



Quasi-stationary distribution for Hamiltonian dynamics with singular potentials

Arnaud Guillin , Boris Nectoux , Liming Wu

► To cite this version:

Arnaud Guillin , Boris Nectoux , Liming Wu. Quasi-stationary distribution for Hamiltonian dynamics with singular potentials. 2022. hal-03276880v2

HAL Id: hal-03276880

<https://hal.science/hal-03276880v2>

Preprint submitted on 24 May 2022

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.



Distributed under a Creative Commons Attribution 4.0 International License

QUASI-STATIONARY DISTRIBUTION FOR HAMILTONIAN DYNAMICS WITH SINGULAR POTENTIALS

ARNAUD GUILLIN[◇], BORIS NECTOUX[◇], AND LIMING WU[◇]

ABSTRACT. In this work, we prove the existence and the uniqueness of a quasi-stationary distribution for hypoelliptic Hamiltonian dynamics for a system of N particles in \mathbb{R}^d interacting with Lennard-Jones type potentials or with repulsive Coulomb potentials.

AMS 2010 Subject classifications. 37A60, 60B10, 60F99, 60J60, 37A30.

Key words and Phrases. Quasi-stationary distribution, Lyapunov functions, hypoelliptic diffusions, molecular dynamics, Lennard-Jones potential, Coulomb potential.

1. INTRODUCTION

1.1. Setting and purpose. For $d \geq 1$, consider a system of $N \geq 2$ particles in \mathbb{R}^d which cannot collide and let

$$x_t = (x_t^1, \dots, x_t^N) \in (\mathbb{R}^d)^N \text{ and } v_t = (v_t^1, \dots, v_t^N) \in (\mathbb{R}^d)^N,$$

denote respectively the positions of the N particles and their velocities, at time $t \geq 0$. The natural space to consider the time evolution of the positions $(x_t, t \geq 0)$ and of the velocities $(v_t, t \geq 0)$ of the N particles is thus

$$\mathcal{S} = \mathcal{O} \times (\mathbb{R}^d)^N, \tag{1.1}$$

where

$$\begin{cases} \text{if } d = 1, & \mathcal{O} = \{x = (x^1, \dots, x^N) \in (\mathbb{R})^N, x^1 < x^2 < \dots < x^N\}, \\ \text{if } d \geq 2, & \mathcal{O} = \{x = (x^1, \dots, x^N) \in (\mathbb{R}^d)^N, x^i \neq x^j \text{ for all } i \neq j\}. \end{cases} \tag{1.2}$$

Notice that in both cases, \mathcal{O} is open, path connected, and unbounded. In addition,

$$\partial\mathcal{S} = \partial\mathcal{O} \times (\mathbb{R}^d)^N, \text{ with, } \begin{cases} \text{if } d = 1, & \partial\mathcal{O} \subset \cup_{i=1, \dots, N-1} \{x \in \mathbb{R}^N, x^i = x^{i+1}\}, \\ \text{if } d \geq 2, & \partial\mathcal{O} = \cup_{1 \leq i < j \leq N} \{x \in (\mathbb{R}^d)^N, x^i = x^j\}. \end{cases} \tag{1.3}$$

In molecular dynamics, the interatomic potential of the system of N particles is typically of the form, for $x = (x^1, \dots, x^N) \in \mathcal{O}$,

$$V(x) = \sum_{i=1}^N V_c(x^i) + \sum_{1 \leq i < j \leq N} V_I(x^i - x^j) \in \overline{\mathbb{R}}, \tag{1.4}$$

where $V_c : \mathbb{R}^d \rightarrow \mathbb{R}$ is the confining potential of the system and $V_I : \Omega \rightarrow \mathbb{R}$ (where, if $d = 1$, $\Omega = \{y < 0\}$, and if $d \geq 2$, $\Omega = \{y \neq 0\}$) is the potential energy modeling the

interaction between two particles, the latter becoming infinite when (and only when) $y \in \partial\Omega = \{0\}$ (which prevents from collisions). Let $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \geq 0}, \mathbb{P})$ be a filtered probability space. We assume that the evolution of the positions $(x_t, t \geq 0)$ and the velocities $(v_t, t \geq 0)$ of the N particles on \mathcal{S} is described by the following hypoelliptic stochastic differential equation¹

$$\begin{cases} dx_t = v_t dt, \\ dv_t = -\nabla V(x_t) dt - \gamma(x_t, v_t) v_t dt + \Sigma(x_t, v_t) dB_t, \end{cases} \quad (1.5)$$

where $\gamma : (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N \rightarrow M_{Nd}(\mathbb{R})$ (the space of square matrices of size Nd with real coefficients) is the friction matrix, $(B_t, t \geq 0)$ is a standard dN -dimensional Brownian motion, and $\Sigma : (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N \rightarrow \mathbb{R}$. We set $X_t = (x_t, v_t)$ for $t \geq 0$. Throughout this paper, we assume that

- (Ac) $\gamma : (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N \rightarrow M_{Nd}(\mathbb{R})$ is a locally Lipschitz function such that:
- (i) there exists $\gamma^* > 0$, $\forall x, v \in (\mathbb{R}^d)^N : \frac{1}{2}[\gamma(x, v) + \gamma^T(x, v)] \geq \gamma^* I_{(\mathbb{R}^d)^N}$, where γ^T is the transpose matrix of γ ,
 - (ii) $\sup_{x, v \in (\mathbb{R}^d)^N, k, \ell=1, \dots, Nd} |\gamma_{k, \ell}(x, v)| < +\infty$.
- (A Σ) $\Sigma : (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N \rightarrow \mathbb{R}$ is a \mathcal{C}^∞ function, uniformly Lipschitz over $(\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$, and such that for some $\Sigma_0 > 0$ and $\Sigma_\infty > 0$,

$$\forall x \in (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N, \quad \Sigma_0 \leq \Sigma(x) \leq \Sigma_\infty.$$

Let us mention that in many applications where the equation (1.5) is used, the functions γ and Σ are constant. However, in certain cases, γ and Σ can indeed be state-dependent, see for instance [7, 33, 34, 48, 5, 46, 45] and references therein.

Let us also mention that for many intermediate results, Assumption (Ac) can be relaxed, see Remark 2.14.

In this work, we prove the existence and the uniqueness of a quasi-stationary distribution for the process (1.5) when V_I is the Lennard-Jones type potential or the Coulomb potential (see (1.7) for the definition of a quasi-stationary distribution). These two pair potentials are widely used in molecular dynamics simulation. Such a setting is motivated by what follows. Due to energetic barriers of the potential V , the process $(x_t, t \geq 0)$ spends a lot of time in a neighborhood \mathcal{O} (bounded or not) of a local minimum of V in \mathcal{O} . Thus, the process (1.5) is stuck during long period of times in regions \mathcal{D} of the form $\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N$. For this reason, the set \mathcal{D} is called a metastable region (modelling in practice a macroscopic state). It is thus expected that when the process starts inside \mathcal{D} , its law becomes quickly close to a local equilibrium inside \mathcal{D} . This local equilibrium inside \mathcal{D} is described by a quasi-stationary distribution. In addition, starting from the quasi-stationary distribution, the first exit time from \mathcal{D} and the exit location on $\partial\mathcal{D}$ are independent, and the first exit time from \mathcal{D} is exponentially distributed. For this reason, the notion of quasi-stationary distribution is a central object to justify the use of kinetic Monte Carlo processes (also called Markov jump processes) to model the exit event from a metastable region [42, 35, 21, 1, 37].

¹Existence and uniqueness will be proved later, under additional assumptions on V , see Propositions 2.3 and 3.1.

The main results of this work are Theorem 2.4 and Theorem 3.2 which provide existence and uniqueness (in some weighted spaces) of a quasi-stationary distribution (see (1.7)) for the process (1.5) on $\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N$ (where $\mathcal{O} \subset \mathcal{O}$) when V_I is respectively a Lennard-Jones type potential and when V_I is the Coulomb potential. The results cover the case when $\overline{\mathcal{O}}$ contains some subset of singular points of V , namely some subset of $\partial\mathcal{O}$. The starting point of the proofs is [28, Theorem 2.2]. To use these results, we will in particular construct Lyapunov functions W on \mathcal{S} for such processes which provide an asymptotic return from $+\infty$. Let us mention that these Lyapunov functions are much smaller, to the best of our knowledge, than those already constructed in the literature for such processes. Indeed, they satisfy, for any $\eta \in (0, 1)$, $W \leq \exp(mH^\eta)$ on \mathcal{S} , where H is the Hamiltonian of the process (1.5). Let us also mention that since the potentials V we consider are singular and $\partial\mathcal{O} \cap \{V = +\infty\}$ is not necessarily nonempty, it turns out that most of the arguments used in [28, Section 6] do not apply here.

Remark 1.1. The long time behavior of the law of the process (1.5) has been investigated in [30, 38, 3, 6] when γ and Σ are constant, and V is \mathcal{C}^∞ on \mathcal{S} (see also [18, 19, 27, 41, 47, 10] and references therein).

Remark 1.2. From the proof of Theorem 2.4 and Theorem 3.2, we also deduce that large deviation principles hold for the non killed process (i.e. the process $(X_t, t \geq 0)$ on \mathcal{S}) with Lennard-Jones and Coulomb potential interactions, as well as the exponential convergence of its law towards its invariant measure, see Corollary 4.1.

Remark 1.3. The notion of quasi-stationary distribution has initially been introduced to investigate long time behavior of biological systems and we refer for instance to [8, 22, 9, 16, 39, 17, 23, 15, 12]. For existence and uniqueness of a quasi-stationary distribution for elliptic processes, we refer to [43, 26, 35, 32, 13, 11, 29]. See also [2, 25, 14] for general criteria implying existence uniqueness of a quasi-stationary distribution.

We refer to [28] for existence and uniqueness of a quasi-stationary distribution for the process (1.5) when the coefficients of (1.5) are continuous on \mathbb{R}^{2dN} . We also refer to [36] (see also [44, Chapter 4]) when γ and Σ are constant on \mathbb{R}^{2dN} , the drift in (1.5) is smooth on \mathbb{R}^{2dN} , and \mathcal{O} is bounded. Existence and uniqueness of quasi-stationary distribution for hypoelliptic diffusions on a bounded subdomain D of \mathbb{R}^m have also been very recently investigated in [4] when D satisfies a boundary condition (see (ii)-(a) in Theorem 1 there), and the coefficients of the diffusions are smooth and satisfy some Hörmander conditions.

1.2. Notation and definition of a quasi-stationary distribution. Let $\mathcal{B}(\mathcal{S})$ be the Borel σ -algebra of \mathcal{S} , $b\mathcal{B}(\mathcal{S})$ the space of all bounded and Borel measurable functions f on \mathcal{S} (its norm will be denoted by $f \in b\mathcal{B}(\mathcal{S}) \mapsto \|f\|_{b\mathcal{B}(\mathcal{S})} = \sup_{x \in \mathcal{S}} |f(x)|$). If $u : \mathcal{S} \rightarrow [1, +\infty)$ is a continuous function, we denote by $b_u\mathcal{B}(\mathcal{S})$ the Banach space of all $\mathcal{B}(\mathcal{S})$ -measurable functions on \mathcal{S} with norm $\|f\|_{b_u\mathcal{B}(\mathcal{S})} := \sup_{x \in \mathcal{S}} |f(x)|/u(x) < +\infty$. The function 1_K will denote the indicator function of $K \subset (\mathbb{R}^d)^N$.

Consider $(X_t, t \geq 0)$ the (strong) Markov process solution in the strong sense of the stochastic differential equation (1.5) with values in an open subset \mathcal{S} of $(\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$ (existence and uniqueness of such a process will be proved later, see Propositions 2.3

and 3.1). Its transition probability semigroup is denoted by $(P_t, t \geq 0)$ where we recall that it is defined by:

$$P_t f(\mathbf{x}) = \mathbb{E}_{\mathbf{x}}[f(X_t)],$$

for $f \in b\mathcal{B}(\mathcal{S})$ and $\mathbf{x} \in \mathcal{S}$. We will denote by $(X_t(\mathbf{x}), t \geq 0)$ the process $(X_t, t \geq 0)$ when $X_0 = \mathbf{x} \in \mathcal{S}$. Given an initial distribution ν on \mathcal{S} , we write $\mathbb{P}_{\nu}(\cdot) = \int_{\mathcal{S}} \mathbb{P}_{\mathbf{x}}(\cdot) \nu(d\mathbf{x})$. Under \mathbb{P}_{ν} , the distribution of X_0 is ν .

Now let \mathcal{D} be a non-empty subdomain of \mathcal{S} (i.e. a non-empty connected open subset of \mathcal{S}), different from \mathcal{S} . Consider the first exit time of \mathcal{D}

$$\sigma_{\mathcal{D}} := \inf\{t \geq 0, X_t \in \mathcal{D}^c\}$$

where $\mathcal{D}^c = \mathcal{S} \setminus \mathcal{D}$ is the complement of \mathcal{D} . The transition semigroup of the killed process $(X_t, 0 \leq t < \sigma_{\mathcal{D}})$ is for $t \geq 0$ and $\mathbf{x} \in \mathcal{D}$,

$$P_t^{\mathcal{D}} f(\mathbf{x}) = \mathbb{E}_{\mathbf{x}}[1_{t < \sigma_{\mathcal{D}}} f(X_t)], \quad (1.6)$$

for $f \in b\mathcal{B}(\mathcal{D})$. Let us now recall the definition of a quasi-stationary distribution.

Definition 1.4. *A quasi-stationary distribution (QSD in short) of the Markov process $(X_t, t \geq 0)$ in the domain \mathcal{D} is a probability measure on \mathcal{D} such that*

$$\mu_{\mathcal{D}}(A) = \mathbb{P}_{\mu_{\mathcal{D}}}(X_t \in A | t < \sigma_{\mathcal{D}}) = \frac{\mathbb{P}_{\mu_{\mathcal{D}}}(X_t \in A, t < \sigma_{\mathcal{D}})}{\mathbb{P}_{\mu_{\mathcal{D}}}(t < \sigma_{\mathcal{D}})}, \quad \forall t > 0, A \in \mathcal{B}(\mathcal{D}). \quad (1.7)$$

where $\mathcal{B}(\mathcal{D}) := \{A \cap \mathcal{D}; A \in \mathcal{B}(\mathcal{S})\}$.

We say that a continuous function f belongs to the extended domain $\mathbb{D}_e(\mathcal{L})$ of the generator \mathcal{L} of $(P_t, t \geq 0)$ if there is some measurable function g on \mathcal{S} such that $\int_0^t |g|(X_s) ds < +\infty, \mathbb{P}_{\mathbf{x}} - a.e.$ for all $\mathbf{x} \in \mathcal{S}$, and

$$M_t(f) = f(X_t) - f(X_0) - \int_0^t g(X_s) ds$$

is a $\mathbb{P}_{\mathbf{x}}$ -local martingale for all \mathbf{x} . Such a function g , denoted by $\mathcal{L}f$, is not unique in general. But it is unique up to the equivalence of *quasi-everywhere* (q.e.): two functions g_1, g_2 are said to be equal q.e., if $g_1 = g_2$ almost everywhere in the (resolvent) measure $R_1(\mathbf{x}, \cdot) = \int_0^{+\infty} e^{-t} P_t(\mathbf{x}, \cdot) dt$ for every $\mathbf{x} \in \mathcal{S}$ (see for instance [20, Definition (14.15)]).

Finally, we say that a class \mathcal{A} of bounded continuous functions on \mathcal{D} is *measure-separable*, if for any bounded (signed) measure ν on \mathcal{D} , if $\nu(f) = 0$ for all $f \in \mathcal{A}$, then $\nu = 0$.

1.3. Organization. The rest of the paper is organized as follows. In Section 2, we focus on Lennard-Jones type interactions (see (2.1)): we state and prove Theorem 2.4. Section 3 is dedicated to the case when V_1 is the Coulomb potential. The main result of Section 3 is Theorem 3.2. Let us mention that we treat Lennard-Jones type interactions and the Coulomb potential in two different sections mainly because the construction of the Lyapunov function is not the same (this separate treatment follows the separate treatments of [30, 38]).

2. QUASI-STATIONARY DISTRIBUTIONS FOR LENNARD-JONES TYPE INTERACTIONS

In this section, we state and prove Theorem 2.4, which is concerned with existence and uniqueness of the process (1.5) with Lennard-Jones type interactions.

2.1. Main result.

2.1.1. Lennard-Jones type interactions. Recall that $\Omega = \{y \in \mathbb{R}, y < 0\}$ if $d = 1$, and $\Omega := \{y \in \mathbb{R}^d, |y| \neq 0\}$ if $d \geq 2$. Let $\Phi_{1,I} : \Omega \rightarrow \mathbb{R}$, $B > 0$, and $\beta_1 > 0$. Define for $y \in \bar{\Omega}$:

$$V_{1,I}(y) = \begin{cases} \frac{B}{|y|^{\beta_1}} + \Phi_{1,I}(y) & \text{if } y \in \Omega \\ +\infty & \text{if } y = 0. \end{cases}$$

Recall that the potential function V_1 we consider is, for $x = (x^1, \dots, x^N) \in \bar{\mathcal{O}}$ (see (1.2)),

$$V_1(x) = \sum_{i=1}^N V_{1,c}(x^i) + \sum_{1 \leq i < j \leq N} V_{1,I}(x^i - x^j) \in \bar{\mathbb{R}}, \quad (2.1)$$

where $V_{1,c} : \mathbb{R}^d \rightarrow \mathbb{R}$ and $V_{1,I} : \bar{\Omega} \rightarrow \bar{\mathbb{R}}$. We assume the following on $V_{1,c}$ and $\Phi_{1,I}$.

Assumption (H-LJ). Let $A > 0$ and $\alpha_1 > 1$. The function $V_{1,c} \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R})$ and for some $r > 0$, it holds:

$$\forall y \in \mathbb{R}^d, |y| \geq r, \quad V_{1,c}(y) = A|y|^{\alpha_1} + \Phi_{1,c}(y),$$

where $\Phi_{1,c} \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R})$ satisfies:

$$\lim_{|y| \rightarrow +\infty} \frac{|\Phi_{1,c}(y)|}{|y|^{\alpha_1}} = \lim_{|y| \rightarrow +\infty} \frac{|\nabla \Phi_{1,c}(y)|}{|y|^{\alpha_1-1}} = \lim_{|y| \rightarrow +\infty} \frac{|\text{Hess } \Phi_{1,c}(y)|}{|y|^{\alpha_1-2}} = 0.$$

In addition, $\Phi_{1,I} : \Omega \rightarrow \mathbb{R}$ is \mathcal{C}^2 and satisfies:

$$\lim_{y \in \Omega, |y| \rightarrow 0} |y|^{\beta_1} |\Phi_{1,I}(y)| = \lim_{y \in \Omega, |y| \rightarrow 0} |y|^{\beta_1+1} |\nabla \Phi_{1,I}(y)| = \lim_{y \in \Omega, |y| \rightarrow 0} |y|^{\beta_1+2} |\text{Hess } \Phi_{1,I}(y)| = 0. \quad (2.2)$$

Finally, for some $r > 0$,

$$\Phi_{1,I}, \nabla \Phi_{1,I}, \text{ and } \text{Hess } \Phi_{1,I} \text{ are bounded on } \Omega \cap \{|y| \geq r\}. \quad (2.3)$$

Remark 2.1. The Lennard-Jones potential $V_{1,I}$ corresponds to $\beta_1 = 12$ and $\Phi_{1,I}(y) = -C/|y|^6$, $C > 0$, $y \in \Omega$. When $d \geq 3$, the Coulomb potential is also covered here by choosing $\beta_1 = d - 2$ and $\Phi_{1,I} = 0$. The Coulomb potential when $d = 1, 2$ is treated in Section 3.

In this section, we assume that **(H-LJ)** is satisfied. Recall that (see (1.1)), $\mathcal{S} = \mathcal{O} \times (\mathbb{R}^d)^N$ is the natural state space on which the evolution of the N particles can be considered. By assumption **(H-LJ)** (see (1.2)),

$$\mathcal{O} = \{x \in \bar{\mathcal{O}}, V_1(x) < \infty\}.$$

Notice also that the set \mathcal{S} is open and path connected. Let us now give some properties of V_1 which are direct consequences of **(H-LJ)** and which will be used throughout this work. Note first that $V_1 : \mathcal{O} \rightarrow \mathbb{R}$ is \mathcal{C}^2 .

Remark 2.2. We have assumed that V_1 is at least \mathcal{C}^2 on \mathcal{S} to ensure existence and uniqueness of a local strong solution to (1.5) when $V = V_1$, see indeed the proof of Proposition 2.3.

Notice also that by **(H-LJ)**, for all $\epsilon > 0$, there exist $k, K > 0$ such that for all $y \in \mathbb{R}^d$,

$$-k + \frac{A}{1+\epsilon}|y|^{\alpha_1} \leq V_{1,c}(y) \leq K + (1+\epsilon)A|y|^{\alpha_1}, \quad (2.4)$$

and, for all $y \in \Omega$,

$$-k + \frac{B}{1+\epsilon}|y|^{-\beta_1} \leq V_{1,I}(y) \leq K + (1+\epsilon)B|y|^{-\beta_1}. \quad (2.5)$$

In particular, $V_{1,c}$ and $V_{1,I}$ are lower bounded respectively on \mathbb{R}^d and on Ω . Therefore, V_1 is also lower bounded on \mathcal{O} , i.e.

$$\inf_{\mathcal{O}} V_1 > -\infty.$$

In addition, by (2.4) and (2.5), $V_{1,I}(y) \rightarrow +\infty$ ($y \in \Omega$) if and only if $|y| \rightarrow 0$, and $V_{1,c}(y) \rightarrow +\infty$ if and only if $|y| \rightarrow +\infty$. This implies that, when $x \in \mathcal{O}$ (see (2.1)):

$$V_1(x) \rightarrow +\infty \text{ iff } \begin{cases} (1) \exists i \in \{1, \dots, N\} \text{ s.t. } |x^i| \rightarrow +\infty \text{ or,} \\ (2) \text{ for some } i \neq j \in \{1, \dots, N\}, |x^i - x^j| \rightarrow 0 \end{cases}, \quad (2.6)$$

or equivalently, $V_1(x) \rightarrow +\infty$ iff either (1) $|x| \rightarrow +\infty$ or (2) $x \rightarrow \partial\mathcal{O}$ (see (1.3)), that we write $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$. In the following and up to changing V_1 into $V_1 - \inf_{\mathcal{O}} V_1 + 1$, we assume that

$$V_1 \geq 1 \text{ on } \mathcal{O}.$$

Let us denote for $(x, v) \in \mathcal{S}$,

$$\mathcal{L}_1 = \frac{\Sigma^2(x, v)}{2} \Delta_v + v \cdot \nabla_x - \nabla V_1(x) \cdot \nabla_v - \gamma(x, v) v \cdot \nabla_v, \quad (2.7)$$

the infinitesimal generator of the diffusion (1.5) when $V = V_1$. The Hamiltonian of the process (1.5) when $V = V_1$ is, for $(x, v) \in \mathcal{S}$,

$$H_1(x, v) = V_1(x) + \frac{1}{2}|v|^2 \geq 1. \quad (2.8)$$

Notice that for $(x, v) \in \mathcal{S}$, $H_1(x, v) \rightarrow +\infty$ if and only if $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$ or $|v| \rightarrow +\infty$. Existence and uniqueness of the process (1.5) on \mathcal{S} (see also [30, Proposition 2.2 and Section 4]) follows from the following result.

Proposition 2.3. *Assume that **(H-LJ)** is satisfied as well as **(Ac)** and **(A Σ)**. For all $R > 0$, the set $\{x \in \mathcal{O}, V_1(x) < R\}$ is open, bounded, and its closure is included in \mathcal{O} . Furthermore, for all $(x_0, v_0) \in \mathcal{S}$, there exists a unique pathwise solution $(X_t = (x_t, v_t), t \geq 0)$ of*

$$\begin{cases} dx_t = v_t dt, \\ dv_t = -\nabla V_1(x_t) dt - \gamma(x_t, v_t) v_t dt + \Sigma(x_t, v_t) dB_t. \end{cases} \quad (2.9)$$

with $X_0 = (x_0, v_0)$, which is moreover non-explosive and remains in \mathcal{S} for all $t \geq 0$.

Notice that by Proposition 2.3, the process (2.9) is a (strong) Markov process.

Proof. Clearly, for $R > 0$, the set $\{x \in \mathcal{O}, V_1(x) < R\}$ is open, and its closure is included in \mathcal{O} since $\partial\mathcal{O} = \{V_1 = +\infty\}$. It is bounded, by (2.6). Even if it is standard, let us write the proof of the second statement since we will need Eq. (2.12) below for further computations. By definition of H_1 (see (2.8)), for $r > 0$, the set

$$\mathcal{H}_r^1 := \{(x, v) \in \mathcal{S}, H_1(x, v) < r\}, \quad (2.10)$$

is open, bounded, and its closure is included in \mathcal{S} . Let $\mathbf{x} = (x, v) \in \mathcal{S}$ and $r_x > 0$ be such that $\mathbf{x} \in \{(x, v) \in \mathcal{S}, H_1(x, v) < r_x\}$. Since the coefficients of the stochastic differential equations (1.5) are locally Lipschitz on \mathcal{S} , for any $r \geq r_x$, there exists a unique strong solution $(X_t = (x_t, v_t), t \geq 0)$ of (2.9) with initial condition \mathbf{x} up to time

$$\tau_r(\mathbf{x}) = \inf\{t \geq 0, X_t(\mathbf{x}) \notin \mathcal{H}_r^1\}. \quad (2.11)$$

Let $\tau = \lim_{r \rightarrow +\infty} \tau_r = \sup_{r \geq r_x} \tau_r$. Then, using $(\mathbf{A}\Sigma)$ and the fact that $\gamma + \gamma^T \geq 0$ on $(\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$ (see $(\mathbf{A}\mathbf{c})$), we have for all $(x, v) \in \mathcal{S}$:

$$\mathcal{L}_1 H_1(x, v) = \frac{1}{2} dN \Sigma^2(x, v) - \gamma(x, v) v \cdot v \leq h H_1(x, v),$$

where $h = dN \Sigma^2/2$. Thus, by Itô formula, $(e^{-ht \wedge \tau_r} H_1(X_{t \wedge \tau_r}), t \geq 0)$ is a supermartingale and then:

$$\text{for } r \geq r_x : H_1(\mathbf{x}) \geq \mathbb{E}_{\mathbf{x}}[1_{\tau_r \leq t} e^{-ht \wedge \tau_r} H_1(X_{t \wedge \tau_r})] \geq e^{-ht} r \mathbb{P}_{\mathbf{x}}(\tau_r \leq t). \quad (2.12)$$

Therefore, $\mathbb{P}_{\mathbf{x}}(\tau_r \leq t) \rightarrow 0$ as $r \rightarrow +\infty$, and then $\mathbb{P}_{\mathbf{x}}(\tau > t) = 1$. That is $\mathbb{P}_{\mathbf{x}}(\tau = +\infty) = 1$. Because² $\{\tau = +\infty\} \subset \{X_t \in \mathcal{S}, \forall t \geq 0\}$, it holds $\mathbb{P}_{\mathbf{x}}(\{X_t \in \mathcal{S}, \forall t \geq 0\}) = 1$, which concludes the proof of the proposition. \square

2.1.2. Quasi-stationary distribution for Lennard-Jones type interactions. The first main result of this section concerns the existence and uniqueness of a quasi-stationary distribution of the process (2.9) in $\mathcal{D} = \mathcal{O} \times \mathbb{R}^d$ with the potential V_1 (see (2.1)).

Theorem 2.4. *Assume that $(\mathbf{H-LJ})$, (\mathbf{Ac}) , and $(\mathbf{A}\Sigma)$ are satisfied. Let \mathcal{O} be a subdomain of \mathcal{O} such that $\mathcal{O} \setminus \overline{\mathcal{O}}$ is nonempty and $\partial\mathcal{O} \cap \mathcal{O}$ is \mathcal{C}^2 . Set $\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N \subset \mathcal{S}$ (see (1.1)). Consider the process $(X_t, t \geq 0)$ solution of (2.9) with potential V_1 on \mathcal{S} (see Proposition 2.3). Let*

$$\eta_1 \in (0, 1].$$

If $\alpha_1 \in (1, 2)$, we assume in addition that $\eta_1 > (2 - \alpha_1)/\alpha_1 \in (0, 1)$. Then, there exists a continuous and unbounded Lyapunov functional $W_1 : \mathcal{S} \rightarrow [1, +\infty)$ such that $W_1 \leq \exp[mH_1^{\eta_1}]$ on \mathcal{S} , for some $m > 0$ (see Proposition 2.10 for the explicit construction of W_1) and for all $p \in (1, +\infty)$:

- (a) *There is only one QSD $\mu_{\mathcal{D}}$ of the process $(X_t, t \geq 0)$ in \mathcal{D} satisfying $\mu_{\mathcal{D}}(W_1^{1/p}) := \int_{\mathcal{D}} W_1^{1/p}(\mathbf{x}) \mu_{\mathcal{D}}(d\mathbf{x}) < +\infty$.*

²Indeed, on $\{\tau = +\infty\}$, for all $t > 0$, there exists $r > 0$ such that $t < \tau_r$. Therefore, for all $s \in [0, t]$, $X_s \in \{H_1 < r\} \subset \mathcal{S}$.

(b) There exists $\lambda_{\mathcal{D}} > 0$ such that for all $t \geq 0$, the spectral radius of $P_t^{\mathcal{D}}$ on $b_{W_1^{1/p}}\mathcal{B}(\mathcal{D})$ is given by

$$r(P_t^{\mathcal{D}}|_{b_{W_1^{1/p}}\mathcal{B}(\mathcal{D})}) = e^{-\lambda_{\mathcal{D}}t}.$$

In addition, $\mu_{\mathcal{D}}P_t^{\mathcal{D}} = e^{-\lambda_{\mathcal{D}}t}\mu_{\mathcal{D}}$, for all $t \geq 0$, and $\mu_{\mathcal{D}}(O) > 0$ for all non-empty open subsets O of \mathcal{D} . Furthermore, there is a unique continuous function $\varphi : \mathcal{D} \rightarrow \mathbb{R}$ bounded by $cW_1^{1/p}$ (for some $c > 0$) such that $\mu_{\mathcal{D}}(\varphi) = 1$ and

$$P_t^{\mathcal{D}}\varphi = e^{-\lambda_{\mathcal{D}}t}\varphi \text{ on } \mathcal{D}, \forall t \geq 0. \quad (2.13)$$

Moreover, $\varphi > 0$ everywhere on \mathcal{D} .

(c) There exist $\delta > 0$ and $C \geq 1$ such that for any initial distribution ν on \mathcal{D} with $\nu(W_1^{1/p}) < +\infty$,

$$|\mathbb{P}_{\nu}(X_t \in A | t < \sigma_{\mathcal{D}}) - \mu_{\mathcal{D}}(A)| \leq Ce^{-\delta t} \frac{\nu(W_1^{1/p})}{\nu(\varphi)}, \quad \forall A \in \mathcal{B}(\mathcal{D}), t > 0. \quad (2.14)$$

(d) $\mathbb{P}_{\mathbf{x}}(\sigma_{\mathcal{D}} < +\infty) = 1$ for all $\mathbf{x} \in \mathcal{D}$, $X_{\sigma_{\mathcal{D}}}$ and $\sigma_{\mathcal{D}}$ are $\mathbb{P}_{\mu_{\mathcal{D}}}$ -independent, and $\mathbb{P}_{\mu_{\mathcal{D}}}(t < \sigma_{\mathcal{D}}) = e^{-\lambda_{\mathcal{D}}t}$.

Notice that \mathcal{O} is not necessarily bounded in Theorem 2.4, and its closure may contain singularities of \mathbf{V} , namely some subset of $\partial\mathcal{O}$. The Lyapunov function W_1 given in (2.25) satisfies thanks to (2.31), for $(x, v) \in \mathcal{S}$,

$$W_1(x, v) = \exp[(\mathbf{a}H_1(x, v) + o(H_1(x, v)))^{\eta_1}],$$

as $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$ or $|v| \rightarrow +\infty$. If $\alpha_1 \geq 2$, there is no restriction on η_1 (i.e. one can choose any η_1 in $(0, 1]$). Notice that if \mathcal{O} is bounded, we can modify $V_{1,c}$ outside \mathcal{O} with $\alpha_1 \geq 2$, so that we can take any $\eta_1 \in (0, 1]$ such that W_1 satisfies **(C3)**. In addition, because W_1 is continuous over \mathcal{S} , the set of probability measures ν such that $\nu(W_1^{1/p}) < +\infty$ contains the set of compactly supported probability measures in \mathcal{D} (and in particular Dirac measures $\delta_{\mathbf{x}}$ with $\mathbf{x} \in \mathcal{D}$). Theorem 2.4 will be a consequence of Lemma 2.7, Corollary 2.13, and Propositions 2.9, 2.10, and 2.12 below.

Remark 2.5. Apart from the fact that V_1 is assumed to be only \mathcal{C}^2 on \mathcal{S} , Assumption **(H-LJ)** differs from those adopted in [30, Example 4.4] because (2.3) is not assumed there. We have added Assumption (2.3) so that in particular [30, Lemma A.1] implies that

$$|\text{Hess } V_1|/|\nabla V_1|^2 \rightarrow 0 \text{ as } x \rightarrow \partial\mathcal{O} \cup \{\infty\}, \quad (2.15)$$

a property we will use³. Indeed, without (2.3) one can consider, when $d = 1$ and $N = 2$, $\Phi_{1,I}(y) = y^6$ for $y < 0$, and $\alpha_1 = 2$. To simplify the computations, choose $\beta_1 = 1$, $\mathbf{B} = \mathbf{A} = 1$, and $\Phi_{1,c} \equiv 0$. Then, it holds for $x^1 < x^2 \in \mathbb{R}$, $V_1(x^1, x^2) = (x^1)^2 + (x^2)^2 + 1/(x_1 - x_2) + (x^1 - x^2)^6$. Thus, for $x^1 < x^2 \in \mathbb{R}$:

$$\partial_1^2 V_1(x^1, x^2) = 2 + \frac{2}{(x_1 - x_2)^3} + 30(x^1 - x^2)^4.$$

Set $x^2 = 0$ and $x^1 = -\lambda$, for $\lambda > 0$. Then, one has $\partial_1^2 V_1(-\lambda, 0) \sim 30\lambda^4$, when $\lambda \rightarrow +\infty$. Then, we cannot conclude with [30, Lemma A.1] that $|\partial_1^2 V_1(-\lambda, 0)|/|\nabla V_1(-\lambda, 0)|^2 \rightarrow 0$

³Eq. (2.3) also ensures that $V_{1,I}$ is lower bounded (see (2.5)), and Lemma A.1 in [30] holds when **(HLJ)** is satisfied (see Remark 2.6).

as $\lambda \rightarrow +\infty$, since $\alpha_1 - 1 = 1$ here. However, when assuming (2.3), Eq. (2.30) below holds, and then [30, Lemma A.1] implies that (2.15) holds. Assumption (2.3) is natural since it states that the interaction potential does not blow up when the particles are far from each other (this the case for the potential functions of interest, see Remark 2.1).

Remark 2.6. Let us explain why [30, Lemma A.1] (that we will use) is valid when **(H-LJ)** holds. Lemma A.1 in [30] is proved there when $\Phi_{1,c} \equiv 0$ and $\Phi_{1,I} \equiv 0$. Fix $C > 0$. By (2.3), for all $r > 0$, there exists $m > 0$, for all $y \in \Omega$,

$$\frac{C}{|y|^{\beta_1+1}} - |\nabla \Phi_{1,I}(y)| \geq \frac{1_{|y| \leq r}}{|y|^{\beta_1+1}} \left[C - |y|^{\beta_1+1} |\nabla V_{1,I}(y)| \right] - m.$$

Then, by (2.2), choosing $r > 0$ small enough, there exists $m > 0$, $C/|y|^{\beta_1+1} - |\nabla \Phi_{1,I}(y)| \geq C/(2|y|^{\beta_1+1}) - m$. Similarly, one has $C|y|^{\alpha_1-1} - |\nabla \Phi_{1,c}(y)| \geq C|y|^{\alpha_1-1}/2 - R$ for some $R > 0$ and all $y \in \mathbb{R}^d$. Thus, [30, Lemma A.1] holds under **(H-LJ)**.

2.2. Proof of Theorem 2.4. The proof of Theorem 2.4 is based on the recent results from [28].

2.2.1. Result from [28]. Let us recall the previous result from [28]. We consider in this section, the framework of Section 1.2. Introduce the following set of assumptions:

- (C1) There exists $t_0 > 0$ such that for each $t \geq t_0$, P_t is strong Feller, i.e. $P_t f$ is continuous on \mathcal{S} for any $f \in b\mathcal{B}(\mathcal{S})$.
- (C2) For every $T > 0$, $\mathbf{x} \mapsto \mathbb{P}_{\mathbf{x}}(X_{[0,T]} \in \cdot)$ (the law of $X_{[0,T]} := (X_t)_{t \in [0,T]}$) is continuous from \mathcal{S} to the space $\mathbf{M}_1(\mathcal{C}^0([0,T], \mathcal{S}))$ of probability measures on $\mathcal{C}^0([0,T], \mathcal{S})$, equipped with the weak convergence topology.
- (C3) There exist a continuous function $W : \mathcal{S} \rightarrow [1, +\infty)$, belonging to the extended domain $\mathbb{D}_e(\mathcal{L})$, two sequences of positive constants (r_n) and (b_n) where $r_n \rightarrow +\infty$, and an increasing sequence of compact subsets (K_n) of \mathcal{S} , such that

$$-\mathcal{L}W(\mathbf{x}) \geq r_n W(\mathbf{x}) - b_n \mathbf{1}_{K_n}(\mathbf{x}), \text{ q.e.}$$

Let \mathcal{D} be a nonempty subdomain of \mathcal{S} different from \mathcal{S} . Assume in addition that the killed process $(X_t, 0 \leq t < \sigma_{\mathcal{D}})$ satisfies:

- (C4) For $t \geq 0$, $P_t^{\mathcal{D}}$ is weakly Feller, i.e. for a measure-separable class \mathcal{A} of continuous bounded functions f with support contained in \mathcal{D} , $P_t^{\mathcal{D}} f$ is continuous on \mathcal{D} .
- (C5) $(P_t^{\mathcal{D}}, t \geq 0)$ is topologically irreducible on \mathcal{D} , that is: there exists $t_1 > 0$ such that for all $t \geq t_1$, for all $\mathbf{x} \in \mathcal{D}$ and non-empty open subsets O of \mathcal{D} , $P_t^{\mathcal{D}}(\mathbf{x}, O) > 0$ (where $P_t^{\mathcal{D}}(\mathbf{x}, O) := \mathbb{P}_{\mathbf{x}}(X_t \in O, t < \sigma_{\mathcal{D}})$). In addition, there exists $\mathbf{x}_0 \in \mathcal{D}$ such that $\mathbb{P}_{\mathbf{x}_0}(\sigma_{\mathcal{D}} < +\infty) > 0$.

Notice that (C1), (C2), and (C3) are independent of the domain \mathcal{D} . Let us recall [28, Theorem 2.2] when one considers the process (1.5) on \mathcal{S} .

Lemma 2.7. *If (C1), (C2), (C3), (C4), and (C5) hold, then, items (a)→(d) in Theorem 2.4 are satisfied with W given by (C3).*

Remark 2.8. *The intuition behind the assumptions (C1)→(C5) is the following. It is now well known that a Lyapunov condition provides a spectral gap for a non killed semigroup in some weighted Banach spaces [24, 40]. Using results of [50] characterizing the essential spectral radius of a positive operator (combined with the regularity conditions*

(C1) and **(C2)** on the non killed process $(X_t, t \geq 0)$, the Lyapunov type condition **(C3)** is used in [28] to get a spectral gap for P_t^D in $b_W \mathcal{B}(\mathcal{D})$. It is also known that an irreducibility condition and a regularity condition on a non killed semigroup ensure the uniqueness of the invariant measure. It is similar for killed processes: in [28] we show that the regularity condition **(C4)** on P_t^D and the irreducibility condition **(C5)** imply that P_t^D admits a principal eigenvalue.

The purpose of the next sections is to check that **(C1)**→**(C5)** are satisfied when $\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N$ with \mathcal{O} a subdomain of \mathcal{O} (see (1.1) and the lines after).

2.2.2. Assumptions (C2) and (C3) on $(P_t, t \geq 0)$. In this section, we prove that assumptions **(C2)** and **(C3)** are satisfied for the process (2.9) with potential function V_1 (see (2.1)).

Proposition 2.9. *Assume that **(H-LJ)** is satisfied as well as **(Ac)** and **(A Σ)**. Then, Assumption **(C2)** is satisfied for the solution $(X_t, t \geq 0)$ of (2.9) on \mathcal{S} (see Proposition 2.3).*

Proof. Let $T > 0$. Let $\mathbf{x}_n \rightarrow \mathbf{x} \in \mathcal{S}$, where $(\mathbf{x}_n)_{n \geq 0}$ is a sequence in \mathcal{S} . We want to prove that $\mathbb{P}_{\mathbf{x}_n}[X_{[0,T]} \in \cdot] \rightarrow \mathbb{P}_{\mathbf{x}}[X_{[0,T]} \in \cdot]$ weakly in $\mathbf{M}_1(\mathcal{C}^0([0,T], \mathcal{S}))$ as $n \rightarrow +\infty$. To this end, we first construct a candidate limit \mathbf{P} using a compactness argument, and we then identify this limit using a martingale problem. Let $r_{\mathbf{x}} > 0$ be such that

$$\{\mathbf{x}_n, n \geq 0\} \cup \{\mathbf{x}\} \subset \mathcal{H}_{r_{\mathbf{x}}}^1 = \{(x, v) \in \mathcal{S}, H_1(x, v) < r_{\mathbf{x}}\}. \quad (2.16)$$

In what follows we consider $r \geq r_{\mathbf{x}}$.

Step 1. Construct of a candidate limit \mathbf{P} .

We claim that the sequence of probability measures $(\mathbb{P}_{\mathbf{x}_n}[X_{[0,T]} \in \cdot])_{n \geq 0}$ on $\mathcal{C}^0([0, T])$ is tight. Let us prove this claim. Recall that (see (2.11)),

$$\tau_r(\mathbf{z}) = \inf\{t \geq 0, X_t(\mathbf{z}) \notin \mathcal{H}_r^1\},$$

is the first exit time for the process (2.9) from \mathcal{H}_r^1 (see (2.10)) when $X_0 = \mathbf{z} \in \mathcal{S}$. Define for $(x, v) \in \mathcal{S}$:

$$\mathbf{b}(x, v) = \left(-\nabla V_1(x) \cdot v - \gamma(x, v) v \right), \quad (2.17)$$

which is the drift of the stochastic differential equation (2.9). Set for $r > 0$,

$$\mathbf{c}_r = \sup_{(x,v) \in \mathcal{H}_r^1} |\mathbf{b}(x, v)|.$$

Notice that \mathbf{c}_r is finite because \mathcal{H}_r^1 is bounded, with closure included in \mathcal{S} (see (2.10) and the lines below), and \mathbf{b} is locally bounded on \mathcal{S} since it is continuous on \mathcal{S} . Then, for all $n \geq 0$, $0 \leq s \leq t \leq \tau_r(\mathbf{x}_n)$, it holds:

$$\int_s^t |\mathbf{b}(x_u(\mathbf{x}_n), v_u(\mathbf{x}_n))| du \leq \mathbf{c}_r(t - s).$$

Because Σ is uniformly bounded on $(\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$ (see **(A Σ)**), using in addition the BDG inequalities and the Kolmogorov-Chentsov criterion (see for instance [31, Corollary 14.9 and Proposition 15.7]), it follows that $(\mathbb{P}_{\mathbf{x}_n}[X_{[0, T \wedge \tau_r]} \in \cdot])_{n \geq 0}$ is tight in

$\mathbf{M}_1(\mathcal{C}^0([0, T], \mathcal{S}))$, for any $r \geq r_x$ fixed. On the other hand, by (2.12) (see also (2.16)), one has for all $n \geq 0$ and $r \geq r_x$:

$$\mathbf{H}_1(\mathbf{x}_n) \geq e^{-hT} r \mathbb{P}_{\mathbf{x}_n}(T \geq \tau_r). \quad (2.18)$$

Thus, since \mathbf{H}_1 is continuous at \mathbf{x} , $\sup_{n \geq 0} \mathbb{P}_{\mathbf{x}_n}(\tau_r \leq T) \rightarrow 0$ as $r \rightarrow +\infty$. Let K be compact subset of $\mathcal{C}^0([0, T], \mathcal{S})$. Then,

$$\begin{aligned} \mathbb{P}_{\mathbf{x}_n}(X_{[0, T \wedge \tau_r]} \in K) &= \mathbb{P}_{\mathbf{x}_n}(X_{[0, T]} \in K, T < \tau_r) + \mathbb{P}_{\mathbf{x}_n}(X_{[0, \tau_r]} \in K, T \geq \tau_r) \\ &= \mathbb{P}_{\mathbf{x}_n}(X_{[0, T]} \in K) - \mathbb{P}_{\mathbf{x}_n}(X_{[0, T]} \in K, T \geq \tau_r) \\ &\quad + \mathbb{P}_{\mathbf{x}_n}(X_{[0, \tau_r]} \in K, T \geq \tau_r). \end{aligned} \quad (2.19)$$

Let $\epsilon > 0$. Take $r(\epsilon) \geq r_x$ in (2.18) such that $\sup_{n \geq 0} \mathbb{P}_{\mathbf{x}_n}(\tau_{r(\epsilon)} \leq T) \leq \epsilon/2$. For this fixed $r(\epsilon) > 0$, let $K_\epsilon \subset \mathcal{C}^0([0, T], \mathcal{S})$ be a compact set such that for all $n \geq 0$, $\inf_{n \geq 0} \mathbb{P}_{\mathbf{x}_n}(X_{[0, T \wedge \tau_{r(\epsilon)}]} \in K_\epsilon) > 1 - \epsilon/2$ (this is possible by tightness of the sequence of probability measures $(\mathbb{P}_{\mathbf{x}_n}[X_{[0, T \wedge \tau_{r(\epsilon)}]} \in \cdot])_{n \geq 0}$). By (2.19),

$$\begin{aligned} \mathbb{P}_{\mathbf{x}_n}(X_{[0, T]} \in K_\epsilon) &\geq \mathbb{P}_{\mathbf{x}_n}(X_{[0, T \wedge \tau_{r(\epsilon)}]} \in K_\epsilon) - \mathbb{P}_{\mathbf{x}_n}(X_{[0, \tau_{r(\epsilon)}]} \in K_\epsilon, T \geq \tau_{r(\epsilon)}) \\ &\geq \mathbb{P}_{\mathbf{x}_n}(X_{[0, T \wedge \tau_{r(\epsilon)}]} \in K_\epsilon) - \mathbb{P}_{\mathbf{x}_n}(T \geq \tau_{r(\epsilon)}) \end{aligned}$$

and therefore,

$$\inf_{n \geq 0} \mathbb{P}_{\mathbf{x}_n}[X_{[0, T]} \in K_\epsilon] > 1 - \epsilon.$$

Thus, by Prokhorov's theorem [31, Theorem 14.3], $(\mathbb{P}_{\mathbf{x}_n}[X_{[0, T]} \in \cdot])_{n \geq 0}$ is sequentially compact in the space $\mathbf{M}_1(\mathcal{C}^0([0, T], \mathcal{S}))$ equipped with the topology of weak convergence. Let \mathbf{P} and $(\mathbb{P}_{\mathbf{x}_{m'}}[X_{[0, T]} \in \cdot])_{m' \geq 0}$ a subsequence such that

$$\mathbb{P}_{\mathbf{x}_{m'}}[X_{[0, T]} \in \cdot] \rightarrow \mathbf{P} \text{ (weakly in } \mathbf{M}_1(\mathcal{C}^0([0, T], \mathcal{S}))) \text{ as } m' \rightarrow +\infty.$$

Denote by $Y_{[0, T]} = (Y_t, t \in [0, T])$ the canonical process associated with \mathbf{P} .

Step 2. In this step we prove that $\mathbf{P} = \mathbb{P}_x[X_{[0, T]} \in \cdot]$.

For each m' , $X_{[0, T]}(\mathbf{x}_{m'}) = (X_t(\mathbf{x}_{m'}), t \in [0, T])$ is the solution of the martingale problem associated with (2.9) and with initial condition $\mathbf{x}_{m'}$. For $f : \mathcal{S} \rightarrow \mathbb{R}$ a smooth compactly supported function, $0 \leq s \leq t \leq T$, $g : \mathcal{C}^0([0, s], \mathcal{S}) \rightarrow \mathbb{R}$ a bounded and continuous function, and $\mu \in \mathcal{C}^0([0, T], \mathcal{S})$, set

$$\Phi_{s,t}(\mu) = \left(f(\mu(t)) - f(\mu(s)) - \int_s^t \mathcal{L}_1 f(\mu(r)) dr \right) g(\mu|_{[0, s]}) \in \mathbb{R}.$$

It thus holds for all $m' \geq 0$, $\mathbb{E}[\Phi_{s,t}(X_{[0, T]}(\mathbf{x}_{m'}))] = 0$. Because $\Phi_{s,t}(\mu_{m'}) \rightarrow \Phi_{s,t}(\mu)$ when $\mu_{m'} \rightarrow \mu$ in $\mathcal{C}^0([0, T], \mathcal{S})$ (because \mathbf{b} and Σ are continuous over \mathcal{S}), and $\mathbb{P}_{\mathbf{x}_{m'}}[X_{[0, T]} \in \cdot] \rightarrow \mathbf{P}$ (weakly in $\mathbf{M}_1(\mathcal{C}^0([0, T], \mathcal{S}))$), $\Phi_{s,t}$ is bounded (by $\|g\|_{L^\infty}[2\|f\|_{L^\infty} + (t-s)(\|\nabla f\|_{L^\infty} \sup_{\mathbf{x} \in \text{supp } f} |\mathbf{b}(\mathbf{x})| + \|\Delta_v f\|_{L^\infty} \sup_{\mathbf{x} \in \text{supp } f} |\Sigma(\mathbf{x})|)]$), one has as $m' \rightarrow +\infty$

$$\mathbb{E}[\Phi_{s,t}(X_{[0, T]}(\mathbf{x}_{m'}))] \rightarrow \mathbb{E}[\Phi_{s,t}(Y_{[0, T]})].$$

Consequently, $\mathbb{E}[\Phi_{s,t}(Y_{[0, T]})] = 0$, i.e. $Y_{[0, T]}$ solves the martingale problem (2.9) with initial condition \mathbf{x} . By uniqueness of the martingale problem for (2.9)⁴, $Y_{[0, T]} = X_{[0, T]}(\mathbf{x})$

⁴Recall that pathwise uniqueness and weak existence imply uniqueness in law, and thus uniqueness of the martingale problem (see for instance [31, Theorems 18.7 and 18.14]).

in law and then, $\mathbb{P}_{x_n}[X_{[0,T]} \in \cdot] \rightarrow \mathbb{P}_x[X_{[0,T]} \in \cdot]$ weakly in $\mathbf{M}_1(\mathcal{C}^0([0,T], \mathcal{S}))$ as $n \rightarrow +\infty$. This concludes the proof of the proposition. \square

Let us now check that **(C3)** is satisfied. To this end, let us introduce some functionals. Recall that $\alpha_1 > 1$. Let

$$\eta_1 \in (0, 1].$$

and assume moreover that, if $\alpha_1 \in (1, 2)$, $\eta_1 > (2 - \alpha_1)/\alpha_1$ (notice that in this case $(2 - \alpha_1)/\alpha_1 \in (0, 1)$). Let us define for $x = (x^1, \dots, x^N) \in \mathcal{O}$,

$$\kappa(x) = \kappa_c(x) + \kappa_I(x) \quad (2.20)$$

with

$$\kappa_c(x) = \sum_{i=1}^N \mathbf{U}(x^i) \quad \text{and} \quad \kappa_I(x) = \sum_{1 \leq i < j \leq N} |x^i - x^j|^{-\beta_1},$$

and where $\mathbf{U} : \mathbb{R}^d \rightarrow \mathbb{R}^+$ is smooth and is such that,

$$\text{for all } y \in \mathbb{R}^d, |y| \geq 1, \mathbf{U}(y) = |y|^{\alpha_1 - \epsilon_1},$$

with

$$\max(0, 2 - \alpha_1) < \epsilon_1 < \min(1, \alpha_1 \eta_1). \quad (2.21)$$

The function \mathbf{U} is a confinement potential weaker than $\mathbf{V}_{1,c}$ at infinity and κ_I is the sum of the dominant parts of the interaction potential $\mathbf{V}_{1,I}$ when $x \rightarrow \partial\mathcal{O}$. The function κ is a smooth function over \mathcal{O} and is lower bounded. Notice that the function $\kappa(x) \rightarrow +\infty$ if and only if $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$ (since $\alpha_1 - \epsilon_1 > 0$).

We now claim that there exists $r > 0$ such that $|\nabla \mathbf{V}_1(x)| \geq 1$ if $\mathbf{V}_1(x) \geq r$, $x \in \mathcal{O}$. This is a simple consequence of what follows. By [30, Lemma A.1] (see also Remark 2.6), it holds for some $C > 0$ and $m > 0$, and all $x \in \mathcal{O}$:

$$|\nabla \mathbf{V}_1(x)| \geq C \left(|x|^{\alpha_1 - 1} + \sum_{1 \leq i < j \leq N} |x^i - x^j|^{-\beta_1 - 1} \right) - m. \quad (2.22)$$

Consequently, since $\alpha_1 > 1$ and $\beta_1 > 0$, $|\nabla \mathbf{V}_1(x)| \rightarrow +\infty$ (when $x \in \mathcal{O}$) if one of the two conditions (1) or (2) in (2.6) is satisfied. The reverse is also true since $|\nabla \mathbf{V}_1|$ is continuous over \mathcal{O} . Hence, one has:

$$|\nabla \mathbf{V}_1(x)| \rightarrow +\infty \text{ iff } x \rightarrow \partial\mathcal{O} \cup \{\infty\} \text{ (equivalently iff } \mathbf{V}_1(x) \rightarrow +\infty, \text{ by (2.6)).}$$

Therefore, there exists $r > 0$ such that $|\nabla \mathbf{V}_1(x)| \geq 1$ if $\mathbf{V}_1(x) \geq r$. Then, inspired by [30], we set for $x \in \mathcal{O}$:

$$\mathbf{G}_1(x) = \kappa(x) \alpha(\mathbf{V}_1(x)) \frac{\nabla \mathbf{V}_1(x)}{|\nabla \mathbf{V}_1(x)|^2}, \quad (2.23)$$

where $\alpha \in \mathcal{C}^\infty(\mathbb{R}, [0, 1])$ is such that $\alpha(u) = 1$ if $u \geq R_2$ and $\alpha(u) = 0$ if $u \leq R_1$ ($0 < R_1 < R_2$), where R_1 is chosen large enough such that $|\nabla \mathbf{V}_1(x)| \geq 1$ if $\mathbf{V}_1(x) \geq R_1$. The function \mathbf{G}_1 is then \mathcal{C}^1 over \mathcal{O} . Recall that the Hamiltonian of the process (2.9) is, for $(x, v) \in \mathcal{S}$ (see (2.8)),

$$\mathbf{H}_1(x, v) = \mathbf{V}_1(x) + \frac{1}{2}|v|^2.$$

Let us introduce for $(x, v) \in \mathcal{S}$, the modified Hamiltonian [49, Eq. (3.3)],

$$F_1(x, v) = \mathbf{a} H_1(x, v) + \mathbf{b} v \cdot G_1(x), \quad (2.24)$$

where $\mathbf{a} > 0$ and $\mathbf{b} > 0$. For all $(x, v) \in \mathcal{S}$, set:

$$W_1(x, v) = \exp \left[(F_1(x, v) + \mathbf{m})^{\eta_1} \right] \geq 1, \quad (2.25)$$

where $\mathbf{m} = -\inf_{\mathcal{S}} F_1 + 1$. It will be proved in the next proposition that F_1 is indeed lower bounded on \mathcal{S} .

When $\eta_1 = 1$ and κ is a (well chosen) constant function (i.e. κ is independent of x), it is proved in [30] that for some $\mathbf{a}, \mathbf{b} > 0$:

$$\frac{\mathcal{L}_1 W_1}{W_1} \leq -c_1 |v|^2 - c_2 \text{ on } \mathcal{S}, \quad (2.26)$$

where $c_1, c_2 > 0$. To get Assumption **(C3)**, one needs in particular a stronger version of (2.26). More precisely, we need an asymptotic return to $+\infty$ in the x -variable in the sense that we need that (2.26) holds replacing c_2 in (2.26) by a function L of $x \in \mathcal{O}$ satisfying

$$\lim_{x \in \mathcal{O}, x \rightarrow \partial \mathcal{O} \cup \{\infty\}} L(x) = +\infty.$$

It turns out that the function κ defined in (2.20) will provide this asymptotic behavior as $V_1 \rightarrow +\infty$, as shown by the following result.

Proposition 2.10. *Assume that **(H-LJ)** is satisfied as well as **(Ac)** and **(AΣ)**, and consider the solution $(X_t, t \geq 0)$ of (2.9) on \mathcal{S} (see Proposition 2.3). Then, the function F_1 is lower bounded on \mathcal{S} . Moreover, for each*

$$\eta_1 \in (0, 1] \text{ with moreover, if } \alpha_1 \in (1, 2), \eta_1 > (2 - \alpha_1)/\alpha_1,$$

*we can choose parameters $\mathbf{a}, \mathbf{b}, \epsilon_1 > 0$ (see (2.38), (2.39), (2.21)) such that **(C3)** is satisfied for the process (2.9) on \mathcal{S} with the Lyapunov function $W_1 : \mathcal{S} \rightarrow [1, +\infty)$ defined in (2.25) (see also (2.23) and (2.20)).*

Proof. We prove that F_1 is lower bounded over \mathcal{S} and that, for $\mathbf{a}, \mathbf{b} > 0$ small enough, W_1 defined by (2.25) satisfies **(C3)**. The proof is divided into two steps.

Step 1. Properties of G_1 and F_1 is lower bounded over \mathcal{S} .

In this step, $C > 0$ is a constant independent of $(x, v) \in \mathcal{S}$, which can change from one occurrence to another.

For all $x \in \mathcal{O}$, $G_1(x) \cdot \nabla V_1(x) = \kappa(x) \alpha(V_1(x))$. Therefore, if $V_1(x) \geq R_2$,

$$G_1(x) \cdot \nabla V_1(x) = \kappa(x).$$

Thus, since the closure of $\{x \in \overline{\mathcal{O}}, V_1(x) \leq R_2\}$ is a compact subset of \mathcal{O} , it holds on \mathcal{O} ,

$$\nabla V_1 \cdot G_1 \geq \kappa - M, \quad (2.27)$$

for some $M > 0$. Let us now prove that ∇G_1 is bounded over \mathcal{O} . One has on \mathcal{O} :

$$|\nabla G_1| \leq C \left[\alpha(V_1) |\kappa| \frac{|\text{Hess } V_1|}{|\nabla V_1|^2} + \alpha(V_1) \frac{|\nabla \kappa|}{|\nabla V_1|} + |\kappa| |\alpha'(V_1)| \right].$$

By definition of κ (see (2.20)), for all $x \in \mathcal{O}$,

$$|\kappa(x)| \leq C \left(1 + \sum_{i=1}^N |x^i|^{\alpha_1 - \epsilon_1} + \sum_{1 \leq i < j \leq N} |x^i - x^j|^{-\beta_1} \right) \quad (2.28)$$

and

$$|\nabla \kappa(x)| \leq C \left(1 + \sum_{i=1}^N |x^i|^{\alpha_1 - \epsilon_1 - 1} + \sum_{1 \leq i < j \leq N} |x^i - x^j|^{-\beta_1 - 1} \right). \quad (2.29)$$

Using **(H-LJ)**, for all $y \in \Omega$, $|\text{Hess } \mathbf{V}_{1,\text{I}}(y)| \leq C(1/|y|^{\beta_1+2} + 1)$ and for all $y \in \mathbb{R}^d$, $|\text{Hess } \mathbf{V}_{1,\text{c}}(y)| \leq C(|y|^{\alpha_1-2} + 1)$. Then, by definition of \mathbf{V}_1 (see (2.1)) for all $x \in \mathcal{O}$:

$$|\text{Hess } \mathbf{V}_1(x)| \leq C \left(1 + \sum_{i=1}^N |x^i|^{\alpha_1-2} + \sum_{1 \leq i < j \leq N} |x^i - x^j|^{-\beta_1-2} \right). \quad (2.30)$$

Because $\alpha'(\mathbf{V}_1) = 0$ if $\mathbf{V}_1 \geq R_2$ and since $\{x \in \mathcal{O}, \mathbf{V}_1 \leq R_2\}$ is bounded,

the function $|\kappa| |\alpha'(\mathbf{V}_1)|$ is bounded over \mathcal{O} .

A continuous function $\mathbf{Q} : \mathcal{O} \rightarrow \mathbb{R}$ is bounded if and only if it is bounded when $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$. For this reason, and using (2.29) and (2.22) together with the fact that $0 \leq \alpha \leq 1$,

$$\alpha_1 - \epsilon_1 - 1 - (\alpha_1 - 1) = -\epsilon_1 < 0 \text{ and } \beta_1 + 1 - (\beta_1 + 1) = 0,$$

the function $\alpha(\mathbf{V}_1) |\nabla \kappa| / |\nabla \mathbf{V}_1|$ is bounded over \mathcal{O} . Furthermore, using (2.28), (2.22) and (2.30) together with

$$\alpha_1 - \epsilon_1 + \alpha_1 - 2 - 2(\alpha_1 - 1) = -\epsilon_1 < 0$$

and

$$\beta_1 + \beta_1 + 2 - 2(\beta_1 + 1) = 0,$$

the function $\alpha(\mathbf{V}_1) |\kappa| |\text{Hess } \mathbf{V}_1| / |\nabla \mathbf{V}_1|^2$ is bounded over \mathcal{O} . In conclusion, the function $\nabla \mathbf{G}_1$ is bounded over \mathcal{O} .

Let us now prove that as $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$ or $v \rightarrow \{\infty\}$,

$$|v \cdot \mathbf{G}_1(x)| = o(\mathbf{H}_1(x, v)). \quad (2.31)$$

First of all, since $\alpha(\mathbf{V}_1) |\kappa| / |\nabla \mathbf{V}_1|$ is bounded over \mathcal{O} (by definition of κ_{I} and (2.22)), for all $(x, v) \in \mathcal{S}$:

$$|v \cdot \mathbf{G}_1(x)| \leq |v| \alpha(\mathbf{V}_1)(x) \frac{|\kappa_{\text{c}}(x)|}{|\nabla \mathbf{V}_1(x)|} + C|v|.$$

In addition, for all $x \in \mathcal{O}$,

$$\alpha(\mathbf{V}_1)(x) \frac{|\kappa_{\text{c}}(x)|}{|\nabla \mathbf{V}_1(x)|} \leq C(1 + |x|^{1-\epsilon_1}). \quad (2.32)$$

Let p be such that $2 < p < (\alpha_1 - \epsilon_1)/(1 - \epsilon_1)$ (notice that $(\alpha_1 - \epsilon_1)/(1 - \epsilon_1) > 2$ since $\epsilon_1 > 2 - \alpha_1$). Set $q = p/(p-1) < 2$. By Young's inequality, for all $(x, v) \in \mathcal{S}$,

$$|v \cdot \mathbf{G}_1(x)| \leq C|v| + C|v|^q + C\alpha(\mathbf{V}_1)(x) \frac{|\kappa_{\text{c}}(x)|^p}{|\nabla \mathbf{V}_1(x)|^p}. \quad (2.33)$$

In conclusion, by (2.32) and (2.33) together with the definition of V_1 (see (2.1), (2.4), and (2.5)), since $1 < q < 2$ and $p(1 - \epsilon_1) < \alpha_1 - \epsilon_1 < \alpha_1$ for all $(x, v) \in \mathcal{S}$,

$$\frac{|v \cdot G_1(x)|}{|v|^2/2 + V_1(x)} \leq \frac{C(1 + |v|^q)}{|v|^2/2 + V_1(x)} + \frac{C(1 + |x|^{1-\epsilon_1})^p}{|v|^2/2 + V_1(x)} \rightarrow 0$$

as $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$ or $v \rightarrow \{\infty\}$. This proves (2.31). Equation (2.31) implies that

$$\inf_{\mathcal{S}} F_1 > -\infty.$$

Step 2. W_1 satisfies **(C3)**.

Let us now prove that **(C3)** is satisfied for the process (2.9) on \mathcal{S} with $W_1 : \mathcal{S} \rightarrow [1, +\infty)$ (see (2.25)). Because $W_1 \in \mathcal{C}^{1,2}(\mathcal{S}, \mathbb{R})$ (i.e. W_1 is \mathcal{C}^1 in the variable x and \mathcal{C}^2 in the variable v), $W_1 \in \mathbb{D}_e(\mathcal{L})$ and $\mathcal{L}W_1 = \mathcal{L}_1W_1$ quasi-everywhere (where we recall that \mathcal{L} is the extended generator of the solution of (2.9) and \mathcal{L}_1 is defined in (2.7)). In the following, for ease of notation and with a slight abuse of notation, we denote by F_1 the function $F_1 + m$. One then has on \mathcal{S} ,

$$\begin{aligned} \frac{\mathcal{L}_1W_1}{W_1} &= \mathcal{L}_1F_1^{\eta_1} + \frac{\Sigma^2}{2} |\nabla_v F_1^{\eta_1}|^2 \\ &= \eta_1 F_1^{\eta_1-1} \mathcal{L}_1F_1 + \frac{\Sigma^2}{2} \left[\eta_1(\eta_1 - 1) |\nabla_v F_1|^2 F_1^{\eta_1-2} + \eta_1^2 F_1^{2(\eta_1-1)} |\nabla_v F_1|^2 \right] \\ &\leq \frac{\eta_1}{F_1^{1-\eta_1}} \left[\mathcal{L}_1F_1 + \eta_1 \frac{\Sigma^2}{2 F_1^{1-\eta_1}} |\nabla_v F_1|^2 \right] \\ &\leq \frac{\eta_1}{F_1^{1-\eta_1}} \left[\mathcal{L}_1F_1 + \eta_1 \frac{\Sigma^2}{2} |\nabla_v F_1|^2 \right], \end{aligned} \tag{2.34}$$

where we have used that $\eta_1 - 1 \leq 0$ and that over \mathcal{S} , $0 \leq 1/F_1^{1-\eta_1} \leq 1$ (because $F_1 \geq 1$). In addition, for all $(x, v) \in \mathcal{S}$:

$$\begin{aligned} \mathcal{L}_1F_1(x, v) + \eta_1 \frac{\Sigma^2}{2} |\nabla_v F_1|^2(x, v) &= \frac{\Sigma^2(x, v)}{2} \Delta_v F_1(x, v) + v \cdot \nabla_x F_1(x, v) \\ &\quad - [\nabla V_1(x) + \gamma(x, v)v] \cdot \nabla_v F_1(x, v) \\ &\quad + \eta_1 \frac{\Sigma^2(x, v)}{2} |\nabla_v F_1(x, v)|^2 \\ &= \mathfrak{a}Nd \frac{\Sigma^2(x, v)}{2} - \mathfrak{a}\gamma(x, v)v \cdot v + \mathfrak{b} \sum_{i,j=1}^N v^i \cdot \partial_{x_i}(G_1)^j(x) v^j \\ &\quad - \mathfrak{b}\gamma(x, v)v \cdot G_1(x) - \mathfrak{b}\nabla V_1(x) \cdot G_1(x) \\ &\quad + \eta_1 \frac{\Sigma^2(x, v)}{2} |\mathfrak{a}v + \mathfrak{b}G_1(x)|^2. \end{aligned} \tag{2.35}$$

For all $\varepsilon > 0$ and for $(x, v) \in \mathcal{S}$, one has:

$$|\mathfrak{a}v + \mathfrak{b}G_1(x)|^2 \leq \mathfrak{a}^2|v|^2(1 + \varepsilon) + \mathfrak{b}^2(1 + \varepsilon^{-1})|G_1(x)|^2. \tag{2.36}$$

By (2.32) and (2.33), and since $\alpha(\mathbf{V}_1)|\kappa_I|/|\nabla \mathbf{V}_1|$ is bounded over \mathcal{O} , $|v| \leq |v|^q + 1$, and γ is bounded over $(\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$ (see **(Ac)**), there exists $\mathbf{C}_1 > 0$ such that for $(x, v) \in \mathcal{S}$,

$$-\gamma(x, v)v \cdot \mathbf{G}_1(x) \leq \mathbf{C}_1(1 + |v|^q + |x|^{p(1-\epsilon_1)}),$$

and

$$|\mathbf{G}_1(x)|^2 \leq \mathbf{C}_1(1 + |x|^{2(1-\epsilon_1)}).$$

In addition, since $\nabla \mathbf{G}_1$ is bounded over \mathcal{O} , there exists $\mathbf{C}_2 > 0$ such that for $(x, v) \in \mathcal{S}$

$$\sum_{i,j=1}^N v^i \cdot \partial_{x_i}(\mathbf{G}_1)^j(x) v^j \leq \mathbf{C}_2 |v|^2. \quad (2.37)$$

Consequently, using also (2.27), **(Ac)**, and **(AS)**, one has for all $(x, v) \in \mathcal{S}$:

$$\begin{aligned} \mathcal{L}_1 \mathbf{F}_1(x, v) + \eta_1 \frac{\Sigma^2}{2} |\nabla_v \mathbf{F}_1|^2(x, v) &\leq \mathbf{a} N d \frac{\Sigma_\infty^2}{2} - [\mathbf{a}(\gamma^* - \mathbf{a}\eta_1 \Sigma_\infty^2(1 + \varepsilon)/2) - \mathbf{b}\mathbf{C}_2] |v|^2 \\ &\quad + \mathbf{b}\mathbf{C}_1 |v|^q + \eta_1 \mathbf{b}^2 \Sigma_\infty^2(1 + \varepsilon^{-1}) \mathbf{C}_1(1 + |x|^{2(1-\epsilon_1)})/2 \\ &\quad - \mathbf{b}(\kappa(x) - M) + \mathbf{b}\mathbf{C}_1(1 + |x|^{p(1-\epsilon_1)}). \end{aligned}$$

Choose $\mathbf{a} > 0$ such that

$$\mathbf{a} < 2\gamma^*/(\eta_1 \Sigma_\infty^2). \quad (2.38)$$

For $\varepsilon > 0$ small enough, one has $(\gamma^* - \mathbf{a}\eta_1 \Sigma_\infty^2(1 + \varepsilon)/2) > 0$, and then for $\mathbf{b} > 0$ small enough:

$$\mathbf{a}(\gamma^* - \mathbf{a}\eta_1 \Sigma_\infty^2(1 + \varepsilon)/2) - \mathbf{b}\mathbf{C}_2 > 0. \quad (2.39)$$

Fix such parameters $\mathbf{a} > 0$ and $\mathbf{b} > 0$. Since $p(1 - \epsilon_1) < \alpha_1 - \epsilon_1$ and $2(1 - \epsilon_1) < \alpha_1 - \epsilon_1$ (because $\epsilon_1 > 2 - \alpha_1$), it holds

$$\max(|x|^{2(1-\epsilon_1)}, |x|^{p(1-\epsilon_1)}) = o(\kappa_c(x)) \text{ as } x \rightarrow \partial\mathcal{O} \cup \{\infty\},$$

and since $q < 2$, $|v|^q = o(|v|^2)$ as $|v| \rightarrow +\infty$. Consequently, using in addition (2.38) and (2.39), there exist constants $\mathbf{c}_i > 0$ ($i = 1, 2, 3$) such that for all $(x, v) \in \mathcal{S}$,

$$\mathcal{L}_1 \mathbf{F}_1(x, v) + \eta_1 \frac{\Sigma^2}{2} |\nabla_v \mathbf{F}_1|^2(x, v) \leq \mathbf{c}_1 - \mathbf{c}_2 |v|^2 - \mathbf{c}_3 \kappa(x),$$

so that

$$\frac{\mathcal{L}_1 \mathbf{W}_1}{\mathbf{W}_1}(x, v) \leq -\mathbf{K}_1(x, v),$$

where

$$\mathbf{K}_1(x, v) := \frac{\eta_1 \left[-\mathbf{c}_1 + \mathbf{c}_2 |v|^2 + \mathbf{c}_3 \kappa(x) \right]}{\mathbf{F}_1^{1-\eta_1}(x, v)}.$$

The function \mathbf{K}_1 is continuous over \mathcal{S} . By (2.31), for all $(x, v) \in \mathcal{S}$, $\mathbf{F}_1(x, v) \leq M \mathbf{H}_1(x, v)$, for some $M > 0$. Consequently, it holds, for $(x, v) \in \mathcal{S}$ outside a compact set of \mathcal{S} (so that the numerator in the definition of \mathbf{K}_1 is positive):

$$\mathbf{K}_1(x, v) \geq \frac{2\eta_1 \left[-\mathbf{c}_1 + \mathbf{c}_2 |v|^2 + \mathbf{c}_3 \kappa(x) \right]}{M^{1-\eta_1} (|v|^2/2 + \mathbf{V}_1(x))^{1-\eta_1}}.$$

By definition of κ (see (2.20)) and \mathbf{V}_1 (see (2.1), (2.4), and (2.5)), since $\alpha_1 - \epsilon_1 > \alpha_1(1 - \eta_1)$ (recall that $\epsilon_1 < \alpha_1\eta_1$, see (2.21)), $\beta_1(1 - \eta_1) < \beta_1$, and $2 > 2(1 - \eta_1)$, we deduce that, for $(x, v) \in \mathcal{S}$,

$$\lim_{x \rightarrow \partial\mathcal{O} \cup \{\infty\} \text{ or } v \rightarrow \{\infty\}} \mathbf{K}_1(x, v) = +\infty,$$

or equivalently,

$$\lim_{(x, v) \in \mathcal{S}, \mathbf{H}_1(x, v) \rightarrow +\infty} \mathbf{K}_1(x, v) = +\infty.$$

Let us now consider, for $n \in \mathbb{N}$, K_n as the closure of the bounded set $\mathcal{H}_n^1 = \{(x, v) \in \mathcal{S}, \mathbf{H}_1(x, v) < n\}$, which is a compact subset of \mathcal{S} (see the lines after (2.10)). For all $(x, v) \in \mathcal{S}$, one has:

$$\begin{aligned} \frac{\mathcal{L}_1 \mathbf{W}_1}{\mathbf{W}_1}(x, v) &\leq -\mathbf{K}_1(x, v) \mathbf{1}_{\mathcal{S}/K_n}(x, v) - \mathbf{K}_1(x, v) \mathbf{1}_{K_n}(x, v) \\ &\leq -\mathbf{1}_{\mathcal{S}/K_n}(x, v) \inf_{\mathcal{S}/K_n} \mathbf{K}_1 - \mathbf{m}_1 \mathbf{1}_{K_n}(x, v) \\ &\leq -\inf_{\mathcal{S}/K_n} \mathbf{K}_1 + (\inf_{\mathcal{S}/K_n} \mathbf{K}_1 - \mathbf{m}_1) \mathbf{1}_{K_n}(x, v) \\ &\leq -\inf_{\mathcal{S}/K_n} \mathbf{K}_1 + (\inf_{\mathcal{S}/K_n} \mathbf{K}_1 - \mathbf{m}_1) \frac{\sup_{K_n} \mathbf{W}_1}{\mathbf{W}_1(x, v)} \mathbf{1}_{K_n}(x, v), \end{aligned}$$

where $\mathbf{m}_1 = \inf_{\mathcal{S}} \mathbf{K}_1$ (the function \mathbf{K}_1 is indeed lower bounded on \mathcal{S}). Set $r_n := \inf_{\mathcal{S}/K_n} \mathbf{K}_1 \rightarrow +\infty$ as $n \rightarrow +\infty$, and $b_n = (\inf_{\mathcal{S}/K_n} \mathbf{K}_1 - \mathbf{m}_1) \sup_{K_n} \mathbf{W}_1 \geq 0$. The proof of the proposition is complete. \square

2.2.3. On Assumptions (C1), (C4), and (C5). Let us now consider a subdomain \mathcal{O} of \mathcal{O} . Set

$$\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N \subset \mathcal{S}. \quad (2.40)$$

Recall that $\sigma_{\mathcal{D}}$ is the first exit time from \mathcal{D} for the process (2.9):

$$\sigma_{\mathcal{D}}(\mathbf{x}) = \inf \{t \geq 0, X_t(\mathbf{x}) \notin \mathcal{D}\} = \inf \{t \geq 0, x_t(\mathbf{x}) \notin \mathcal{O}\},$$

and that the semigroup of the killed process $(X_t, t \in [0, \sigma_{\mathcal{D}}))$ is

$$P_t^{\mathcal{D}} f(\mathbf{x}) = \mathbb{E}_{\mathbf{x}}[f(X_t) \mathbf{1}_{t < \sigma_{\mathcal{D}}}],$$

for $f \in b\mathcal{B}(\mathcal{D})$ and $\mathbf{x} \in \mathcal{D}$. Introduce the process $(X_t^0 = (x_t^0, v_t^0), t \geq 0)$ solution (in the strong sense) to the stochastic differential equation over $(\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$:

$$\begin{cases} dx_t^0 = v_t^0 dt, \\ dv_t^0 = \Sigma(x_t^0, v_t^0) dB_t. \end{cases} \quad (2.41)$$

That is $(X_t^0, t \geq 0)$ is the process (2.9) when $\mathbf{V}_1 = 0$ and $\gamma = 0$. We denote by $\sigma_{\mathcal{D}}^0$ the first exit time from \mathcal{D} for the process $(X_t^0, t \geq 0)$. For $r > 0$, we also denote by τ_r^0 the first exit time from \mathcal{H}_r^1 for the process $(X_t^0, t \geq 0)$ (i.e. $\tau_r^0 = \inf\{t \geq 0, X_t^0 \notin \mathcal{H}_r^1\}$, see (2.11)), and we set $\tau^0 = \lim_{r \rightarrow +\infty} \tau_r^0 = \sup_{r \geq 0} \tau_r^0$. Notice that $\sigma_{\mathcal{D}}^0(\mathbf{x}) \leq \tau^0(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{D}$. One has the following (local) Girsanov formula.

Proposition 2.11. *Assume that $(\mathbf{H-LJ})$, (\mathbf{Ac}) , and $(\mathbf{A}\Sigma)$ are satisfied, and consider the solution $(X_t, t \geq 0)$ of (2.9) on \mathcal{S} (see Proposition 2.3). Let \mathbf{O} be a subdomain of \mathcal{O} and set $\mathcal{D} = \mathbf{O} \times (\mathbb{R}^d)^N$ (see (2.40)). Let $f \in b\mathcal{B}(\mathcal{D})$ (see (2.40)), $t > 0$, and $\mathbf{x} \in \mathcal{D}$. Then, it holds:*

$$\mathbb{E}_{\mathbf{x}}[f(X_t)1_{t < \sigma_{\mathcal{D}}}] = \mathbb{E}_{\mathbf{x}}[f(X_t^0)1_{t < \sigma_{\mathcal{D}}^0} \mathbf{M}_t], \quad (2.42)$$

where \mathbf{M}_t is the exponential martingale defined by $\mathbf{M}_t = 1_{t < \tau^0} \exp \mathbf{F}_t^0$ with

$$\begin{aligned} \mathbf{F}_t^0 = & - \int_0^t \Sigma^{-1}(x_s^0, v_s^0) (\gamma(x_s^0, v_s^0) v_s^0 + \nabla \mathbf{V}_1(x_s^0)) dB_s \\ & - \frac{1}{2} \int_0^t |\Sigma^{-1}(x_s^0, v_s^0) [\gamma(x_s^0, v_s^0) v_s^0 + \nabla \mathbf{V}_1(x_s^0)]|^2 ds. \end{aligned} \quad (2.43)$$

Proof. Let us prove (2.42). Let \mathbf{O} be a subdomain of \mathcal{O} . For $n \in \mathbb{N}$, let \mathbf{O}_n be a bounded subdomain (i.e. non-empty, bounded, open, and connected subset) of \mathcal{O} such that $\overline{\mathbf{O}_n} \subset \mathbf{O}_{n+1}$ and $\cup_{n \geq 0} \mathbf{O}_n = \mathbf{O}$ (so $\overline{\mathbf{O}_n} \cap \partial \mathcal{O} = \emptyset$). Then, set

$$\mathcal{D}_n = \mathbf{O}_n \times \{v \in (\mathbb{R}^d)^N, |v| < n\},$$

which is bounded and with closure included in $\mathcal{S} = \mathcal{O} \times (\mathbb{R}^d)^N$. Choose a function $\psi_n \in \mathcal{C}^\infty((\mathbb{R}^d)^N, [0, 1])$ such that $\psi_n = 1$ on \mathbf{O}_n and $\psi_n = 0$ on $(\mathbb{R}^d)^N \setminus \mathbf{O}_{n+1}$ (this is possible since $\overline{\mathbf{O}_n} \subset \mathbf{O}_{n+1}$). Set

$$\mathbf{V}^{(n)} = \psi_n \mathbf{V}_1. \quad (2.44)$$

According to [49, Lemma 1.1], for all $n \geq 0$, there exists a unique non explosive strong solution $(X_t^{(n)} = (x_t^{(n)}, v_t^{(n)}), t \geq 0)$ on $(\mathbb{R}^d)^N \times (\mathbb{R}^d)^N$ of

$$\begin{cases} dx_t^{(n)} = v_t^{(n)} dt, \\ dv_t^{(n)} = -\nabla \mathbf{V}^{(n)}(x_t^{(n)}) dt - \gamma(x_t^{(n)}, v_t^{(n)}) v_t^{(n)} dt + \Sigma(x_t^{(n)}, v_t^{(n)}) dB_t, \end{cases}$$

and for all $t > 0$, $f \in b\mathcal{B}(\mathcal{D}_n)$, $\mathbf{x} \in \mathcal{D}_n$, and $n \geq 0$:

$$\mathbb{E}_{\mathbf{x}}[f(X_t^{(n)})1_{t < \sigma_{\mathcal{D}_n}^{(n)}}] = \mathbb{E}_{\mathbf{x}}[f(X_t^0)1_{t < \sigma_{\mathcal{D}_n^0}^0} \mathbf{M}_t^{(n)}],$$

where $\sigma_{\mathcal{D}_n}^{(n)} = \inf\{t \geq 0, x_t^{(n)} \notin \mathbf{O}_n\}$ is the first exit time from \mathcal{D}_n for the process $(X_t^{(n)}, t \geq 0)$ and $\mathbf{M}_t^{(n)}$ is the exponential martingale given by

$$\begin{aligned} \mathbf{M}_t^{(n)} = & \exp \left[- \int_0^t \Sigma^{-1}(x_s^0, v_s^0) (\gamma(x_s^0, v_s^0) v_s^0 + \nabla \mathbf{V}^{(n)}(x_s^0)) dB_s \right. \\ & \left. - \frac{1}{2} \int_0^t |\Sigma^{-1}(x_s^0, v_s^0) [\gamma(x_s^0, v_s^0) v_s^0 + \nabla \mathbf{V}^{(n)}(x_s^0)]|^2 ds \right]. \end{aligned}$$

Let $f \in b\mathcal{B}(\mathcal{D})$, $t > 0$, and $\mathbf{x} \in \mathcal{D}$ (in the following n is large enough such that $\mathbf{x} \in \mathcal{D}_n$). The process $(X_t, t \geq 0)$ and $(X_t^{(n)}, t \geq 0)$ coincides in law up to the first exit time from \mathcal{D}_n , i.e.

$$\mathbb{E}_{\mathbf{x}}[f(X_t)1_{t < \sigma_{\mathcal{D}_n}}] = \mathbb{E}_{\mathbf{x}}[f(X_t^{(n)})1_{t < \sigma_{\mathcal{D}_n}^{(n)}}].$$

Notice that when $t < \sigma_{\mathcal{D}_n}^0$, $\mathbf{V}^{(n)}(x_s^0) = \mathbf{V}_1(x_s^0)$ for all $s \in [0, t]$, and thus, when $t < \sigma_{\mathcal{D}_n}^0$,

$$\mathbf{M}_t^{(n)} = \exp \mathbf{F}_t^0, \text{ where } \mathbf{F}_t^0 \text{ is defined in (2.43).}$$

Using also that $\sigma_{\mathcal{D}_n}^0(\mathbf{x}) \leq \tau^0(\mathbf{x})$, we deduce that:

$$\mathbb{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}_n}}] = \mathbb{E}_{\mathbf{x}}[f(X_t^0)\mathbf{1}_{t < \sigma_{\mathcal{D}_n}^0} M_t]. \quad (2.45)$$

Notice that $\sigma_{\mathcal{D}_n}(\mathbf{x})$ is increasing in n and

$$\{t < \sigma_{\mathcal{D}}\} = \cup_{n \geq 0} \{t < \sigma_{\mathcal{D}_n}\},$$

and the same holds for $\{t < \sigma_{\mathcal{D}}^0\}$. Consequently, passing to the limit $n \rightarrow +\infty$, one has by the monotone convergence theorem, if $f \geq 0$,

$$\mathbb{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}}] = \mathbb{E}_{\mathbf{x}}[f(X_t^0)\mathbf{1}_{t < \sigma_{\mathcal{D}}^0} M_t]. \quad (2.46)$$

Equation (2.46) then extends to any $f \in b\mathcal{B}(\mathcal{D})$, by linearity.

Let us now prove that $(M_t, t \geq 0)$ is a true martingale. By definition it is a supermartingale, and it is then sufficient to prove that $\mathbb{E}_{\mathbf{x}}[M_t] = 1$ for all $\mathbf{x} \in \mathcal{S}$. Because the closure of \mathcal{H}_r^1 is compact and included in \mathcal{S} , we have from the Girsanov formula: $\mathbb{P}_{\mathbf{x}}(\tau_r > t) = \mathbb{E}_{\mathbf{x}}[M_t \mathbf{1}_{t < \tau_r^0}]$ for all $r \geq r_{\mathbf{x}}$ (this formula is obtained with the same arguments as those to get (2.45)). Since $\tau = +\infty$ a.s. (see the proof of Proposition 2.3), we then deduce that

$$1 = \mathbb{P}_{\mathbf{x}}(\tau > t) = \lim_{r \rightarrow +\infty} \mathbb{P}_{\mathbf{x}}(\tau_r > t) = \lim_{r \rightarrow +\infty} \mathbb{E}_{\mathbf{x}}[M_t \mathbf{1}_{t < \tau_r^0}] = \mathbb{E}_{\mathbf{x}}[M_t],$$

where the last equality follows from the monotone convergence theorem and $\tau_r \uparrow \tau$ as $r \rightarrow +\infty$. The proof of Proposition 2.11 is complete. \square

With Proposition 2.11, we are in position to prove the following result.

Proposition 2.12. *Assume that $(\mathbf{H-LJ})$, (\mathbf{Ac}) , and $(\mathbf{A}\Sigma)$ are satisfied, and consider the solution $(X_t, t \geq 0)$ of (2.9) on \mathcal{S} (see Proposition 2.3). Recall that \mathcal{O} is a subdomain of \mathcal{O} and $\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N$ (see (2.40)). Then:*

- (1) *The semigroup $(P_t^{\mathcal{D}}, t \geq 0)$ is topologically irreducible on \mathcal{D} .*
- (2) *If $\mathcal{O} \setminus \overline{\mathcal{O}}$ is nonempty, then for all $\mathbf{x} \in \mathcal{D}$*

$$\mathbb{P}_{\mathbf{x}}(\sigma_{\mathcal{D}} < +\infty) > 0.$$

- (3) *If $\partial\mathcal{O} \cap \mathcal{O}$ is \mathcal{C}^2 , for $t > 0$, $P_t^{\mathcal{D}}$ is strong Feller on \mathcal{D} (and thus weakly Feller on \mathcal{D}).*

Consequently, **(C4)** and **(C5)** are satisfied for the process (2.9) when $\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N$.

Proof. Let \mathcal{O} be a subdomain of \mathcal{O} .

Step 1. On Assumption **(C5)**.

Consider $\mathbf{x}_0 \in \mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N$. Let $\mathcal{O}_1 \subset \mathcal{O}$ and $\mathcal{O}_2 \subset (\mathbb{R}^d)^N$ be two nonempty open sets. Then, by choosing $f = \mathbf{1}_{\mathcal{O}_1 \times \mathcal{O}_2} \in b\mathcal{B}(\mathcal{D})$ in (2.42), it holds for all $t > 0$,

$$\mathbb{P}_{\mathbf{x}_0}(X_t \in \mathcal{O}_1 \times \mathcal{O}_2, t < \sigma_{\mathcal{D}}) > 0 \text{ if and only if } \mathbb{P}_{\mathbf{x}_0}(X_t^0 \in \mathcal{O}_1 \times \mathcal{O}_2, t < \sigma_{\mathcal{D}}^0) > 0.$$

Consider $\mathbf{x}_1 = (x_1, v_1) \in \mathcal{O}_1 \times \mathcal{O}_2$, and write $\mathbf{x}_0 = (x_0, v_0)$ with $x_0 \in \mathcal{O}$ and $v_0 \in (\mathbb{R}^d)^N$. By the first step of the proof of [28, Lemma 6.5],

$$\mathbb{P}_{\mathbf{x}_0}(X_t^0 \in \mathcal{O}_1 \times \mathcal{O}_2, t < \sigma_{\mathcal{D}}^0) > 0.$$

This implies that for all $t > 0$,

$$P_t^{\mathcal{D}}(\mathbf{x}_0, \mathcal{O}_1 \times \mathcal{O}_2) = \mathbb{P}_{\mathbf{x}_0}(X_t \in \mathcal{O}_1 \times \mathcal{O}_2, t < \sigma_{\mathcal{D}}) > 0.$$

Let us now prove that $\mathbb{P}_{\mathbf{x}_0}(\sigma_{\mathcal{D}} < t) > 0$, for all $t > 0$. Assume that $\mathcal{O} \setminus \overline{\mathcal{O}}$ is not empty. Let us then consider a nonempty open ball B_1 such that $\overline{B_1} \subset \mathcal{O} \setminus \overline{\mathcal{O}}$. Let $\mathbf{x}_1 = (x_1, v_1) \in B_1 \times (\mathbb{R}^d)^N$. By the first step of the proof of [28, Lemma 6.5], for all $t > 0$,

$$\mathbb{P}_{\mathbf{x}_0}(X_t^0 \in B_1 \times (\mathbb{R}^d)^N, t < \sigma_{\mathcal{S}}^0) > 0.$$

Then, using (2.42) with \mathcal{S} instead of \mathcal{D} , it holds for all $t > 0$ and all $\mathbf{x}_0 \in \mathcal{D}$,

$$\mathbb{P}_{\mathbf{x}_0}(X_t \in B_1 \times (\mathbb{R}^d)^N) = \mathbb{P}_{\mathbf{x}_0}(X_t \in B_1 \times (\mathbb{R}^d)^N, t < \sigma_{\mathcal{S}}) > 0,$$

since $\mathbb{P}_{\mathbf{x}_0}(t < \sigma_{\mathcal{S}}) = 1$ by Proposition 2.3. When $X_0 = \mathbf{x}_0$, $\{X_t \in B_1 \times (\mathbb{R}^d)^N\} \subset \{\sigma_{\mathcal{D}} < t\}$ by continuity of the trajectories of the process (2.9) and because $x_0 \in \mathcal{O}$ and $\overline{B_1} \subset \mathcal{O} \setminus \overline{\mathcal{O}}$. Therefore, we have

$$\mathbb{P}_{\mathbf{x}_0}(\sigma_{\mathcal{D}} < +\infty) \geq \mathbb{P}_{\mathbf{x}_0}(\sigma_{\mathcal{D}} < t) > 0.$$

Assumption **(C5)** is then satisfied for the process (2.9).

Step 2. On Assumption **(C4)**.

Let us now prove that **(C4)** is satisfied. Pick $f \in b\mathcal{B}(\mathcal{D})$, $t > 0$, and $x \in \mathcal{D}$. Let $(\mathbf{x}_n)_n$ be a sequence of elements of \mathcal{S} such that $\mathbf{x}_n \rightarrow \mathbf{x} \in \mathcal{D}$ as $n \rightarrow +\infty$. We want to prove that

$$\mathbb{E}_{\mathbf{x}_n}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}}] \rightarrow \mathbb{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}}], \text{ as } n \rightarrow +\infty. \quad (2.47)$$

Assume that $\partial\mathcal{O} \cap \mathcal{O}$ is \mathcal{C}^2 .

Case 1. Let us first consider the case when $\overline{\mathcal{O}} \subset \mathcal{O}$.

By [49, Equation (1.8)],

$$f(X_t^0(\mathbf{x}_n)) \rightarrow f(X_t^0(\mathbf{x})) \text{ in probability as } n \rightarrow +\infty.$$

Let $\psi \in \mathcal{C}^\infty((\mathbb{R}^d)^N, [0, 1])$ such that $\psi = 1$ on \mathcal{O} and $\psi = 0$ on a neighborhood of the closure of $(\mathbb{R}^d)^N \setminus \mathcal{O}$ (which is possible since $\overline{\mathcal{O}} \subset \mathcal{O}$). The function $\psi\mathbf{V}_1$ is lower bounded and \mathcal{C}^1 over $(\mathbb{R}^d)^N$. When $t < \sigma_{\mathcal{D}}^0$, $\mathbf{V}_1(x_s^0) = (\psi\mathbf{V}_1)(x_s^0)$, for all $s \in [0, t]$. Then, one can replace \mathbf{V}_1 by $\psi\mathbf{V}_1$ in the expression of F_t^0 in (2.43) when $t < \sigma_{\mathcal{D}}^0$. The function $\psi\mathbf{V}_1$ satisfies the assumptions of [49, Proposition 1.2] as well as γ and Σ (see indeed **(Ac)** and **(A Σ)**). Consequently, by [49, Equation (1.7)], one has, as $n \rightarrow +\infty$,

$$\exp F_t^0(\mathbf{x}_n) \rightarrow \exp F_t^0(\mathbf{x}) \text{ in } L^1.$$

Finally, since $\partial\mathcal{O}$ is \mathcal{C}^2 , by the first step of the proof of [28, Proposition 6.6], one has, $\mathbf{1}_{t < \sigma_{\mathcal{D}}^0(\mathbf{x}_n)} \rightarrow \mathbf{1}_{t < \sigma_{\mathcal{D}}^0(\mathbf{x})}$ in probability as $n \rightarrow +\infty$. Thus,

$$\mathbb{E}_{\mathbf{x}_n}[f(X_t^0)\mathbf{1}_{t < \sigma_{\mathcal{D}}^0} \exp F_t^0(\mathbf{x}_n)] \rightarrow \mathbb{E}_{\mathbf{x}}[f(X_t^0)\mathbf{1}_{t < \sigma_{\mathcal{D}}^0} \exp F_t^0(\mathbf{x})], \text{ as } n \rightarrow +\infty,$$

which implies (2.47) thanks to (2.42).

Case 2. Let us now consider the case when $\partial\mathcal{O} \cap \partial\mathcal{O} \neq \emptyset$.

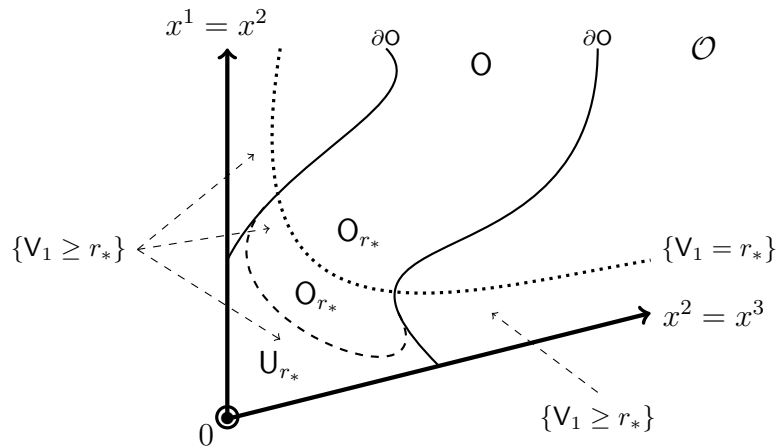
In this case, we cannot argue as previously since the situation when $x_{\sigma_{\mathcal{D}}}^0 \in \partial\mathcal{O} \cap \partial\mathcal{O}$ can occur, and $\partial\mathcal{O} \cap \partial\mathcal{O}$ is not in general \mathcal{C}^2 , a crucial condition to prove that $\mathbf{1}_{t < \sigma_{\mathcal{D}}^0(\mathbf{x}_n)} \rightarrow \mathbf{1}_{t < \sigma_{\mathcal{D}}^0(\mathbf{x})}$ in probability as $n \rightarrow +\infty$ (see indeed the first step of the proof of [28, Proposition 6.6]). To overcome this issue, we use the fact that, roughly speaking, the process $(X_t, t \geq 0)$

$$\{\mathbf{x}_n, n \geq 0\} \cup \{\mathbf{x}\} \subset \mathcal{H}_{r_x}^1 = \{(x, v) \in \mathcal{S}, H_1(x, v) < r_x\},$$
$$\sup_{n \geq 0} \mathbb{P}_{x_n}(\tau_{r_*} \leq t) \leq \frac{\epsilon}{4(1 + \|f\|_{L^\infty})} \text{ and } \mathbb{P}_x(\tau_{r_*} \leq t) \leq \frac{\epsilon}{4(1 + \|f\|_{L^\infty})}.$$
$$\mathcal{D} = \mathcal{D}_{r_*} \cup \Omega_{r_*},$$

- $\mathcal{D}_{r_*} = \mathcal{O}_{r_*} \times (\mathbb{R}^d)^N$ with \mathcal{O}_{r_*} a \mathcal{C}^2 subdomain of \mathcal{O} such that

- $\Omega_{r_*} = \mathbf{U}_{r_*} \times (\mathbb{R}^d)^N$ (where $\mathbf{U}_{r_*} = \mathbf{O} \setminus \mathbf{O}_{r_*}$) with

$$U_{r_*} \subset \{x \in \mathcal{O}, V_1(x) \geq r_*\}.$$



We refer to Figure 1 for a schematic representation of \mathcal{O}_{r_*} and \mathcal{U}_{r_*} . To end the proof of Proposition 2.12, we will treat the part \mathcal{D}_{r_*} as in the first case above, and it will thus remain to control the case when the process $(X_t, t \geq 0)$ reaches Ω_{r_*} , but reaching Ω_{r_*}

occurs with small probability. By continuity of the trajectories of the process (2.9) on \mathcal{S} , when $X_0 \in \mathcal{D}_{r_*}$ and on $\{t < \sigma_{\mathcal{D}}, t \geq \sigma_{\mathcal{D}_{r_*}}\}$,

$$\exists s \in (0, t], X_s \in \Omega_{r_*} \subset \{(x, v) \in \mathcal{S}, H_1(x, v) \geq r_*\},$$

so that $\{t < \sigma_{\mathcal{D}}, t \geq \sigma_{\mathcal{D}_{r_*}}\} \subset \{\tau_{r_*} \leq t\}$, where we recall that τ_{r_*} is defined by (2.11). Since $r_* > r_x$,

$$\{\mathbf{x}_n, n \geq 0\} \cup \{\mathbf{x}\} \subset \mathcal{D}_{r_*}.$$

Therefore, when $X_0 \in \{\mathbf{x}_n, n \geq 0\} \cup \{\mathbf{x}\}$,

$$\{t < \sigma_{\mathcal{D}}, t \geq \sigma_{\mathcal{D}_{r_*}}\} \subset \{\tau_{r_*} \leq t\}.$$

Furthermore, by (2.42), and since \mathbf{O}_{r_*} is \mathcal{C}^2 and $\overline{\mathbf{O}_{r_*}} \subset \mathcal{O}$, by the first case above, there exists $n_0 \geq 0$ such that for all $n \geq n_0$,

$$|\mathbb{E}_{\mathbf{x}_n}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}_{r_*}}}] - \mathbb{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}_{r_*}}}]| \leq \epsilon/2.$$

Then, since $\mathbf{1}_{t < \sigma_{\mathcal{D}}}\mathbf{1}_{t < \sigma_{\mathcal{D}_{r_*}}} = \mathbf{1}_{t < \sigma_{\mathcal{D}_{r_*}}}$ when $X_0 \in \mathcal{D}_{r_*}$, one has for all $n \geq n_0$,

$$\begin{aligned} & |\mathbb{E}_{\mathbf{x}_n}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}}] - \mathbb{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}}]| \\ & \leq |\mathbb{E}_{\mathbf{x}_n}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}_{r_*}}}] - \mathbb{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}_{r_*}}}]| \\ & \quad + |\mathbb{E}_{\mathbf{x}_n}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}, t \geq \sigma_{\mathcal{D}_{r_*}}}] - \mathbb{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}, t \geq \sigma_{\mathcal{D}_{r_*}}}]| \\ & \leq \epsilon/2 + \|f\|_{L^\infty} [\mathbb{P}_{\mathbf{x}_n}(t < \sigma_{\mathcal{D}}, t \geq \sigma_{\mathcal{D}_{r_*}}) + \mathbb{P}_{\mathbf{x}}(t < \sigma_{\mathcal{D}}, t \geq \sigma_{\mathcal{D}_{r_*}})] \\ & \leq \epsilon/2 + \|f\|_{L^\infty} [\mathbb{P}_{\mathbf{x}_n}(\tau_{r_*} \leq t) + \mathbb{P}_{\mathbf{x}}(\tau_{r_*} \leq t)] \\ & \leq \epsilon. \end{aligned}$$

Consequently, $\mathbb{E}_{\mathbf{x}_n}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}}] \rightarrow \mathbb{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}}]$ as $\mathbf{x}_n \rightarrow \mathbf{x} \in \mathcal{D}$. In conclusion, Assumption **(C4)** is satisfied when $\partial\mathbf{O} \cap \mathcal{O}$ is \mathcal{C}^2 . This concludes the proof of Proposition 2.12. \square

Choosing $\mathbf{O} = \mathcal{O}$ in items (1) and (3) in Proposition 2.12, we have the following direct consequence of Proposition 2.12 together with the fact that $\mathbb{P}_{\mathbf{x}}(t < \sigma_{\mathcal{S}}) = 1$, for all $\mathbf{x} \in \mathcal{S}$, by Proposition 2.3.

Corollary 2.13. *Assume that **(H-LJ)**, **(Ac)**, and **(A Σ)** are satisfied. Consider the solution $(X_t, t \geq 0)$ of (2.9) on \mathcal{S} (see Proposition 2.3). Then, for all $t > 0$, P_t is strong Feller, i.e. Assumption **(C1)** is satisfied. In addition, $(P_t, t \geq 0)$ is topologically irreducible on \mathcal{S} .*

When γ and Σ are constant, and \mathbf{V} is \mathcal{C}^∞ on \mathcal{S} , this results is a direct consequence of the Hörmander's hypoellipticity theorem (see for instance [30, Proposition 2.5]).

Let us now recall that Theorem 2.4 is a consequence of Lemma 2.7, Corollary 2.13, and Propositions 2.9, 2.10, and 2.12. The proof of Theorem 2.4 is thus complete.

Remark 2.14. Notice that for Corollary 2.13 and Propositions 2.9 and 2.12, we can replace **(Ac)** by the less stringent assumption $\gamma : (\mathbb{R}^d)^N \times (\mathbb{R}^d)^N \rightarrow \mathbf{M}_{Nd}(\mathbb{R})$ is a locally Lipschitz function such that for some $m > 0$, $\forall x, v \in (\mathbb{R}^d)^N : \frac{1}{2}[\gamma(x, v) + \gamma^T(x, v)] \geq -m I_{(\mathbb{R}^d)^N}$.

3. QUASI-STATIONARY DISTRIBUTIONS FOR COULOMB INTERACTIONS

In this section we consider N particles in \mathbb{R}^d interacting through the Coulomb potential. Recall that the case of Coulomb potential when $d \geq 3$ is covered by Theorem 2.4 (see Remark 2.1), and therefore, it remains to deal with the case when $d = 1, 2$. Thus, in this section, we assume that

$$d \in \{1, 2\}.$$

The purpose of this section is to prove Theorem 3.2 below which provides existence and uniqueness of a quasi-stationary distribution for the process (1.5) with Coulomb type interactions when $d = 1, 2$. Let us introduce more precisely the process we consider. For $x = (x^1, \dots, x^N) \in \overline{\mathcal{O}}$ (see (1.2)), set:

$$V_2(x) = \sum_{i=1}^N V_{2,c}(x^i) + \sum_{1 \leq i < j \leq N} V_{2,I}(x^i - x^j) \in \overline{\mathbb{R}}, \quad (3.1)$$

where $V_{2,I}$ is the potential:

$$\text{for all } y \in \mathbb{R}^d: V_{2,I}(y) = -\log |y| \text{ if } y \neq 0, \text{ else } V_{2,I}(y) = +\infty, \quad (3.2)$$

where $V_{2,c} : (\mathbb{R}^d)^N \rightarrow \mathbb{R}$ is a confining potential which satisfies:

Assumption (H-C). *Let $A > 0$ and $\alpha_2 \geq 2$. The function $V_{2,c} \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R})$ and for some $r > 0$, it holds:*

$$\forall y \in \mathbb{R}^d, |y| \geq r, V_{2,c}(y) = A|y|^{\alpha_2} + \Phi_{2,c}(y),$$

where $\Phi_{2,c} \in \mathcal{C}^2(\mathbb{R}^d, \mathbb{R})$ satisfies: $\lim_{|y| \rightarrow +\infty} \frac{|\Phi_{2,c}(y)|}{|y|^{\alpha_2}} = \lim_{|y| \rightarrow +\infty} \frac{|\nabla \Phi_{2,c}(y)|}{|y|^{\alpha_2-1}} = 0$.

Let us mention that here we have assumed that $\alpha_2 \geq 2$ in **(H-C)** (whereas α_1 was chosen larger than 1 in **(H-LJ)**), which is explained by the specific choice of Lyapunov function later. Notice that for some $M > 0$,

$$A|y|^{\alpha_2}/2 - M \leq V_{2,c}(y) \leq 2A|y|^{\alpha_2} + M \text{ for all } y \in \mathbb{R}^d. \quad (3.3)$$

When $d = 2$, $V_{2,I}$ is the Coulomb potential, and when $d = 1$, $V_{2,I}$ corresponds to a log singularity pairwise potential. Notice that since $V_{2,I}(y) = V_{2,I}(-y)$ for all $y \neq 0$, V_2 also writes

$$V_2(x) = \sum_{i=1}^N V_{2,c}(x^i) + \frac{1}{2} \sum_{1 \leq i \neq j \leq N} V_{2,I}(x^i - x^j), \quad x \in \mathcal{O}.$$

3.1. Properties of V_2 and definition of the process. Recall $d = 1, 2$. Let us give some properties of V_2 . Note first that $V_2 : \mathcal{S} \rightarrow \mathbb{R}$ is a \mathcal{C}^2 function. In addition, V_2 is lower bounded on \mathcal{S} , since, using the inequality $\log z \leq z$ for $z > 0$, and (3.3), one has for all $x \in \mathcal{O}$:

$$V_2(x) \geq \frac{A}{2} \sum_{i=1}^N |x^i|^{\alpha_2} - MN - \sum_{i < j} |x^i - x^j| \geq \frac{A}{2} \sum_{i=1}^N |x^i|^{\alpha_2} - C|x| - MN. \quad (3.4)$$

Moreover, for all $x \in \mathcal{O}$, $V_2(x) \geq -MN - \sum_{i < j} \log(|x^i - x^j|)$. Consequently, $V_2(x) \rightarrow +\infty$ as $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$ (see (1.3)), $x \in \mathcal{O}$. Since $V_{2,c}$ is continuous on \mathcal{O} , the reverse is also true, that is: when $x \in \mathcal{O}$,

$$V_2(x) \rightarrow +\infty \text{ iff } x \rightarrow \partial\mathcal{O} \cup \{\infty\}. \quad (3.5)$$

Let us now introduce

$$\mathcal{L}_2 = \frac{\Sigma^2(x, v)}{2} \Delta_v + v \cdot \nabla_x - \nabla V_2(x) \cdot \nabla_v - \gamma(x, v) v \cdot \nabla_v,$$

the infinitesimal generator of the diffusion (1.5) when $V = V_2$. The Hamiltonian of the process (1.5) when $V = V_2$ is, for $(x, v) \in \mathcal{S}$,

$$H_2(x, v) = V_2(x) + \frac{1}{2}|v|^2. \quad (3.6)$$

Note that $H_2(x, v) \rightarrow +\infty$ if and only if $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$ or $|v| \rightarrow +\infty$. In the following, we assume (up to considering $V_2 - \inf_{\mathcal{O}} V_2 + 1$) that

$$V_2 \geq 1 \text{ on } \mathcal{O},$$

so that $H_2 \geq 1$ on \mathcal{S} . We have (see also [38, Proposition 2.4]):

Proposition 3.1. *Assume $d = 1, 2$ and **(H-C)**. Assume also that **(Ac)** and **(A Σ)** are satisfied. For all $R > 0$, the set $\{x \in \mathcal{O}, V_2(x) < R\}$ is open, bounded, and its closure is included in \mathcal{O} . Furthermore, for all $(x_0, v_0) \in \mathcal{S} = \mathcal{O} \times (\mathbb{R}^d)^N$, there exists a unique pathwise solution $(X_t = (x_t, v_t), t \geq 0)$ of*

$$\begin{cases} dx_t = v_t dt, \\ dv_t = -\nabla V_2(x_t) dt - \gamma(x_t, v_t) v_t dt + \Sigma(x_t, v_t) dB_t. \end{cases} \quad (3.7)$$

with $X_0 = (x_0, v_0)$, which is moreover non-explosive and remains in \mathcal{S} for all $t \geq 0$.

Proof. Thanks to (3.5), and because V_2 is \mathcal{C}^2 and lower bounded on \mathcal{O} , the proof is the same as the proof of Proposition 2.3. Let us mention that we have as in Proposition 2.3,

$$H_2(x) \geq e^{-ht} r \mathbb{P}_x(\tau_r \leq t), \quad (3.8)$$

for some $h > 0$ and where $\tau_r(x) = \inf\{t \geq 0, X_t(x) \notin \mathcal{H}_r^2\}$ and $\mathcal{H}_r^2 = \{(x, v) \in \mathcal{S}, H_2(x, v) < r\}$, $r > 0$. \square

By Proposition 3.1, the process (3.7) is a (strong) Markov process.

3.2. Quasi-stationary distribution for Coulomb interactions. The main result of this section is the following.

Theorem 3.2. *Assume $d = 1, 2$ and **(H-C)**. Assume also that **(Ac)** and **(A Σ)** are satisfied. Let \mathcal{O} be a subdomain of \mathcal{O} such that $\mathcal{O} \setminus \overline{\mathcal{O}}$ is nonempty and $\partial\mathcal{O} \cap \mathcal{O}$ is \mathcal{C}^2 . Set $\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N$. Then, for each $\eta_2 \in (0, 1]$, there exists a continuous and unbounded Lyapunov functional $W_2 : \mathcal{S} \rightarrow [1, +\infty)$ such that $W_2 \leq \exp[mH_2^{\eta_2}]$ on \mathcal{S} , for some $m > 0$ (see Proposition 3.3 for the explicit construction of W_2), and the statements of items (a) \rightarrow (d) in Theorem 2.4 are valid for the process (3.7) on \mathcal{S} (see Proposition 3.1) and with the Lyapunov function W_2 (in place of W_1 there).*

When $\alpha_2 > 2$, by (3.12), the Lyapunov function W_2 defined in (3.11) satisfies, for $(x, v) \in \mathcal{S}$,

$$W_2(x, v) = \exp \left[\left(\mathbf{a} H_2(x, v) + o(H_2(x, v)) \right)^{\eta_2} \right],$$

as $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$ or $v \rightarrow \{\infty\}$. The o above is O when $\alpha_2 = 2$. Let us also mention that there is no restriction on η_2 (i.e. one can choose any η_2 in $(0, 1]$).

3.3. Proof of Theorem 3.2. To prove Theorem 3.2, we use Lemma 2.7. To this end, we need to check that the assumptions **(C1)**–**(C5)** are satisfied for the process (3.7) with potential V_2 when $\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N$ with \mathcal{O} a subdomain of \mathcal{O} such that $\mathcal{O} \setminus \overline{\mathcal{O}}$ is nonempty and $\partial\mathcal{O} \cap \mathcal{O}$ is \mathcal{C}^2 . It is clear that, in view of their proofs, Corollary 2.13, Proposition 2.9, and Proposition 2.12 are still valid for the process (3.7) on \mathcal{S} . It thus just remains to prove **(C3)** for such a process.

Notice first that if we choose as we did in the previous section, a functional of the form $G = \kappa \alpha(V_2) \nabla V_2 / |\nabla V_2|^2$, because here the function $|\text{Hess } V_2| / |\nabla V_2|^2$ does not converge to 0 as $x \rightarrow \partial\mathcal{O}$ (as already observed in [38]), it will not be possible to take a function κ growing at infinity as $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$. Let us rather consider the function $G_2 = ((G_2)^1, \dots, (G_2)^N)^T \in (\mathbb{R}^d)^N$ constructed in [38] which is defined as follows: for $x = (x^1, \dots, x^N) \in \mathcal{O}$ and $i \in \{1, \dots, N\}$, set:

$$(G_2)^i(x) = -\mathbf{b} \sum_{j=1, j \neq i}^N \frac{x^i - x^j}{|x^i - x^j|} + \mathbf{c} x^i,$$

where $\mathbf{b} > 0$ and $\mathbf{c} > 0$ will be chosen later. Let us introduce for $(x, v) \in \mathcal{S}$, the modified Hamiltonian $F_2(x, v) = \mathbf{a} H_2(x, v) + v \cdot G_2(x)$, where $\mathbf{a} > 0$ will be chosen later. Notice that for all $i = 1, \dots, N$ and all $x \in \mathcal{O}$,

$$|(G_2)^i(x)| \leq \mathbf{b}N + \mathbf{c}|x^i|. \quad (3.9)$$

Then, by **(H-C)** and using (3.4), one has for $(x, v) \in \mathcal{S}$:

$$\begin{aligned} F_2(x, v) &\geq \mathbf{a}(V_2(x) + |v|^2/2) - \sum_{i=1}^N |v^i| |(G_2)^i(x)| \\ &\geq \frac{|v|^2}{2} (\mathbf{a} - \mathbf{c}) - \mathbf{b}N \sum_{i=1}^N |v^i| + \sum_{i=1}^N (\mathbf{a}A|x^i|^{\alpha_2}/2 - \mathbf{c}|x^i|^2/2) - \mathbf{a}C|x| - \mathbf{a}MN. \end{aligned}$$

Then, if

$$\mathbf{c} < 1_{\alpha_2=2} \min(\mathbf{a}A, \mathbf{a}) + 1_{\alpha_2>2} \mathbf{a} \quad (3.10)$$

the function F_2 is lower bounded on \mathcal{S} . Finally, set for all $(x, v) \in \mathcal{S}$:

$$W_2(x, v) = \exp \left[\left(F_2(x, v) - \inf_{\mathcal{S}} F_2 + 1 \right)^{\eta_2} \right] \geq 1. \quad (3.11)$$

where

$$\eta_2 \in (0, 1].$$

When $\alpha_2 > 2$ in **(H-C)**, using (3.9) and Young's inequality with $p \in (2, \alpha_2)$ (so that $q = p/(p-1) < 2$), for $(x, v) \in \mathcal{S}$,

$$v \cdot G_2(x, v) = o(H_2(x, v)) \quad \text{as } x \rightarrow \partial\mathcal{O} \cup \{\infty\} \text{ or } v \rightarrow \{\infty\}. \quad (3.12)$$

If $\alpha_2 = 2$, the o in (3.12) is O .

Proposition 3.3. *Assume $d = 1, 2$ and **(H-C)**. For each $\eta_2 \in (0, 1]$, we can choose parameters $\mathbf{a}, \mathbf{b}, \mathbf{c} > 0$ (see more precisely (3.10), (3.13), (3.14) (3.15)), such that Assumption **(C3)** is satisfied for the process (3.7) on \mathcal{S} with the Lyapunov function $\mathbf{W}_2 : \mathcal{S} \rightarrow [1, +\infty)$ defined in (3.11).*

Proof. Because $\mathbf{W}_2 \in \mathcal{C}^{1,2}(\mathcal{S})$, $\mathbf{W}_2 \in \mathbb{D}_e(\mathcal{L})$ and $\mathcal{L}\mathbf{W}_2 = \mathcal{L}_2\mathbf{W}_2$ quasi-everywhere. For ease of notation and with a slight abuse of notation, we will denote by \mathbf{F}_2 the function $\mathbf{F}_2 - \inf_{\mathcal{S}} \mathbf{F}_2 + 1$. The same computations as those to get (2.34) imply that on \mathcal{S} ,

$$\frac{\mathcal{L}_2\mathbf{W}_2}{\mathbf{W}_2} \leq \frac{\eta_2}{\mathbf{F}_2^{1-\eta_2}} \left[\mathcal{L}_2\mathbf{F}_2 + \eta_2 \frac{\Sigma^2}{2} |\nabla_v \mathbf{F}_2|^2 \right].$$

Using **(Ac)** and (3.9), there exists $\mathbf{K}_\gamma > 0$ depending only on γ , such that for all $(x, v) \in \mathcal{S}$,

$$-\gamma(x, v) v \cdot \mathbf{G}_2(x) \leq \mathbf{K}_\gamma [\mathbf{b}N|v| + \mathbf{c}|v||x|].$$

Then, one has, with the almost identical computations to those leading to (2.35), for all $(x, v) \in \mathcal{S}$, using **(A Σ)** and **(Ac)**:

$$\begin{aligned} \mathcal{L}_2\mathbf{F}_2(x, v) + \eta_2 \frac{\Sigma^2}{2} |\nabla_v \mathbf{F}_2|^2(x, v) &= \mathbf{a}Nd \frac{\Sigma^2(x, v)}{2} - \mathbf{a}\gamma(x, v) v \cdot v \\ &\quad + \sum_{i=1}^N v^i \cdot \partial_{x_i} \sum_{j=1}^N (\mathbf{G}_2)^j(x) v^j - \gamma(x, v) v \cdot \mathbf{G}_2(x) \\ &\quad - \nabla \mathbf{V}_2(x) \cdot \mathbf{G}_2(x) + \eta_2 \frac{\Sigma^2(x, v)}{2} |\mathbf{a}v + \mathbf{G}_2(x)|^2 \\ &\leq \mathbf{a}Nd \frac{\Sigma_\infty^2}{2} - \mathbf{a}\gamma^*|v|^2 + \sum_{i,j=1}^N v^i \cdot \partial_{x_i} (\mathbf{G}_2)^j(x) v^j + \mathbf{b}N\mathbf{K}_\gamma|v| \\ &\quad + \mathbf{c}\mathbf{K}_\gamma|v||x| - \nabla \mathbf{V}_2(x) \cdot \mathbf{G}_2(x) + \eta_2 \frac{\Sigma_\infty^2}{2} |\mathbf{a}v + \mathbf{G}_2(x)|^2. \end{aligned}$$

In addition, one has:

$$\begin{aligned} \frac{\Sigma_\infty^2}{2} |\mathbf{a}v + \mathbf{G}_2(x)|^2 &\leq \frac{\Sigma_\infty^2}{2} [2\mathbf{a}^2|v|^2 + 2|\mathbf{G}_2(x)|^2] \leq \mathbf{a}^2\Sigma_\infty^2|v|^2 + \Sigma_\infty^2 \sum_{i=1}^N |(\mathbf{G}_2)^i(x)|^2 \\ &\leq \mathbf{a}^2\Sigma_\infty^2|v|^2 + \Sigma_\infty^2 \sum_{i=1}^N [2\mathbf{b}^2N^2 + 2\mathbf{c}^2|x^i|^2] \\ &\leq \mathbf{a}^2\Sigma_\infty^2|v|^2 + 2\mathbf{c}^2\Sigma_\infty^2|x|^2 + 2\mathbf{b}^2N^3\Sigma_\infty^2. \end{aligned}$$

Furthermore, by **(H-C)**, $|\nabla \mathbf{V}_{2,c}(y)| \leq C(1 + |y|^{\alpha_2-1})$ and $\nabla \mathbf{V}_{2,c}(y) \cdot y \geq \alpha_2 \mathbf{A}|y|^{\alpha_2}/2 - M$, for some $M, C > 0$ and all $y \in \mathbb{R}^d$. Thus, by following the computations made in [38, Section 4]⁵ (notice that the computations there also works when $d = 1$), it holds for all $(x, v) \in \mathcal{S}$,

$$\sum_{i,j=1}^N v^i \cdot \partial_{x_i} (\mathbf{G}_2)^j(x) v^j \leq \mathbf{c}|v|^2,$$

⁵See more precisely the the computations for the terms $\mathbf{p} \cdot \nabla_{\mathbf{q}} \Psi$ and $-\nabla_{\mathbf{q}} U \cdot \nabla_{\mathbf{p}} \Psi$ there.

and, denoting by $m = \alpha_2 A/4$,

$$-\nabla V_2(x) \cdot G_2(x) \leq -\mathfrak{c}m|x|_{\alpha_2} - C_0 \mathfrak{b} \sum_{i \neq j} \frac{1}{|x^i - x^j|} + C_1,$$

for some finite constant $C_0, C_1 > 0$ and where $|x|_{\alpha_2} := \sum_i |x^i|^{\alpha_2}$. Therefore, since $|x|^2 \leq |x|_{\alpha_2} + 1$, for all $(x, v) \in \mathcal{S}$,

$$\begin{aligned} \mathcal{L}_2 F_2(x, v) + \eta_2 \frac{\Sigma^2}{2} |\nabla_v F_2|^2(x, v) &\leq (\mathfrak{c} - \mathfrak{a}(\gamma^* - \mathfrak{a}\eta_2 \Sigma_\infty^2))|v|^2 + \mathfrak{c}K_\gamma |v||x| + \mathfrak{b}K_\gamma N|v| \\ &\quad - \mathfrak{c}(m - 2\eta_2 \mathfrak{c} \Sigma_\infty^2)|x|_{\alpha_2} - C_0 \mathfrak{b} \sum_{i \neq j} \frac{1}{|x^i - x^j|} + C_2, \end{aligned}$$

for some constant $C_2 > 0$. Thus, for all $\epsilon > 0$, it holds for $(x, v) \in \mathcal{S}$:

$$\begin{aligned} \mathcal{L}_2 F_2(x, v) + \eta_2 \frac{\Sigma^2}{2} |\nabla_v F_2|^2(x, v) &\leq \left[\mathfrak{c} + \epsilon - \mathfrak{a}(\gamma^* - \mathfrak{a}\eta_2 \Sigma_\infty^2) \right] |v|^2 + \mathfrak{b}K_\gamma N|v| \\ &\quad + \left[\mathfrak{c}^2 K_\gamma^2 / (4\epsilon) - \mathfrak{c}(m - \eta_2 \mathfrak{c} \Sigma_\infty^2) \right] |x|_{\alpha_2} \\ &\quad - C_0 \mathfrak{b} \sum_{i \neq j} \frac{1}{|x^i - x^j|} + C_2. \end{aligned}$$

Fix $\mathfrak{b} > 0$. Choose first $\mathfrak{a} > 0$ sufficiently small such that

$$\mathfrak{a} < \gamma^* / (\eta_2 \Sigma_\infty^2). \quad (3.13)$$

Then, take $\epsilon > 0$ sufficiently small such that

$$\epsilon - \mathfrak{a}(\gamma - \mathfrak{a}\eta_2 \Sigma_\infty^2 / 2) < 0 \quad (3.14)$$

Finally, for such fix parameters $\mathfrak{a}, \mathfrak{b}$, and ϵ , choose $\mathfrak{c} > 0$ sufficiently small such that

$$\mathfrak{c} + \epsilon - \mathfrak{a}(\gamma^* - \mathfrak{a}\eta_2 \Sigma_\infty^2 / 2) < 0 \text{ and } \mathfrak{c}^2 K_\gamma^2 / (4\epsilon) - \mathfrak{c}(m - \mathfrak{c}\eta_2 \Sigma_\infty^2) < 0. \quad (3.15)$$

Notice that the second inequality in (3.15) is satisfied for $\mathfrak{c} > 0$ small enough since $\mathfrak{c}^2 K_\gamma^2 / (4\epsilon) - \mathfrak{c}(m - \mathfrak{c}\eta_2 \Sigma_\infty^2) = O(\mathfrak{c}^2) - \mathfrak{c}m$ as $\mathfrak{c} \rightarrow 0$. One then has for some constants $\mathfrak{c}_i > 0$ ($i = 1, 2, 3$) and for all $(x, v) \in \mathcal{S}$,

$$\frac{\mathcal{L}_1 W_2}{W_2}(x, v) \leq -K_2(x, v),$$

where

$$K_2(x, v) = \frac{\eta_2 [-\mathfrak{c}_3 + \mathfrak{c}_1 |v|^2 + \mathfrak{c}_2 |x|_{\alpha_2} + C_0 \mathfrak{b} \sum_{i \neq j} |x^i - x^j|^{-1}]}{F_2^{1-\eta_2}(x, v)}. \quad (3.16)$$

By (3.12) (see also the line just after), there exists $M > 0$ such that for $(x, v) \in \mathcal{S}$

$$F_2(x, v) \leq M H_2(x, v). \quad (3.17)$$

By (3.3), for some $C > 0$, $H_2(x, v) \leq |v|^2/2 + 2A|x|_{\alpha_2} - \sum_{i < j} \mathbf{1}_{|x^i - x^j| \leq 1} \log |x^i - x^j| + C$, for $(x, v) \in \mathcal{S}$. Thus, using (3.17) and since $1 - \eta_2 < 1$, using (3.16) and (3.17), one deduces that for $(x, v) \in \mathcal{S}$,

$$\lim_{H_2(x, v) \rightarrow +\infty} K_2(x, v) = +\infty \text{ or equivalently (see (3.5)), } \lim_{x \rightarrow \partial \mathcal{O} \cup \{\infty\} \text{ or } v \rightarrow \{\infty\}} K_2(x, v) = +\infty.$$

This concludes the proof of Proposition 3.3. \square

Assumptions **(C1)**→**(C5)** are thus satisfied for the process (3.7) with potential V_2 when $\mathcal{D} = \mathcal{O} \times (\mathbb{R}^d)^N$ with \mathcal{O} a subdomain of \mathcal{O} as in Theorem 3.2. Theorem 3.2 is then a direct consequence of Lemma 2.7. The proof of Theorem 3.2 is thus complete.

4. ADDITIONAL RESULTS

4.1. Large deviations for the processes (2.9) and (3.7). The purpose of this section is to show that the two (non killed) Markov processes (2.9) and (3.7) satisfy large deviation principles on \mathcal{S} , see Corollary 4.1 below, which is of independent interest. Before, we recall some definitions related to large deviation principles and a result from [49].

4.1.1. Some generalities on large deviations principles. In this section, we introduce the definitions and the result we need to state Corollary 4.1.

Recall that $(X_t, t \geq 0)$ denotes either the solution to (2.9) (in this case $d \in \mathbb{N}^*$) or the solution of (3.7) (in this case $d = 1, 2$) on $\mathcal{S} = \mathcal{O} \times (\mathbb{R}^d)^N$. Let $\mathbf{M}_b(\mathcal{S})$ (resp. $\mathbf{M}_1(\mathcal{S})$) be the space of all σ -additive (resp. probability) measures of bounded variation on $(\mathcal{S}, \mathcal{B}(\mathcal{S}))$. The pair relation between $\nu \in \mathbf{M}_b(\mathcal{S})$ and $f \in b\mathcal{B}(\mathcal{S})$ is

$$\langle \nu, f \rangle := \nu(f) := \int_{\mathcal{S}} f(x) d\nu(x).$$

Using the pair above, $\mathbf{M}_b(\mathcal{S})$ is a subspace of the dual Banach space $(b\mathcal{B}(\mathcal{S}))^*$. On $\mathbf{M}_b(\mathcal{S})$ we consider the following two topologies:

- The weak topology $\sigma(\mathbf{M}_b(\mathcal{S}), b\mathcal{B}(\mathcal{S}))$. It will be called τ -topology, and is simply denoted by τ . The σ -algebra on $\mathbf{M}_b(\mathcal{S})$ we consider is $\mathcal{M}^\tau = \sigma(\nu \mapsto \nu(f), f \in b\mathcal{B}(\mathcal{S}))$.
- The weak topology $\sigma(\mathbf{M}_b(\mathcal{S}), \mathcal{C}_b(\mathcal{S}))$ will be denoted by w ($\mathcal{C}_b(\mathcal{S})$ is the space of all functions $f \in b\mathcal{B}(\mathcal{S})$ such that f is continuous on \mathcal{S}).

We now introduce the *Donsker and Varadhan level-3 entropy functional*. To this end, we define:

$$\Omega = \mathcal{C}(\mathbb{R}_+, \mathcal{S}) \text{ and for } t \geq 0, \mathfrak{F}_t = \sigma(X_s, s \in [0, t]).$$

The set $b\mathfrak{F}_t(\Omega)$ denotes the space of all real bounded \mathfrak{F}_t -measurable functions on Ω . On $\mathbf{M}_1(\Omega)$, we consider the *projective limit* τ -topology τ_p generated by $\{Q \mapsto \int F dQ; F \in b\mathfrak{F}_t(\Omega), \forall t \geq 0\}$. The σ -field on $\mathbf{M}_1(\Omega)$ generated by $\{Q \mapsto \int F dQ; F \in b\mathfrak{F}_t(\Omega), \forall t \geq 0\}$ is denoted by \mathcal{M}^{τ_p} . Define for $t > 0$, the random elements

$$L_t = \frac{1}{t} \int_0^t \delta_{X_s} ds \in \mathbf{M}_1(\mathcal{S}) \text{ and } R_t = \frac{1}{t} \int_0^t \delta_{X_{s+}} ds \in \mathbf{M}_1(\Omega),$$

where X_{s+} denotes the path $t \mapsto X_{s+t}$ (which is a random element in Ω). The Donsker and Varadhan level-3 entropy functional $H : \mathbf{M}_1(\Omega) \rightarrow [0, +\infty]$ is given by

$$H(Q) = \mathbb{E}^{\bar{Q}}[h_{\mathfrak{F}_1}(\bar{Q}_{\omega(-\infty, 0]}; \mathbb{P}_{\omega(0)})] \text{ if } Q \in \mathbf{M}_1^s(\Omega), \text{ and } H(Q) = +\infty \text{ else,}$$

where $\omega(t) = X_t(\omega)$, $\mathbf{M}_1^s(\Omega)$ is the set of $Q \in \mathbf{M}_1(\Omega)$ which are stationary, \bar{Q} is the unique stationary extension of $Q \in \mathbf{M}_1^s(\Omega)$ to $\bar{\Omega} := \mathcal{C}(\mathbb{R}, \mathcal{S})$, $\bar{Q}_{\omega(-\infty, 0]} = \bar{Q}(\cdot | X_t, t \leq 0)$ is the regular conditional distribution, and $h_{\mathfrak{F}_1}(\cdot; \mathbb{P}_z)$ is the Kullback entropy w.r.t. \mathbb{P}_z on the σ -field \mathfrak{F}_1 .

The *Donsker and Varadhan level-2 entropy functional* $J : \mathbf{M}_1(\mathcal{S}) \rightarrow [0, +\infty]$ is given by

$$J(\nu) = \inf\{H(Q), Q(X_0 \in \cdot) = \nu\}, \quad \nu \in \mathbf{M}_1(\mathcal{S}),$$

with convention $\inf \emptyset = +\infty$.

We now recall a result from [49] on the equivalence between large deviation principles. Recall that P_t is strong Feller and topologically irreducible (see Corollary 2.13). Then, we can use [49, Theorem 2.1] that we recall: the following large deviation principles $(\mathbf{L}\tau)$, $(\mathbf{R}\tau_p)$, and $(\mathbf{L}w)$ are equivalent:

$(\mathbf{L}\tau)$ $\mathbb{P}_z(L_t \in \cdot)$ satisfies the large deviation principle on $\mathbf{M}_1(\mathcal{S})$ w.r.t the τ -topology with the rate functional J , uniformly for initial states z in the compacts of \mathcal{S} . More precisely, the three properties below hold:

- For all $k \geq 0$, $\{J \leq k\}$ is compact in $(\mathbf{M}_1(\mathcal{S}), \tau)$.
- For any τ -open $G \in \mathcal{M}^\tau$ and any compact $K \subset \mathcal{S}$,

$$\liminf_{t \rightarrow +\infty} \frac{1}{t} \log \inf_{z \in K} \mathbb{P}_z(L_t \in G) \geq - \inf_{\nu \in G} J(\nu).$$

- For any τ -closed $F \in \mathcal{M}^\tau$ and any compact $K \subset \mathcal{S}$,

$$\limsup_{t \rightarrow +\infty} \frac{1}{t} \log \sup_{z \in K} \mathbb{P}_z(L_t \in F) \leq - \inf_{\nu \in F} J(\nu).$$

$(\mathbf{R}\tau_p)$ $\mathbb{P}_z(R_t \in \cdot)$ satisfies the large deviation principle on $\mathbf{M}_1(\Omega)$ w.r.t the τ_p -topology with the rate functional H , uniformly for initial states z in the compacts of \mathcal{S} .

$(\mathbf{L}w)$ $\mathbb{P}_z(L_t \in \cdot)$ satisfies the large deviation principle on $\mathbf{M}_1(\mathcal{S})$ w.r.t the w -topology with the rate functional J , uniformly for initial states z in the compacts of \mathcal{S} .

4.1.2. *Large deviations principles for the processes (2.9) and (3.7).* According to the following result, the processes (2.9) and (3.7) satisfy the large deviations principles $(\mathbf{L}\tau)$, $(\mathbf{R}\tau_p)$, and $(\mathbf{L}w)$.

Corollary 4.1. *Let $d \geq 1$ (resp. $d = 1, 2$). Assume that $(\mathbf{HL-J})$ (resp. $(\mathbf{H-C})$) is satisfied. Assume also that (\mathbf{Ac}) and $(\mathbf{A}\Sigma)$ hold. Let $\mathbf{W}_1 : \mathcal{S} \rightarrow [1, +\infty)$ (resp. $\mathbf{W}_2 : \mathcal{S} \rightarrow [1, +\infty)$) be such that $(\mathbf{C3})$ is satisfied for the process (2.9), see Proposition 2.10 (resp. the process (3.7), see Proposition 3.3). Then,*

- The large deviations principles $(\mathbf{L}\tau)$, $(\mathbf{R}\tau_p)$, and $(\mathbf{L}w)$ hold for the process (2.9) (resp. the process (3.7)) uniformly for initial states in the compacts of \mathcal{S} , and also uniformly over any family of initial measures of \mathcal{S} in $\{\nu \in \mathbf{M}_1(\mathcal{S}), \int_{\mathcal{S}} \mathbf{W}_1 d\nu \leq L\}$ (resp. $\{\nu \in \mathbf{M}_1(\mathcal{S}), \int_{\mathcal{S}} \mathbf{W}_2 d\nu \leq L\}$) where $L > \inf_{\mathcal{S}} \mathbf{W}_1$ (resp. $L > \inf_{\mathcal{S}} \mathbf{W}_2$) is arbitrary.*
- The process (2.9) (resp. the process (3.7)) has a unique invariant probability measure μ_1 on \mathcal{S} (resp. μ_2).*

In addition:

- It holds:*

$$\int_{\mathcal{S}} \mathbf{W}_1 d\mu_1 < +\infty \text{ (resp. } \int_{\mathcal{S}} \mathbf{W}_2 d\mu_2 < +\infty).$$

- There exist $\delta > 0$ and $C \geq 1$ such that for all $t \geq 0$,*

$$\|P_t - \mu_1(\cdot)\|_{b_{\mathbf{W}_1}\mathcal{B}(\mathcal{S})} \leq C e^{-\delta t} \text{ (resp. } \|P_t - \mu_2(\cdot)\|_{b_{\mathbf{W}_2}\mathcal{B}(\mathcal{S})} \leq C e^{-\delta t}).$$

Corollary 4.1 is an extension of [49, Theorem 3.1] to singular potentials.

Proof. The proof is divided into two steps.

Step 1. Proofs of items (a) and (b).

The functions $-\mathcal{L}_1 W_1/W_1$ and $-\mathcal{L}_2 W_2/W_2$ converges to $+\infty$ when $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$ or $v \rightarrow \{\infty\}$, $(x, v) \in \mathcal{S}$. These two functions are thus inf-compact on \mathcal{S} . In addition, P_t is strong Feller and topologically irreducible by Corollary 2.13. Items (a) and (b) in Corollary 4.1 are then direct consequences of [49, Corollary 2.2].

Step 2. Proofs of items (c) and (d).

Let us denote by $r_{ess}(\mathbf{T})$ (resp. $r_{sp}(\mathbf{T})$) the (Wolf) essential spectral radius (resp. the spectral radius) of a bounded linear map \mathbf{T} on a Banach space \mathbf{X} (see for instance [50] for a definition). Let us consider the process (2.9) on \mathcal{S} . The case of the process (2.9) is treated similarly. For $p > 1$ sufficiently close to 1, by choice of $\mathfrak{a} > 0$ and $\mathfrak{b} > 0$ (see (2.38) and (2.39)) in the definition of W_1 , the function W_1^p satisfies **(C3)** (indeed the parameters \mathfrak{a} and \mathfrak{b} are then changed into $\mathfrak{a}p^{1/\delta_1}$ and $\mathfrak{b}p^{1/\delta_1}$). Then, for all $n \geq 0$,

$$\mathcal{L}(W_1^p) \leq b_n 1_{K_n} \leq b_n W_1^p.$$

Therefore, since in addition **(C1)** and **(C2)** are satisfied, by [28, Theorem 3.5], it holds for all $t > 0$ and $n \geq 0$, $r_{ess}(P_t|_{b_{W_1}\mathcal{B}(\mathcal{S})}) \leq e^{-r_n t}$. Because $r_n \rightarrow +\infty$ as $n \rightarrow +\infty$, this implies that for all $t > 0$:

$$r_{ess}(P_t|_{b_{W_1}\mathcal{B}(\mathcal{S})}) = 0.$$

Since P_t is a Markov transition kernel, by [49, Proposition 4.5], one deduces that:

$$r_{sp}(P_t|_{b_{W_1}\mathcal{B}(\mathcal{S})}) = 1.$$

Items (c) and (d) in Corollary 4.1 are then direct consequences of [28, Theorem 4.1] (P_t is strong Feller, topologically irreducible, and has a spectral gap on $b_{W_1}\mathcal{B}(\mathcal{S})$) and of the uniqueness of the invariant measure for the process (2.9) on \mathcal{S} (notice also that $\varphi = 1$ there because $P_t 1 = 1$, $\mu_1(1) = 1$, and $1 \in b_{W_1}\mathcal{B}(\mathcal{S})$, where $1(x) = 1$ for all $x \in \mathcal{S}$). This concludes the proof of Corollary 4.1. \square

4.2. Elliptic diffusions with singular potential. In this section, we extend the results of Section 2 to the elliptic diffusion process $(Y_t, t \geq 0)$ solution of the following stochastic differential equation on \mathcal{O} :

$$dY_t = -\nabla V_1(Y_t)dt + \sqrt{2}dB_t, \quad (4.1)$$

where $V_1 : \overline{\mathcal{O}} \rightarrow \overline{\mathbb{R}}$ is the \mathcal{C}^2 potential function given by (2.1) (under the assumption **(H-LJ)**). In the elliptic case, **(C1)**→**(C5)** are much easier to check. For all $x \in \mathcal{O}$, set

$$\text{if } \alpha_1 > 2, W_3(x) = V_1(x) \geq 1 \text{ and, if } \alpha_1 \in (1, 2], W_3(x) = e^{\epsilon V_1(x)} \geq 1, \quad (4.2)$$

for $\epsilon \in (0, 1)$. The infinitesimal generator of the diffusion (4.1) is denoted by $L = -\nabla V_1 \cdot \nabla + \Delta$. By (2.22) and (2.30), $\Delta V_1 = o(|\nabla V_1(x)|^2)$, as $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$. Thus, if $\alpha_1 \in (1, 2]$, for $x \in \mathcal{O}$, $LW_3(x)/W_3(x) = -(\epsilon - \epsilon^2)|\nabla V_1(x)|^2 + \epsilon\Delta V_1 \rightarrow -\infty$, as

$x \rightarrow \partial\mathcal{O} \cup \{\infty\}$. Assume now that $\alpha_1 > 2$. Then, using (2.22), and since $2(\alpha_1 - 1) > \alpha_1$ and $2(\beta_1 + 1) > \beta_1$,

$$-\frac{|\nabla V_1(x)|^2}{V_1(x)} \rightarrow -\infty, \text{ as } x \rightarrow \partial\mathcal{O} \cup \{\infty\}.$$

Thus, one has for all $x \in \mathcal{O}$, $LW_3(x)/W_3(x) \rightarrow -\infty$ as $x \rightarrow \partial\mathcal{O} \cup \{\infty\}$. In both cases, there exists $M > 0$ such that on \mathcal{O} , $LW_3/W_3 \leq M$. Thus, for all $x_0 \in \mathcal{O}$ and $r > 0$, it holds

$$W_3(x_0) \geq e^{-Mt} r \mathbb{P}_{x_0}(\mathbf{t}_r \leq t), \quad (4.3)$$

where $\mathbf{t}_r \geq 0$ is the first exit time from $\{x \in \mathcal{O}, W_3(x) < r\}$ (whose closure is compact and included in \mathcal{O}) of the local solution $(Y_t, t \in [0, \mathbf{t}_\ell))$ to (4.1) with $Y_0 = x_0$ ($\mathbf{t}_\ell \in [\mathbf{t}_r, \infty]$ being the life time of such a solution). By (4.3), $\mathbf{t}_\ell = +\infty$ almost surely.

Let now \mathfrak{D} be a subdomain of \mathcal{O} and denote by $\sigma_{\mathfrak{D}}$ the first exit time of $(Y_t, t \geq 0)$ from \mathfrak{D} . Then, for all $f \in b\mathcal{B}(\mathcal{O})$ (see (1.2)), $t > 0$, and $x \in \mathfrak{D}$, $\mathbb{E}_x[f(X_t)1_{t < \sigma_{\mathfrak{D}}}] = \mathbb{E}_x[f(B_t^0)1_{t < \sigma_{\mathfrak{D}}^0} \mathfrak{M}_t]$, where $\sigma_{\mathfrak{D}}^0$ is the first exit time of $(B_t, t \geq 0)$ from \mathfrak{D} and \mathfrak{M}_t is the exponential martingale defined by

$$\mathfrak{M}_t = \exp \left[-\frac{1}{\sqrt{2}} \int_0^t \nabla V_1(B_s) dB_s - \frac{1}{4} \int_0^t |\nabla V_1(B_s)|^2 ds \right], \quad t < \sigma_{\mathfrak{D}}^0.$$

Then, arguing similarly as we did to prove Corollary 2.13 and Proposition 2.12, one deduces that **(C1)** is satisfied for the process $(Y_t, t \geq 0)$ on \mathcal{O} , and **(C2)** and **(C4)** are satisfied for the process $(Y_t, t \in [0, \sigma_D))$ when $\mathcal{O} \setminus \overline{\mathfrak{D}}$ is nonempty and $\partial\mathfrak{D} \cap \mathcal{O}$ is \mathcal{C}^2 . By Lemma 2.7, one then has the following result.

Proposition 4.2. *Assume that **(H-C)** holds. Let \mathfrak{D} be a subdomain of \mathcal{O} such that $\mathcal{O} \setminus \overline{\mathfrak{D}}$ is nonempty and $\partial\mathfrak{D} \cap \mathcal{O}$ is \mathcal{C}^2 . Then, there exists a continuous and unbounded Lyapunov function $W_3 : \mathcal{O} \rightarrow [1, +\infty)$ (explicitly given by (4.2) for instance), such that the statements of items (a)–(d) in Theorem 2.4 are valid for the process (4.1) on \mathcal{O} (replacing there \mathcal{D} by \mathfrak{D}) and with the Lyapunov function W_3 (in place of W_1 there).*

Acknowledgement.

B.N. is supported by the grant IA20Nectoux from the Projet I-SITE Clermont CAP 20-25.

REFERENCES

- [1] D. Aristoff and T. Lelièvre. Mathematical Analysis of Temperature Accelerated Dynamics. *Multi-scale Modeling and Simulation*, 12(1):290–317, 2014.
- [2] V. Bansaye, B. Cloez, P. Gabriel, and A. Marguet. A Non-Conservative Harris’ Ergodic Theorem. *Preprint arXiv:1903.03946*, 2019.
- [3] F. Baudoin, M. Gordina, and D. P. Herzog. Gamma Calculus Beyond Villani and Explicit Convergence Estimates for Langevin Dynamics with Singular Potentials. *Archive for Rational Mechanics and Analysis*, 241(2):765–804, 2021.
- [4] M. Benaïm, N. Champagnat, W. Oçafrain, and D. Villemonais. Degenerate processes killed at the boundary of a domain. *Preprint arXiv:2103.08534*, 2021.
- [5] R. B. Best and G. Hummer. Coordinate-dependent diffusion in protein folding. *Proceedings of the National Academy of Sciences*, 107(3):1088–1093, 2010.
- [6] E. Camrud, D. P. Herzog, G. Stoltz, and M. Gordina. Weighted L^2 -contractivity of Langevin dynamics with singular potentials. *Nonlinearity*, 35(2):998–1035, 2021.

- [7] B. Carmeli and A. Nitzan. Theory of activated rate processes: Position dependent friction. *Chemical Physics Letters*, 102(6):517–522, 1983.
- [8] P. Cattiaux, P. Collet, A. Lambert, S. Martínez, S. Méléard, and J. San Martín. Quasi-Stationary Distributions and Diffusion Models in Population Dynamics. *The Annals of Probability*, 37(5):1926–1969, 2009.
- [9] P. Cattiaux and S. Méléard. Competitive or weak cooperative stochastic Lotka–Volterra systems conditioned on non-extinction. *Journal of Mathematical Biology*, 60(6):797–829, 2010.
- [10] D. Chafaï, G. Ferré, and G. Stoltz. Coulomb Gases Under Constraint: Some Theoretical and Numerical Results. *SIAM Journal on Mathematical Analysis*, 53(1):181–220, 2021.
- [11] N. Champagnat, K. A. Coulibaly-Pasquier, and D. Villemonais. Criteria for exponential convergence to quasi-stationary distributions and applications to multi-dimensional diffusions. In *Séminaire de Probabilités XLIX*, pages 165–182. Springer, 2018.
- [12] N. Champagnat and D. Villemonais. Exponential convergence to quasi-stationary distribution and Q-process. *Probability Theory and Related Fields*, 164(1-2):243–283, 2016.
- [13] N. Champagnat and D. Villemonais. General criteria for the study of quasi-stationarity. *Preprint arXiv:1712.08092*, 2017.
- [14] N. Champagnat and D. Villemonais. Lyapunov criteria for uniform convergence of conditional distributions of absorbed Markov processes. *Stochastic Processes and their Applications*, 135:51–74, 2021.
- [15] J-R. Chazottes, P. Collet, and S. Méléard. Sharp asymptotics for the quasi-stationary distribution of birth-and-death processes. *Probability Theory and Related Fields*, 164(1-2):285–332, 2016.
- [16] P. Collet, S. Martínez, S. Méléard, and J. San Martín. Quasi-stationary distributions for structured birth and death processes with mutations. *Probability Theory and Related Fields*, 151(1-2):191–231, 2011.
- [17] P. Collet, S. Martínez, and J. San Martín. *Quasi-Stationary Distributions: Markov Chains, Diffusions and Dynamical Systems*. Springer Science & Business Media, 2012.
- [18] F. Conrad and M. Grothaus. Construction, ergodicity and rate of convergence of N-particle Langevin dynamics with singular potentials. *Journal of Evolution Equations*, 10(3):623–662, 2010.
- [19] B. Cooke, D.P. Herzog, J.C. Mattingly, S.A. McKinley, and S.C. Schmidler. Geometric ergodicity of two-dimensional Hamiltonian systems with a Lennard–Jones-like repulsive potential. *Communications in Mathematical Sciences*, 15:1987–2025, 2011.
- [20] M.H.A Davis. *Markov Models & Optimization*, volume 49. CRC Press, 1993.
- [21] G. Di Gesù, T. Lelièvre, D. Le Peutrec, and B. Nectoux. Jump Markov models and transition state theory: the quasi-stationary distribution approach. *Faraday Discussions*, 195:469–495, 2017.
- [22] P. Diaconis and L. Miclo. On times to quasi-stationarity for birth and death processes. *Journal of Theoretical Probability*, 22(3):558–586, 2009.
- [23] P. Diaconis and L. Miclo. On quantitative convergence to quasi-stationarity. *Annales de la Faculté des Sciences de Toulouse: Mathématiques*, 24(4):973–1016, 2015.
- [24] D. Down, S. P. Meyn, and R. L. Tweedie. Exponential and Uniform Ergodicity of Markov Processes. *The Annals of Probability*, 23(4):1671–1691, 1995.
- [25] G. Ferré, M. Rousset, and G. Stoltz. More on the long time stability of Feynman–Kac semigroups. *Stochastics and Partial Differential Equations: Analysis and Computations*, 9(3):630–673, 2021.
- [26] G. Gong, M. Qian, and Z. Zhao. Killed diffusions and their conditioning. *Probability Theory and Related Fields*, 80(1):151–167, 1988.
- [27] M. Grothaus and P. Stilgenbauer. A Hypocoercivity Related Ergodicity Method for Singularly Distorted Non-Symmetric Diffusions. *Integral Equations and Operator Theory*, 83(3):331–379, 2015.
- [28] A. Guillin, B. Nectoux, and L. Wu. Quasi-stationary distribution for strongly Feller Markov processes by Lyapunov functions and applications to hypoelliptic Hamiltonian systems. *Preprint hal-03068461*.
- [29] A. Hening, Q. Qi, Z. Shen, and Y. Li. Quasistationary distributions of multidimensional diffusion processes. *Preprint arXiv:2102.05785*, 2021.
- [30] D.P. Herzog and J.C. Mattingly. Ergodicity and Lyapunov functions for Langevin dynamics with singular potentials. *Communications on Pure and Applied Mathematics*, 72(10):2231–2255, 2019.

- [31] O. Kallenberg. *Foundations of Modern Probability*, volume 2. Springer, 1997.
- [32] M. Kolb and D. Steinsaltz. Quasilimiting behavior for one-dimensional diffusions with killing. *The Annals of Probability*, 40(1):162–212, 2012.
- [33] P. Lançon, G. Batrouni, L. Lobry, and N. Ostrowsky. Drift without flux: Brownian walker with a space-dependent diffusion coefficient. *EPL (Europhysics Letters)*, 54(1):28, 2001.
- [34] A. W.C. Lau and T. C. Lubensky. State-Dependent Diffusion: Thermodynamic Consistency and its Path Integral Formulation. *Physical Review E*, 76(1):011123, 2007.
- [35] C. Le Bris, T. Lelièvre, M. Luskin, and D. Perez. A mathematical formalization of the parallel replica dynamics. *Monte Carlo Methods and Applications*, 18(2):119–146, 2012.
- [36] T. Lelièvre, M. Ramil, and J. Reygner. Quasi-stationary distribution for the Langevin process in cylindrical domains, part I: existence, uniqueness and long-time convergence. *Stochastic Processes and their Applications*, 144:173–201, 2022.
- [37] T. Lelièvre and G. Stoltz. Partial differential equations and stochastic methods in molecular dynamics. *Acta Numerica*, 25:681–880, 2016.
- [38] Y. Lu and J.C. Mattingly. Geometric ergodicity of Langevin dynamics with Coulomb interactions. *Nonlinearity*, 33(2):675, 2019.
- [39] S. Méléard and D. Villemonais. Quasi-stationary distributions and population processes. *Probability Surveys*, 9:340–410, 2012.
- [40] S. P. Meyn and R. L. Tweedie. *Markov Chains and Stochastic Stability*. Communications and Control Engineering Series. Springer-Verlag London, 1993.
- [41] A. Nonnenmacher and M. Grothaus. Overdamped limit of generalized stochastic Hamiltonian systems for singular interaction potentials. *Journal of Evolution Equations*, 20(2):577–605, 2020.
- [42] D. Perez, E. D Cubuk, A. Waterland, E. Kaxiras, and A.F. Voter. Long-Time Dynamics Through Parallel Trajectory Splicing. *Journal of Chemical Theory and Computation*, 12(1):18–28, 2016.
- [43] R.G. Pinsky. On The Convergence of Diffusion Processes Conditioned to Remain in a Bounded Region for Large Time to Limiting Positive Recurrent Diffusion Processes. *The Annals of Probability*, 13(2):363–378, 1985.
- [44] M. Ramil. *Processus cinétiques dans les domaines à bord et quasi-stationnarité*. PhD thesis, Ecole des Ponts ParisTech, 2020.
- [45] M. Sachs, B. Leimkuhler, and V. Danos. Langevin dynamics with variable coefficients and nonconservative forces: from stationary states to numerical methods. *Entropy*, 19(12):647, 2017.
- [46] Z. Schuss. *Brownian Dynamics at Boundaries and Interfaces*. Springer, 2015.
- [47] R. Song and L. Xie. Well-posedness and long time behavior of singular Langevin stochastic differential equations. *Stochastic Processes and their Applications*, 130(4):1879–1896, 2020.
- [48] G. Stoltz. *Some mathematical methods for molecular and multiscale simulation*. PhD thesis, Ecole Nationale des Ponts et Chaussées, 2007.
- [49] L. Wu. Large and moderate deviations and exponential convergence for stochastic damping Hamiltonian systems. *Stochastic Processes and their Applications*, 91(2):205–238, 2001.
- [50] L. Wu. Essential spectral radius for Markov semigroups. I. Discrete time case. *Probability Theory and Related Fields*, 128(2):255–321, 2004.

Arnaud Guillin. UNIVERSITÉ CLERMONT AUVERGNE, CNRS, LMBP, F-63000 CLERMONT-FERRAND, FRANCE

Email address: arnaud.guillin@uca.fr

Boris Nectoux. UNIVERSITÉ CLERMONT AUVERGNE, CNRS, LMBP, F-63000 CLERMONT-FERRAND, FRANCE

Email address: boris.nectoux@uca.fr

Liming Wu. UNIVERSITÉ CLERMONT AUVERGNE, CNRS, LMBP, F-63000 CLERMONT-FERRAND, FRANCE

Email address: Li-Ming.Wu@uca.fr