin{aligned}
\left\| \frac{\psi^\xi}{\psi^\xi_\infty} - 1 \right\|_{L^\infty(K)} &\leq c \left(\left\| \frac{\psi^\xi}{\psi^\xi_\infty} - 1 \right\|_{L^2(K)} + \left\| \partial_z \left(\frac{\psi^\xi}{\psi^\xi_\infty} - 1 \right) \right\|_{L^2(K)} \right), \\
&\leq \frac{c}{\inf_K \sqrt{\psi^\xi_\infty}} \left(\sqrt{\int_{\mathbb{R}} \left(\frac{\psi^\xi}{\psi^\xi_\infty} - 1 \right)^2 \psi^\xi_\infty} + \sqrt{\int_{\mathbb{R}} \left(\partial_z \left(\frac{\psi^\xi}{\psi^\xi_\infty} - 1 \right) \right)^2 \psi^\xi_\infty} \right).
\end{aligned}$$

Thus, for any $\varepsilon \in (0, \overline{r})$, there exists $C > 0$ such that

$$\left\| \frac{\psi^\xi}{\psi^\xi_\infty} - 1 \right\|_{L^\infty(K)} \leq C \exp(-rt),$$

with $r = \overline{r} - \varepsilon$. This inequality is obtained from the fact that since ψ^ξ_∞ satisfies LSI($\overline{r}$), then ψ^ξ_∞ also satisfies a Poincaré inequality with the same constant $\overline{r}$ (see for example [2]), and a proof similar to that of Lemma 13 for the convergence of the Fisher information $\int_{\mathbb{R}} \left(\partial_z \left(\frac{\psi^\xi}{\psi^\xi_\infty} - 1 \right) \right)^2 \psi^\xi_\infty$ associated with the Poincaré inequality. Now, we write

$$\begin{aligned}
\int_K |A'_t - A'| \psi^\xi_\infty &= \int_K |A'_t - A'| \psi^\xi - \int_K |A'_t - A'| \left(\frac{\psi^\xi}{\psi^\xi_\infty} - 1 \right) \psi^\xi_\infty, \\
&\leq \int_{\mathbb{R}} |A'_t - A'|^2 \psi^\xi + C \exp(-rt) \int_K |A'_t - A'| \psi^\xi_\infty.
\end{aligned}$$

Thus, for t sufficiently large, $\int_K |A'_t - A'| \psi^\xi_\infty$ is bounded from above by some constant times $\int_{\mathbb{R}} |A'_t - A'|^2 \psi^\xi$, which yields (24) (using (23) and (21)).

3.4 Proof of Theorem 2

Let us now prove Theorem 2. We still assume, up to a change of variable, that $\beta = 1$. We have:

$$\begin{aligned}
\frac{dE}{dt} &= -\int_{\mathcal{D}} \left| \nabla \ln \left(\frac{\psi}{\psi_\infty} \right) \right|^2 \psi + \int_{\mathcal{D}} (A'_t - A') \circ \xi \nabla \xi \cdot \nabla \ln \left(\frac{\psi}{\psi_\infty} \right) \psi, \\
&\leq -\int_{\mathcal{D}} \left| \nabla \ln \left(\frac{\psi}{\psi_\infty} \right) \right|^2 \psi + \sqrt{\int_{\mathcal{M}} |A'_t - A'|^2 \psi^\xi} \sqrt{\int_{\mathcal{D}} \left| \nabla \xi \cdot \nabla \ln \left(\frac{\psi}{\psi_\infty} \right) \right|^2 \psi}.
\end{aligned}$$

Since, by Lemmas 10 and 11,

$$\int_{\mathcal{M}} |A'_t - A'|^2 \psi^\xi \le \frac{M^2}{\rho} \int_{\mathcal{D}} \left| \nabla_{\Sigma_z} \ln \left(\frac{\psi}{\psi_\infty} \right) \right|^2 \psi,$$

we thus obtain

$$\begin{aligned}\frac{dE}{dt} &\le - \int_{\mathcal{D}} \left| \nabla \ln \left(\frac{\psi}{\psi_\infty} \right) \right|^2 \psi + \frac{Mm}{\sqrt{\rho}} \sqrt{\int_{\mathcal{D}} \left| \nabla_{\Sigma_z} \ln \left(\frac{\psi}{\psi_\infty} \right) \right|^2 \psi} \sqrt{\int_{\mathcal{D}} \left| \frac{\nabla \xi}{|\nabla \xi|} \cdot \nabla \ln \left(\frac{\psi}{\psi_\infty} \right) \right|^2 \psi} \\ &\le \left(-1 + \frac{Mm}{2\sqrt{\rho}} \right) \int_{\mathcal{D}} \left| \nabla \ln \left(\frac{\psi}{\psi_\infty} \right) \right|^2 \psi,\end{aligned}$$

where we have used the fact that, for any function $f : \mathcal{D} \to \mathbb{R}$, $|\nabla f|^2 = |\nabla_{\Sigma_z} f|^2 + \left| \frac{\nabla \xi}{|\nabla \xi|} \cdot \nabla f \right|^2$. The logarithmic Sobolev inequality with respect to ψ_∞ (see [H5]) concludes the proof.

A The co-area formula

The aim of this section is to state the co-area formula for a function $\xi : \mathcal{D} \to \mathbb{R}^p$, (where $1 \le p < n$) such that rank$(\nabla \xi) = p$. Classical proofs for the co-area formula can be found in the books [1, 8]. These proofs are however quite involved since they assume only Lipschitz-regularity for ξ. The proof is simpler in the case of a smooth ξ: it can be done by an adequate parameterization and a simple change of variables.

Lemma 14 (co-area formula) *For any smooth function $\phi : \mathbb{R}^n \to \mathbb{R}$,*

$$\int_{\mathbb{R}^n} \phi(x) \sqrt{\det G(x)} dx = \int_{\mathbb{R}^p} \int_{\Sigma_z} \phi \, d\sigma_{\Sigma_z} \, dz, \tag{38}$$

where G is a $p \times p$ matrix with $G_{i,j} = \nabla \xi_i \cdot \nabla \xi_j$. In the case $p = 1$, Equation (38) reads:

$$\int_{\mathbb{R}^n} \phi(x) |\nabla \xi|(x) dx = \int_{\mathbb{R}} \int_{\Sigma_z} \phi \, d\sigma_{\Sigma_z} \, dz, \tag{39}$$

Remark 12 *This formula shows that if the random variable X has law $\psi(x)\,dx$ in $\mathbb{R}^n$, then $\xi(X)$ has law*

$$\int_{\Sigma_z} \psi \, (\det G)^{-1/2} \, d\sigma_{\Sigma_z} \, dz,$$

and the law of X conditioned to a fixed value z of $\xi(X)$ is

$$d\mu_z = \frac{\psi \, (\det G)^{-1/2} \, d\sigma_{\Sigma_z}}{\int_{\Sigma_z} \psi \, (\det G)^{-1/2} \, d\sigma_{\Sigma_z}}.$$

Indeed, for any bounded functions f and g,

$$\begin{aligned}\mathbb{E}(f(\xi(X)) g(X)) &= \int_{\mathbb{R}^n} f(\xi(x)) g(x) \psi(x) \, dx, \\ &= \int_{\mathbb{R}^p} \int_{\Sigma_z} f \circ \xi \, g \, \psi \, (\det G)^{-1/2} d\sigma_{\Sigma_z} \, dz, \\ &= \int_{\mathbb{R}^p} f(z) \frac{\int_{\Sigma_z} g \, \psi \, (\det G)^{-1/2} d\sigma_{\Sigma_z}}{\int_{\Sigma_z} \psi \, (\det G)^{-1/2} d\sigma_{\Sigma_z}} \int_{\Sigma_z} \psi \, (\det G)^{-1/2} d\sigma_{\Sigma_z} \, dz.\end{aligned}$$

The measure $(\det G)^{-1/2} d\sigma_{\Sigma_z}$ is sometimes denoted by $\delta_{\xi(x)-z}$ in the literature.

B Another possible set of assumptions for the convergence of the adaptive dynamics (10)–(11)

It is also possible to state a result similar to Theorem 1 for the dynamics (10)–(11) under slightly different assumptions than [H2] and [H3] by introducing another Riemannian structure on Σ_z (see [15]) than that induced by the scalar product of the ambient space $\mathcal{D}$. Let us introduce the following scalar product: $\forall x \in \Sigma_z$, $\forall u, v \in T_x\Sigma_z$,

$$\langle u, v\rangle_{\Sigma_z} = u \cdot v |\nabla \xi|^2(x), \tag{40}$$

where $\cdot$ denotes as before the scalar product of the ambient space $\mathcal{D}$, and the associated norm: $\forall x \in \Sigma_z$, $\forall u \in T_x\Sigma_z$,

$$|u|^2_{\Sigma_z} = \langle u, u\rangle_{\Sigma_z} = |u|^2 |\nabla \xi|^2(x).$$

Accordingly, the definition of the surface gradient is modified as follows[2] (compare with (19)): For $f : \mathcal{D} \to \mathbb{R}$,

$$\nabla_{\Sigma_z} f = |\nabla \xi|^{-2} P \nabla f. \tag{41}$$

In particular, we have $|\nabla_{\Sigma_z} f|_{\Sigma_z} = |\nabla \xi|^{-1} |P\nabla f|$.

In this case, the Fisher information between the conditioned measures $\mu_{t,z}$ and $\mu_{\infty,z}$ is (see [15]):

$$\begin{aligned} I(\mu_{t,z}|\mu_{\infty,z}) &= \int_{\Sigma_z} \left| \nabla_{\Sigma_z} \ln \left(\frac{\psi(t,\cdot)}{\psi_\infty} \right) \right|^2_{\Sigma_z} \frac{\psi(t,\cdot)|\nabla\xi|^{-1} d\sigma_{\Sigma_z}}{\psi^\xi(t,z)}, \\ &= \int_{\Sigma_z} \left| P\nabla \ln \left(\frac{\psi(t,\cdot)}{\psi_\infty} \right) \right|^2 |\nabla \xi|^{-2} \frac{\psi(t,\cdot)|\nabla\xi|^{-1} d\sigma_{\Sigma_z}}{\psi^\xi(t,z)}, \end{aligned}$$

and the assumption [H3] is stated in terms of this new Fisher information:

$$\textbf{[H3']} \quad \left\{ \begin{array}{c} V \text{ and } \xi \text{ are such that } \exists \rho > 0, \text{ for all } z \in \mathcal{M}, \\ \text{the conditional measure } \mu_{\infty,z} \text{ satisfies LSI}(\rho), \\ \Sigma_z \text{ being endowed with the Riemannian structure (40).} \end{array} \right.$$

Using this Fisher information, Lemma 11 writes:

$$E_m(t) \le \frac{1}{2\rho} \int_{\mathcal{D}} \left| P\nabla \ln \left(\frac{\psi(t,\cdot)}{\psi_\infty} \right) \right|^2 |\nabla \xi|^{-2} \psi.$$

The definition for the Wasserstein distance is now stated using the geodesic distance d_{Σ_z}: $\forall x, y \in \Sigma_z$,

$$d_{\Sigma_z}(x,y) = \inf \left\{ \sqrt{\int_0^1 |\dot{w}(t)|^2_{\Sigma_z} \, dt} \,\middle|\, w \in \mathcal{C}^1([0,1], \Sigma_z),\ w(0) = x,\ w(1) = y \right\}.$$

Thus, the estimate of Lemma 10 is changed to:

$$\begin{aligned} |A_t'(z) - A'(z)| &= \left| \int_{\Sigma_z \times \Sigma_z} (F(x) - F(x')) \pi(dx, dx') \right|, \\ &\le \left\| |\nabla \xi|^{-1} \, |P\nabla F| \right\|_{L^\infty} \sqrt{\int_{\Sigma_z \times \Sigma_z} d_{\Sigma_z}(x,x')^2 \pi(dx,dx')}, \end{aligned}$$

---

[2] With a slight abuse of notation, we still use the same notation ∇_{Σ_z} to denote the surface gradient, or $I(\mu_{t,z}|\mu_{\infty,z})$ to denote the Fisher information, or d_{Σ_z} to denote the geodesic distance, or ρ to denote the microscopic rate of convergence, while these are not the same as in the rest of the paper, since the Riemannian structure has been changed.

where F is defined by (6). Notice that

$$|\nabla \xi|^{-1} \, |P \nabla F| = |\nabla_{\Sigma_z} F|_{\Sigma_z} \, .$$

Thus, assumption [H2] is modified as:

$$\textbf{[H2']} \quad \left\{ \begin{array}{c} V \text{ and } \xi \text{ are sufficiently differentiable functions such that} \\ \left\| |\nabla_{\Sigma_z} F|_{\Sigma_z} \right\|_{L^\infty} \leq M < \infty. \end{array} \right.$$

The rest of the proof remains the same, and exponential convergence is thus obtained, assumptions [H2] and [H3] being respectively replaced by [H2'] and [H3']. With this set of assumptions, the rate of convergence is $\lambda = \beta^{-1} \min(\rho, r)$.

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