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GENERALIZED LANGEVIN AND NOSÉ-HOOVER PROCESSES ABSORBED AT THE BOUNDARY OF A METASTABLE DOMAIN

ARNAUD GUILLIN[†], DI LU[†], BORIS NECTOUX[†], AND LIMING WU[†]

ABSTRACT. In this paper, we prove in a very weak regularity setting existence and uniqueness of quasi-stationary distributions as well as exponential convergence towards the quasi-stationary distribution for the generalized Langevin and the Nosé-Hoover processes, two processes which are widely used in molecular dynamics. The case of singular potentials is considered. With the techniques used in this work, we are also able to greatly improve existing results on quasi-stationary distributions for the kinetic Langevin process to a weak regularity setting.

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1. SETTING AND MAIN RESULTS

1.1. Purpose of this work.

1.1.1. *Introduction.* The basic ingredient in molecular dynamics is a potential energy function $V : (\mathbf{R}^d)^N \rightarrow [1, +\infty]$ which associates to a set of position coordinates of N \mathbf{R}^d -valued particles the energy of the system. With this function V , several continuous state space models exist. When the system is thermostated, the time evolution of the position-velocity pair $(x_t = (x_t^1, \dots, x_t^N), v_t = (v_t^1, \dots, v_t^N)) \in (\mathbf{R}^d)^N \times (\mathbf{R}^d)^N$ of the particles is commonly described by the so-called kinetic Langevin process, which is the solution in $(\mathbf{R}^d)^N \times (\mathbf{R}^d)^N$ to the equation

$$dx_t = v_t dt, \quad dv_t = -\nabla V(x_t) dt - \gamma v_t dt + \sqrt{2\gamma} dW_t, \quad (1.1)$$

where $(W_t, t \geq 0)$ is a standard $(\mathbf{R}^d)^N$ -Brownian motion and $-\nabla V$ is the force field. Due to energetic barriers, the position process $(x_t, t \geq 0)$ remains trapped for very long times in a basin of attraction $\mathcal{B}_V(x_*)$ of some local minimum x_* of V for the dynamics $\dot{x} = -\nabla V(x)$ in $(\mathbf{R}^d)^N$. The process (1.1) is therefore said to be metastable and such subdomains of $(\mathbf{R}^d)^N$, which typically describe the macroscopic states of the system, are the metastable regions. The move from one metastable region to another is typically related to a macroscopic transition. The metastable phenomenon prevents to have access to the macroscopic transitions by simulating directly the trajectories of the process (1.1) since such transitions occur over very long periods of time. In simulation in molecular dynamics, many algorithms have been designed to have access to macroscopic transitions such as e.g. the powerful and widely used *accelerated dynamics algorithms* introduced by A.F. Voter & al. [71, 75, 3, 63]. Recently, it has been shown [39, 62, 19, 20, 45, 66] that the notion of quasi-stationary distribution (see Definition 1.1) is the cornerstone to analyse the mathematical foundations of these accelerated dynamics algorithms. For that reason, the study of quasi-stationary distributions for metastable continuous state space model has recently attracted a lot of attention, especially for the hypoelliptic and non reversible process (1.1), see indeed [28, 29, 47, 48, 4, 46].

In this work, we will address the question of existence, uniqueness, and exponential convergence to the quasi-stationary distribution for two other widely used, for example in molecular dynamics,

metastable continuous state space models which are structurally more complicated than (1.1): the Mori-Zwanzig Markovian approximation of the generalized Langevin process (see (1.4) below) and the Nosé-Hoover process (see (1.5) below), which we introduce now.

The generalized Langevin process, namely the solution $(x_t = (x_t^1, \dots, x_t^N), v_t = (v_t^1, \dots, v_t^N), t \geq 0) \in (\mathbf{R}^d)^N \times (\mathbf{R}^d)^N$ to the integro-differential equation

$$dx_t = v_t dt, \quad dv_t = -\nabla V(x_t) dt - \gamma v_t dt + \int_0^t \mathbf{K}(t-s) v_s ds dt + F_t dt + \sqrt{2\gamma} dW_t, \quad (1.2)$$

has been derived to describe the evolution in time of a system of N \mathbf{R}^d -valued particles interacting with a heat bath (see [79, 80, 60, 55, 56]). Here $\gamma \geq 0$ is the friction parameter. The diagonal square bloc matrix $\mathbf{K}_t = \text{diag}(\mathbf{K}_t^1 I_{(\mathbf{R}^d)^N}, \dots, \mathbf{K}_t^N I_{(\mathbf{R}^d)^N})$ is the memory kernel, where $\mathbf{K}_t^i \in \mathbf{R}_+$, is a characteristic of the bath, which encodes the long memory property of the generalized Langevin process. The process $(F_t = (F_t^1, \dots, F_t^N) \in (\mathbf{R}^d)^N, t \geq 0)$ is a stationary zero mean Gaussian stochastic forcing and the fluctuation-dissipation principle writes $\mathbf{E}[F_s^i \cdot F_u^i] = \mathbf{K}^i(|s-u|)$. The generalized Langevin process, which is non Markovian, is one of the standard models in nonequilibrium statistical mechanics [72, 50, 57] and is widely used in many areas of science such as surface scattering [1, 23], polymer dynamics [70], sampling in molecular dynamics [9, 10], and global optimization using simulated annealing [26, 11]. When $\mathbf{K}_t^i = \sum_{l=1}^{k_i} \lambda_{i,l}^2 e^{-\alpha_{i,l} t}$ (where $\alpha_{i,l}, \lambda_{i,l} > 0$ for all $i \in \{1, \dots, N\}$ and all $l \in \{1, \dots, k_i\}$, $k_i \geq 1$), the process (1.2) is quasi-Markovian, i.e. it can be written as a Markovian process by adding a finite number of additional variables [60] (see also [58, Section 1.2], [27], and references therein). More precisely, for such \mathbf{K}^i 's, (1.2) is equivalent to a Markovian system of stochastic differential equations:

$$\begin{cases} dx_t^i &= v_t^i dt \\ dv_t^i &= -\nabla_{x_i} V(x_t) dt - \gamma v_t^i dt + \sum_{l=1}^{k_i} \lambda_{i,l} z_t^{i,l} dt + \sqrt{2\gamma} dW_t^i \\ dz_t^{i,l} &= -\alpha_{i,l} z_t^{i,l} dt - \lambda_{i,l} v_t^i dt + \sqrt{2\alpha_{i,l}} dB_t^{i,l}, \end{cases} \quad (1.3)$$

where for $i \in \{1, \dots, N\}$ and $l \in \{1, \dots, k_i\}$, $(x_t^i, v_t^i, z_t^{i,l}) \in \mathbf{R}^d \times \mathbf{R}^d \times \mathbf{R}^d$, and where the $(W_t^i, t \geq 0)$'s and the $(B_t^{i,l}, t \geq 0)$'s are mutually independent \mathbf{R}^d -Brownian motions. We also mention that for certain kinds of memory kernels \mathbf{K} , (1.2) can be conveniently approximated by the finite dimensional systems (1.3), see e.g. [60, 38, 59, 57]. For ease of expository and since all our proofs extend trivially to the case when $k_i > 1$, we have decided in this work to only consider the case when $k_i = 1$ for all $i \in \{1, \dots, N\}$. In this case, (1.3) writes:

$$\begin{cases} dx_t &= v_t dt \\ dv_t &= -\nabla V(x_t) dt - \gamma v_t dt + \lambda z_t dt + \sqrt{2\gamma} dW_t \\ dz_t &= -\alpha z_t dt - \lambda v_t dt + \sqrt{2\alpha} dB_t, \end{cases} \quad (1.4)$$

where $(x_t, v_t, z_t) \in (\mathbf{R}^d)^N \times (\mathbf{R}^d)^N \times (\mathbf{R}^d)^N$, $\alpha, \lambda > 0$, $\gamma \geq 0$, and where $(W_t, t \geq 0)$ and $(B_t, t \geq 0)$ are independent $(\mathbf{R}^d)^N$ -Brownian motions. Note that when $\gamma = 0$, which is the case often used in practice, the process (1.4) is more degenerated than (1.1) in the sense that the noise does not act on the positions and on the velocities but on an auxiliary variable. With a slight abuse of language, (1.4) will be referred in this work as the generalized Langevin process.

The second process we will consider is the Nosé-Hoover process which is another extension of the kinetic Langevin process (1.1). The Nosé-Hoover process is the solution on $(\mathbf{R}^d)^N \times (\mathbf{R}^d)^N \times \mathbf{R}$ to the following stochastic differential equation:

$$\begin{cases} dx_t &= v_t dt \\ dv_t &= -\nabla V(x_t) dt - \gamma v_t dt - v_t y_t dt + \sqrt{2\gamma} dB_t \\ dy_t &= |v_t|^2 dt - dN dt, \end{cases} \quad (1.5)$$

where $\gamma > 0$. The process (1.5) is also sometimes referred as the adaptive Langevin process. It has been introduced in the context of sampling in molecular dynamics [37, 41, 36, 44], where y_t acts as a thermostat. See also [22, 69] for applications in Bayesian sampling. The friction parameter in

the kinetic Langevin process (1.1) is considered in (1.5) as a dynamical variable. This stochastic correction, which is renewed according to a negative feedback loop control law (as in the Nosé-Hoover thermostat) models random perturbations of unknown magnitude which can occur on the potential gradient, and serves as variable which restores the canonical distribution associated with the prescribed inverse temperature, see indeed [43].

Studying these two metastable processes, via their quasi-stationary distribution, is thus of paramount importance for practical applications, e.g. in molecular dynamics.

Since V might have singularities, we consider a connected component \mathbf{O}_V of the set $\{x \in (\mathbf{R}^d)^N, V(x) < +\infty\}$. Then, if collisions between particles do not occur, which will be the case in this work, the two processes (1.4) and (1.5) evolve on the state space

$$\mathcal{E} = \mathbf{O}_V \times \mathbf{R}^m,$$

where $m = Nd + Nd$ for the generalized Langevin process (1.4) and $m = Nd + 1$ for the Nosé-Hoover process (1.5).

In this work, we prove, for the two processes (1.4) and (1.5), existence and uniqueness in some weighted spaces of the quasi-stationary distribution on metastable domains \mathcal{D} , which are regions of the forms $\mathcal{D} = \mathcal{O} \times \mathbf{R}^m$, where \mathcal{O} is a subdomain (i.e. a nonempty, connected, and open subset) of \mathbf{O}_V , bounded or not, as well as the exponential convergence towards the quasi-stationary distribution. Our main results are Theorem 1.4 (and its extension to non gradient force fields, Theorem 1.5), and Theorems 1.7, and 1.11. We also mention Theorem 5.1 for a significant extension of existing results on the quasi-stationary distribution for the kinetic Langevin process (1.1).

The first main contribution of this work is the very weak regularity setting we consider on both the domain \mathcal{D} and the force field (see items **a** and **b** just below). One of the main novelty of this setting, compared to previous works on quasi-stationary distributions for hypoelliptic degenerate processes [28, 29, 47, 48, 65, 46] on such domains \mathcal{D} , is that we have managed to get rid of any regularity assumption on the boundary of \mathcal{O} . This is a paramount improvement in order to treat the cases which are considered in practice where \mathcal{O} is defined as a basin of attraction $\mathcal{B}_V(x_*)$ (see e.g. [64, 62, 19, 66]), or as (the interior of the closure of the) union of neighboring basins of attraction. In this case, the properties of $\partial\mathcal{O}$ are very arduous to infer, and even worse, it is known that in this case $\partial\mathcal{O}$ is far from being regular¹, even for smooth potentials V .

More precisely, in the weak regularity setting where:

- a.** \mathcal{O} is any subdomain of \mathbf{O}_V (note that there is thus no assumption on the regularity of $\partial\mathcal{O}$, and that $\partial\mathcal{O}$ can also intersect the set $\partial\mathbf{O}_V$ where the potential V is infinite, due to collisions between particles),
- b.** the force field $-\nabla V$ is only locally Lipschitz over \mathbf{O}_V and infinite on $\partial\mathbf{O}_V$,

we will in particular prove that:

1. The nonkilled semigroup, defined in (1.6), and the killed semigroups, defined in (1.7), are respectively strong Feller and weak Feller (actually it will be shown that the latter is also strong Feller), see respectively the conditions **(C1)** and **(C4)** in Section 1.1.3.
2. The killed semigroup is topologically irreducible (see the condition **(C5)** in Section 1.1.3).

In the weak regularity setting **a** and **b**, the tools used to prove Item **1** in [28, 29] for the kinetic process (1.1) are not adapted anymore. We will rather rely on a different approach to prove Item **1**. This approach, which is explained in details in Section 2.1.1, is fundamentally based on the *energy splitting* Equation (2.1) together with the analysis of the behavior of the process at low and at high energy \mathbf{H} (where \mathbf{H} denotes the Hamiltonian of the processes).

On the other hand, to ensure existence of quasi-stationary distributions and exponential convergence to it, we also have to prove

¹E.g. $\partial\mathcal{O}$ may have corners and/or may contain points at which it does not satisfy the exterior sphere condition. Worst geometric situations can also occur for the boundary of such domains.

3. Enhanced exponential integrability of hitting times of larger and larger sets (see the condition **(C3)** below).

The second main contribution of this work is that we consider singular potentials V for both processes and ensure that Item **3** still holds. To this end, we have in particular to construct Lyapunov functions satisfying a strong return from ∞ (see **(C3)**). The Lyapunov functions we construct are bounded from above by $C \exp(c\mathbf{H}^\delta)$, for $\delta \in (0, 1]$, where we recall that \mathbf{H} denotes the Hamiltonian of the processes. It will turn out that for singular potentials V and for the generalized Langevin process, a right choice of Lyapunov function is $e^{\mathbf{F}^\delta}$, where \mathbf{F} is the modified Hamiltonian introduced in [24] (see Section 3). However, for the Nosé-Hoover process (1.5), the Lyapunov function introduced in [32] does not satisfy **(C3)**, and for that reason we modify it to obtain the asymptotic return from ∞ in the position variable x and also to obtain smaller Lyapunov functions.

The starting point of our analysis is [28, Theorem 2.2] when we will consider the generalized Langevin process, whereas, for the Nosé-Hoover process, we will rely on a more general result, namely Theorem 4.6 (stated and proved in Section 4.3). This extension is required since the Nosé-Hoover process does not satisfy the condition **(C5)** (defined at the end of Section 1.1.3).

The approach used in this work (see Section 2.1.1) is particularly well-suited to checking the regularity conditions **(C1)**, **(C2)**, and **(C4)** on actually any kind of subdomains $\mathcal{D} \subset \mathbf{R}^l$ for solutions to SDEs in \mathbf{R}^l with non smooth drifts (see also Remark 2.1). In particular, we can improve, using this approach and the tools used in this work, the existing results on the kinetic Langevin process [29, Theorems 2.4 and 3.2] with singular potentials, as well as those obtained [48]: they are valid without any regularity assumption on the boundary of the subdomain \mathcal{D} (see respectively Theorems 5.1 and 5.2 below) and when the drift is only locally Lipschitz. As explained, such extensions are of real interest to match with the non smooth domains, namely the basins of attraction $\mathcal{B}_V(x^*)$ of $\dot{x} = -\nabla V(x)$, on which is considered the quasi-stationary distribution in practice. We also refer to Theorems 5.3 and 5.4 when elliptic processes are considered.

We finally mention that the tools used in this work will be also employed in a future work to study the existence and uniqueness of (quasi- or not) stationary distributions for SDEs with different kinds of noises.

1.1.2. Related results. The ergodic properties of the nonkilled semigroup of the generalized Langevin process is now well-known, see for instance [59, 58, 61, 42, 27, 24] and references therein (see also [6, 54, 34]). On the other hand, the long time behavior of nonkilled semigroup of the Nosé-Hoover process has been studied in [32], where we also mention that the case of Lennard-Jones type potentials is also considered there (see also [43] for a similar study for the adaptive Langevin process, through a hypocoercivity analysis). We also refer to [5] (resp. [17]) where the metastable behavior of the process (1.4) (resp. (1.5)) has been studied through the derivation of sharp asymptotic equivalents in the small temperature regime of the smallest eigenvalues of its generator (see also [31]).

Several general criteria have been introduced in the mathematical literature to ensure existence and uniqueness of quasi-stationary distributions, see [53, 13] and references therein (see also the recent works [2, 74, 68]). When dealing with biological systems, we refer e.g. to [7, 21, 8, 14, 35, 12]. As already mentioned, quasi-stationary distributions for the kinetic Langevin process (1.1) have been studied recently in [28, 29, 48, 4] (see also [73]).

1.1.3. Notation. Let $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t \geq 0}, \mathbf{P})$ be a filtered probability space (where the filtration satisfies the usual condition). Consider $(X_t, t \geq 0)$ a time homogeneous continuous strong Markov process valued in \mathcal{E} , where \mathcal{E} is a nonempty open subset of \mathbf{R}^k , $k \geq 1$. Let $\mathcal{B}(\mathcal{E})$ be the Borel σ -algebra of \mathcal{E} , $b\mathcal{B}(\mathcal{E})$ the space of all bounded and Borel measurable (real-valued) functions f on \mathcal{E} , $\mathcal{C}^b(\mathcal{E})$ the space of all bounded and continuous (real-valued) functions on \mathcal{E} , and $\mathcal{P}(\mathcal{E})$ as the set of probability measures on \mathcal{E} . We will denote by $\mathcal{L}_{\text{Lip}}^{1, \text{loc}}(\mathcal{E})$ the set of functions $V : \mathcal{E} \rightarrow \mathbf{R}$ such that over \mathcal{E} , V is differentiable

and ∇V is locally Lipschitz. The transition probability semigroup is denoted by $(P_t, t \geq 0)$, i.e.

$$P_t f(\mathbf{x}) = \mathbf{E}_{\mathbf{x}}[f(X_t)], \quad f \in b\mathcal{B}(\mathcal{E}), \quad \mathbf{x} \in \mathcal{E}. \quad (1.6)$$

$(P_t, t \geq 0)$ will be referred as the nonkilled semigroup. The space $\mathcal{C}([0, T], \mathcal{E})$ of \mathcal{E} -valued continuous functions defined on $[0, T]$ is endowed with the sup-norm over $[0, T]$. When \mathcal{D} is a nonempty open subset of \mathcal{E} , we denote by $(P_t^{\mathcal{D}}, t \geq 0)$ the semigroup of the killed process $(X_t, t \geq 0)$:

$$P_t^{\mathcal{D}} f(\mathbf{x}) = \mathbf{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{D}}}], \quad f \in b\mathcal{B}(\mathcal{D}), \quad \mathbf{x} \in \mathcal{D}, \quad (1.7)$$

where $\sigma_{\mathcal{D}} = \inf\{t \geq 0, X_t \notin \mathcal{D}\}$ is the first exit time of the process $(X_t, t \geq 0)$ from \mathcal{D} ($(P_t^{\mathcal{D}}, t \geq 0)$ will be referred as the killed semigroup). For $\mathbf{W} : \mathcal{E} \rightarrow [1, +\infty)$ and when \mathcal{D} is open subset of \mathcal{E} , we define the set $\mathcal{P}_{\mathbf{W}}(\mathcal{D})$ as the set of probability measures ν over \mathcal{D} such that $\nu(\mathbf{W}) < +\infty$. We also define $b_{\mathbf{W}}\mathcal{B}(\mathcal{D})$ the Banach space of measurable functions $f : \mathcal{D} \rightarrow \mathbf{R}^d$ such that f/\mathbf{W} is bounded over \mathcal{D} (its norm is denoted by $\|f\|_{\mathbf{W}} = \sup_{\mathcal{D}} |f/\mathbf{W}|$). We finally denote by $(\mathcal{L}, \mathbb{D}_e(\mathcal{L}))$ the extended generator of $(X_t, t \geq 0)$ (for a definition, see [28, 29] and references therein).

As already mentioned, to prove existence and uniqueness of quasi-stationary distributions for the generalized Langevin process, we will use [28, Theorem 2.2] (for the Nosé-Hoover process, we will use an extension of [28, Theorem 2.2], see Theorem 4.6 below). To this end, we recall the conditions introduced in [28] which ensure existence and uniqueness of the quasi-stationary distribution as well as the exponential convergence in $\mathcal{P}_{\mathbf{W}^{1/p}}(\mathcal{D})$ towards this quasi-stationary distribution:

- (C1) There exists $t_0 > 0$ such that for each $t \geq t_0$, P_t is strong Feller.
- (C2) For every $T > 0$, $\mathbf{x} \in \mathcal{E} \mapsto \mathbf{P}_{\mathbf{x}}(X_{[0, T]} \in \cdot)$ (the law of $X_{[0, T]} := (X_t)_{t \in [0, T]}$) is continuous from \mathcal{E} to the space $\mathcal{P}(\mathcal{C}([0, T], \mathcal{E}))$ of probability measures on $\mathcal{C}([0, T], \mathcal{E})$, equipped with the weak convergence topology.
- (C3) There exist a continuous function $\mathbf{W} : \mathcal{E} \rightarrow [1, +\infty)$, with $\mathbf{W} \in \mathbb{D}_e(\mathcal{L})$, 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{E} , such that

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

- (C4) For all $t \geq 0$ and all $f \in \mathcal{C}_c^{\infty}(\mathcal{D})$, $P_t^{\mathcal{D}} f \in \mathcal{C}^b(\mathcal{D})$.
- (C5) There exists $t_1 > 0$, for all $t \geq t_1$, $\mathbf{x} \in \mathcal{D}$ and nonempty open subset \mathcal{O} of \mathcal{D} , $P_t^{\mathcal{D}}(\mathbf{x}, \mathcal{O}) > 0$. In addition, there exists $\mathbf{x}_0 \in \mathcal{D}$ such that $\mathbf{P}_{\mathbf{x}_0}(\sigma_{\mathcal{D}} < +\infty) > 0$.

We recall also the definition of a quasi-stationary distribution (see for instance the classical textbook [16]).

Definition 1.1. *A quasi-stationary distribution of the Markov process $(X_t, t \geq 0)$ in the domain \mathcal{D} is a probability measure on \mathcal{D} such that $\mu_{\mathcal{D}}(\mathcal{A}) = \mathbf{P}_{\mu_{\mathcal{D}}}(X_t \in \mathcal{A} | t < \sigma_{\mathcal{D}}), \forall t > 0, \forall \mathcal{A} \in \mathcal{B}(\mathcal{D})$, where $\mathcal{B}(\mathcal{D}) := \{\mathcal{A} \cap \mathcal{D}, \mathcal{A} \in \mathcal{B}(\mathcal{E})\}$.*

We end this section by recalling a powerful general convergence result which will be used many times in this work.

Proposition 1.2. ([76, Lemma 3.2]) *Assume that a sequence of random variables $(Y_n)_{n \geq 0}$ defined on a probability space $(\Omega, \mathcal{F}, \mathbf{P})$ with values in a Polish space \mathcal{S} converges in \mathbf{P} -probability to Y . Assume also that there exists a fixed probability measure μ s.t. for all $n \geq 0$, the law of Y_n writes $\mathbf{P}_{\mathbf{x}}[Y_n \in d\mathbf{x}] = p_n(\mathbf{x})\mu(d\mathbf{x})$. If $(p_n)_n$ is uniformly integrable w.r.t. μ , then as $n \rightarrow +\infty$, $f(Y_n) \rightarrow f(Y)$ in \mathbf{P} -probability for all measurable function $f : \mathcal{S} \rightarrow \mathbf{R}$.*

1.2. Quasi-stationary distributions for the generalized Langevin process. In this section, we study existence and uniqueness of the quasi-stationary distribution for the generalized Langevin equation (1.4). We first consider in Section 1.2.1, the case when $N = 1$ and ∇V is locally Lipschitz on \mathbf{R}^d (see Theorem 1.4). In Section 1.2.2, we then consider the case of $N \geq 2$ particles evolving according to the generalized Langevin equation and interacting through singular potentials (see Theorem 1.7).

The proof of Theorem 1.4 when $N = 1$ and when ∇V is locally Lipschitz over \mathbf{R}^d is very instructive, which explains our choice to split this section.

1.2.1. Generalized Langevin process with locally Lipschitz drifts. In this section, $N = 1$ and $V : \mathbf{R}^d \rightarrow [1, +\infty)$ (thus $\mathbf{O}_V = \mathbf{R}^d$), and we consider the process $(X_t = (x_t, v_t, z_t), t \geq 0)$ solution in $\mathcal{E} = \mathbf{R}^d \times \mathbf{R}^d \times \mathbf{R}^d$ to the generalized Langevin equation (1.4) when $N = 1$ (see Proposition 1.3). Recall that $\lambda, \alpha > 0, \gamma \geq 0$. The basic assumption of this section is the following.

Assumption [V_{loc}]. $N = 1$ and $V : \mathbf{R}^d \rightarrow [1, +\infty)$ belongs to $\mathbf{L}_{\text{Lip}}^{1,\text{loc}}(\mathbf{R}^d)$. In addition V is coercive (i.e. $V(x) \rightarrow +\infty$ as $|x| \rightarrow +\infty$).

In the following, we simply denote $\mathbf{R}^d \times \mathbf{R}^d \times \mathbf{R}^d$ by \mathbf{R}^{3d} . We denote the Hamiltonian function of the process (1.4) by

$$\mathbf{H}_{\text{GL}} : (x, v, z) \in \mathbf{R}^{3d} \mapsto V(x) + \frac{1}{2}|v|^2 + \frac{1}{2}|z|^2, \quad (1.8)$$

and its infinitesimal generator

$$\mathcal{L}_{\text{GL}} = v \cdot \nabla_x + (-\gamma v - \nabla_x V + \lambda z) \cdot \nabla_v + \gamma \Delta_v - (\alpha z + \lambda v) \cdot \nabla_z + \alpha \Delta_z. \quad (1.9)$$

Proposition 1.3. *Assume [V_{loc}]. For all $\mathbf{x}_0 \in \mathbf{R}^{3d}$, there exists a unique strong solution $(X_t = (x_t, v_t, z_t), t \geq 0)$ to (1.4) such that $X_0 = \mathbf{x}_0$ (this process is denoted by $(X_t(\mathbf{x}_0), t \geq 0)$). In addition, $(X_t(\mathbf{x}_0), t \geq 0)$ is a strong Markov process.*

Proof. Note that the coefficients in (1.4) are locally Lipschitz. The proof of the non explosion is very standard, but we write it since Equation (1.10) will play a key role in this work. Let $c > 0$ such that $\mathcal{L}_{\text{GL}} \mathbf{H}_{\text{GL}} \leq c \mathbf{H}_{\text{GL}}$ over \mathbf{R}^{3d} . Set for $R \geq 0$, $\sigma_{\mathcal{H}_R} := \inf\{t \geq 0, X_t \notin \mathcal{H}_R\}$, where $\mathcal{H}_R := \{\mathbf{x} \in \mathbf{R}^{3d}, \mathbf{H}_{\text{GL}}(\mathbf{x}) < R\}$ is open and bounded (since V is coercive). Since $\mathbf{H}_{\text{GL}}(X_{\sigma_{\mathcal{H}_R}}) = R$, it holds by the Itô formula, for all $\mathbf{x} \in \mathcal{H}_R, R > 0$:

$$\mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{H}_R} \leq t] \leq \frac{e^{ct}}{R} \mathbf{H}_{\text{GL}}(\mathbf{x}), \quad \forall t \geq 0. \quad (1.10)$$

The proof is complete. \square

In addition to [V_{loc}], we will assume the following growth condition on V , which basically implies that $V(x)$ behaves like $|x|^k$ as $|x| \rightarrow +\infty$, for some $k > 1$.

Assumption [V_{poly-x^k}]. *In addition to [V_{loc}], there exist $k > 1$ and $M_V, r_V, c_V > 0$ such that for all $x \in \mathbf{R}^d$ with $|x| \geq r_V$:*

$$c_V |x|^k \leq V(x) \leq M_V |x|^k \text{ and } c_V |x|^k \leq x \cdot \nabla V(x).$$

When $\gamma = 0$, we assume moreover that $|\nabla V(x)| \leq M_V |x|^{k-1}$ if $|x| \geq r_V$.

The first main result of this work is the following (see also its note just below).

Theorem 1.4. *Assume [V_{loc}] and [V_{poly-x^k}]. Let $\mathcal{D} = \mathcal{O} \times \mathbf{R}^d \times \mathbf{R}^d$ where \mathcal{O} is a subdomain of \mathbf{R}^d (not necessarily smooth neither bounded) such that $\mathbf{R}^d \setminus \overline{\mathcal{O}}$ is nonempty. Assume moreover that $k \in (1, 2]$ when $\gamma = 0$. For $\delta \in ((1 - \beta)/k, 1]$ fixed, let $\mathbf{W}_\delta : \mathbf{R}^{3d} \rightarrow [1, +\infty)$ be the Lyapunov function defined in (2.22) where the parameter $\beta > 0$ satisfies (2.26) if $\gamma > 0$, and (2.28) when $\gamma = 0$. Then, $\mathbf{P}_{\mathbf{x}}(\sigma_{\mathcal{D}} < +\infty) = 1$ for all $\mathbf{x} \in \mathcal{D}$, and for all $p \in (1, +\infty)$,*

i) *There exists a unique quasi-stationary distribution $\mu_{\mathcal{D}}^{(p)}$ for the process (1.4) on \mathcal{D} in the space $\mathcal{P}_{\mathbf{W}_\delta^{1/p}}(\mathcal{D})$.*

ii) *There exists $\lambda_{\mathcal{D}}^{(p)} > 0$ such that for all $t \geq 0$, the spectral radius of $P_t^{\mathcal{D}}$ equals*

$$r_{sp}(P_t^{\mathcal{D}}|_{\mathcal{B}_{\mathbf{W}_\delta^{1/p}}(\mathcal{D})}) = e^{-\lambda_{\mathcal{D}}^{(p)} t}.$$

In addition, for all $t \geq 0$, $\mu_{\mathcal{D}}^{(p)} P_t^{\mathcal{D}} = e^{-\lambda_{\mathcal{D}}^{(p)} t} \mu_{\mathcal{D}}^{(p)}$ and $\mu_{\mathcal{D}}^{(p)}(\mathbf{O}) > 0$ for all nonempty open subsets \mathbf{O} of \mathcal{D} . Furthermore, there is a unique continuous function $\varphi^{(p)}$ in $b_{W_{\delta}^{1/p}} \mathcal{B}(\mathcal{D})$ such that

$$\varphi^{(p)} > 0 \text{ on } \mathcal{D}, \quad \mu_{\mathcal{D}}^{(p)}(\varphi^{(p)}) = 1, \quad \text{and} \quad P_t^{\mathcal{D}} \varphi^{(p)} = e^{-\lambda_{\mathcal{D}}^{(p)} t} \varphi^{(p)} \text{ on } \mathcal{D}, \quad \forall t \geq 0.$$

iii) There exist $M > 0$ and $C \geq 1$ such that:

$$\sup_{\mathcal{A} \in \mathcal{B}(\mathcal{D})} |\mathbf{P}_{\nu}[X_t \in \mathcal{A} | t < \sigma_{\mathcal{D}}] - \mu_{\mathcal{D}}^{(p)}(\mathcal{A})| \leq C e^{-Mt} \frac{\nu(W_{\delta}^{1/p})}{\nu(\varphi^{(p)})}, \quad \forall t > 0, \forall \nu \in \mathcal{P}_{W_{\delta}^{1/p}}(\mathcal{D}).$$

Comments on Theorem 1.4. Let us recall (see [28]) that $\mu_{\mathcal{D}}^{(p)}$ is independent of p , i.e. $\mu_{\mathcal{D}}^{(p)} = \mu_{\mathcal{D}}^{(q)}$ and $\lambda_{\mathcal{D}}^{(p)} = \lambda_{\mathcal{D}}^{(q)}$ for any $p, q > 1$. We now discuss how to choose $\delta > 0$ depending on the values of the growth parameter $k > 1$ of V in $[\mathbf{V}_{\text{poly-}x^k}]$, and how W_{δ} behaves at high energy.

- When $\gamma > 0$ (resp. $\gamma = 0$) and (2.26) holds (resp. (2.28) holds), there exists $c > 0$ such that $W_{\delta} \leq \exp[c^{\delta} E^{\delta}]$, where $\mathbf{E}(x, v, z) = 1 + |x|^k + |v|^2 + |z|^2$. Hence, the smaller $\delta \in ((1 - \beta)/k, 1]$ is (see (2.22)), the smaller W_{δ} is. Moreover, for any probability measure $\mu(dx) = g(x)dx$ s.t. for some $\kappa, r, K, R > 0$, $g \leq K \exp[-\kappa E^r]$ on $\{x \in \mathbf{R}^{3d}, \mathbf{E}(x) > R\}$, it holds: $\int_{\mathbf{R}^{3d}} W_{\delta}^{1/p}(x) \mu(dx) < +\infty$ for any $r > \delta$ and $p > 1$.
- Let us first consider the case when $\gamma > 0$. In view of (2.26), when $k \geq 2$, one can choose any $\delta \in (0, 1)$ in the definition of W_{δ} in (2.22). Indeed, in this case $\min(1, k/2, k - 1) = 1$ and therefore $\beta > 0$ can be chosen as closed as desired (from below) to 1. Let us now consider the case when $\gamma = 0$ (recall in this case that $k \in (1, 2]$). When $k = 2$, $\beta = 1$ and therefore one can choose any $\delta \in (0, 1)$ in the definition of W_{δ} in (2.22).

The proof of Theorem 1.4 is given in Section 2.

Extension to non gradient force fields. In several cases in molecular dynamics the force field $-\nabla V$ is subject to nonequilibrium perturbations (the dynamics is then said to be out of equilibrium [67, 49, 40]), and this the setting we would like to treat here. To this end we consider the following assumption on the force field.

Assumption $[\mathbf{b}_{\text{non-gradient}}]$. The vector field $\mathbf{b} : \mathbf{R}^d \rightarrow \mathbf{R}^d$ decomposes over \mathbf{R}^d as $\mathbf{b} = -\nabla V + \boldsymbol{\ell}$, where: V satisfies $[\mathbf{V}_{\text{poly-}x^k}]$ and $\boldsymbol{\ell} : \mathbf{R}^d \rightarrow \mathbf{R}^d$ is a locally Lipschitz vector field such that for all $x \in \mathbf{R}^d$, $|\boldsymbol{\ell}(x)| \leq C(|x|^{(k-1)/2} + 1)$ for some $C > 0$.

Theorem 1.5. When $[\mathbf{b}_{\text{non-gradient}}]$ is satisfied, Theorem 1.4 is still valid verbatim for the process $(X_t = (x_t, v_t, z_t), t \geq 0)$ solution to the generalized Langevin equation

$$\begin{cases} dx_t &= v_t dt \\ dv_t &= \mathbf{b}(x_t) dt - \gamma v_t dt + \lambda z_t dt + \sqrt{2\gamma} dW_t \\ dz_t &= -\alpha z_t dt - \lambda v_t dt + \sqrt{2\alpha} dB_t. \end{cases}$$

Theorem 1.5 is proved in Section 2.4.

1.2.2. *Generalized Langevin process: extension of the results to singular interaction potentials.* In this section, we extend the results of the previous section to a system of $N \geq 2$ particles $X_t = (x_t, v_t, z_t) \in \mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}^{dN}$ whose positions $x_t = (x_t^1, \dots, x_t^N) \in \mathbf{R}^{dN}$, velocities $v_t = (v_t^1, \dots, v_t^N) \in \mathbf{R}^{dN}$, and noises $z_t = (z_t^1, \dots, z_t^N) \in \mathbf{R}^{dN}$ evolve in time $t \geq 0$ through the generalized Langevin equation (1.4) and which interact through singular potentials (note that we simply write \mathbf{R}^{dN} for $(\mathbf{R}^d)^N$). Let us more precisely introduce the assumptions on the potential function $V : \mathbf{R}^{dN} \rightarrow \overline{\mathbf{R}}$.

Assumption $[\mathbf{V}_{\text{coercive}}]$. The set $\mathbf{O}_V = \{x \in \mathbf{R}^{dN}, V(x) < +\infty\}$ is a subdomain of \mathbf{R}^{dN} and $V : \mathbf{O}_V \rightarrow [1, +\infty)$ belongs to $L_{\text{Lip}}^{1, \text{loc}}(\mathbf{O}_V)$. In addition, for all $R > 0$, $\mathcal{V}_R := \{y \in \mathbf{R}^{dN}, V(y) < R\}$ has compact closure in \mathbf{O}_V . Finally, $|\nabla V(x)| \rightarrow +\infty$ when $V(x) \rightarrow +\infty$.

Recall that the state space is $\mathcal{E} = \mathbf{O}_V \times \mathbf{R}^{dN} \times \mathbf{R}^{dN}$. Note that under $[\mathbf{V}_{\text{coercive}}]$, V is coercive: if \mathbf{O}_V is unbounded (resp. bounded), $V \rightarrow +\infty$ if and only if $x \rightarrow \{\infty\} \cup \partial\mathbf{O}_V$ (resp. $x \rightarrow \partial\mathbf{O}_V$). Without loss of generality, we can thus assume that $V \geq 1$ over \mathbf{O}_V and consequently $\mathbf{H}_{\text{GL}} \geq 1$ over \mathcal{E} . Assumption $[\mathbf{V}_{\text{coercive}}]$ is more general than $[\mathbf{V}_{\text{loc}}]$ since it allows to consider singular potentials.

To prove existence and uniqueness of quasi-stationary distributions in weighted spaces (see Theorem 1.7 below), the starting point is [28, Theorem 2.2]. The strategy will thus consists in proving $(\mathbf{C1}) \rightarrow (\mathbf{C5})$ for the process (1.4). Assumptions $(\mathbf{C1})$, $(\mathbf{C2})$, $(\mathbf{C4})$, and $(\mathbf{C5})$ will be proved for the process (1.4) when $[\mathbf{V}_{\text{coercive}}]$ holds. However, to construct a Lyapunov function satisfying $(\mathbf{C3})$, we will impose more explicit assumptions on V than $[\mathbf{V}_{\text{coercive}}]$ (see $[\mathbf{V}_{\text{sing1}}]$ below), that we introduce now.

For ease of notation we simply denote by $\{x^i \neq x^j\}$ the set $\{x = (x^1, \dots, x^N) \in \mathbf{R}^{dN}, x^i \neq x^j \text{ if } i \neq j\}$. Since what matters in this section is to treat the interaction potential part of the potential V of the system, we will assume that the confining potential is the simple quadratic function (see also Remark 1.8 below for extensions).

Assumption $[\mathbf{V-2}]$. *The confining potential V_c is the quadratic function on \mathbf{R}^d , i.e. $V_c(y) = a_0|y|^2/2$, $y \in \mathbf{R}^d$, $a_0 > 0$.*

Assumption $[\mathbf{V-int}]$. *The interaction potential $V_{\mathbf{I}} : \mathbf{R}^d \rightarrow \overline{\mathbf{R}}$ satisfies $V_{\mathbf{I}}(0) = +\infty$. In addition, there exist $\mathbf{B}, \beta > 0$ and a symmetric function $\Phi \in \mathbf{L}_{\text{Lip}}^{1,\text{loc}}(\mathbf{R}^d \setminus \{0\})$ s.t.*

$$V_{\mathbf{I}}(y) = \frac{\mathbf{B}}{|y|^\beta} + \Phi(y), \text{ for all } y \in \mathbf{R}^d \setminus \{0\}.$$

Furthermore, there exist $r_\Phi, C_\Phi, c_\Phi > 0$, and $0 \leq q_\Phi < \beta + 1$, such that Φ and $\nabla\Phi$ are bounded on $\{y \in \mathbf{R}^d, |y| > r_\Phi\}$, and $|\nabla\Phi(y)| \leq \frac{C_\Phi}{|y|^{q_\Phi}} + c_\Phi$ and $\lim_{|y| \rightarrow 0} |y|^\beta |\Phi(y)| = 0$.

Note that $V_{\mathbf{I}}$ is a symmetric function. Assumption $[\mathbf{V-int}]$ covers the cases of singular potentials used in molecular dynamics, namely: the Lennard-Jones potentials $V_{\mathbf{I}}(y) = c_1/|y|^{12} - c_2/|y|^6$ as well as Coulomb potentials $V_{\mathbf{I}}(y) = c_3/|x|^{d-2}$ when $d \geq 3$ ($c_1, c_2, c_3 > 0$). Note that in many applications in molecular dynamics, $d = 3$.

Assumption $[\mathbf{V}_{\text{sing1}}]$. *$d \geq 2$ and the potential function $V : \mathbf{R}^{dN} \rightarrow \overline{\mathbf{R}}$ writes*

$$V(x) = \sum_{i=1}^N V_c(x^i) + \sum_{i,j=1;i < j}^N V_{\mathbf{I}}(x^i - x^j) + V_{\mathbf{p}}(x), \quad (1.11)$$

where $V_{\mathbf{p}} \in \mathbf{L}_{\text{Lip}}^{1,\text{loc}}(\mathbf{R}^{dN})$, $\text{supp}(V_{\mathbf{p}}) \subset \{x^i \neq x^j\}$, $V_{\mathbf{I}}$ satisfies $[\mathbf{V-int}]$, and V_c satisfies $[\mathbf{V-2}]$.

When $[\mathbf{V}_{\text{sing1}}]$ is satisfied, it holds:

- (1) $\{V < +\infty\} = \{x^i \neq x^j\}$ which is open and connected (since $d \geq 2$). Hence

$$\mathbf{O}_V = \{x^i \neq x^j\}.$$

- (2) $V \in \mathbf{L}_{\text{Lip}}^{1,\text{loc}}(\mathbf{O}_V)$.

- (3) V is coercive on \mathbf{O}_V , i.e. $V(x) \rightarrow +\infty$ if and only if $|x| \rightarrow +\infty$ or for some $i \neq j$, $|x^i - x^j| \rightarrow 0$, that we write $x \rightarrow \{\infty\} \cup \partial\mathbf{O}_V$. Therefore, in this case:

$$\mathbf{H}_{\text{GL}}(x) \rightarrow +\infty \text{ if and only if } x \rightarrow \{\infty\} \text{ or } x \rightarrow \partial\mathbf{O}_V.$$

- (4) $|\nabla V|$ is coercive on \mathbf{O}_V (by [33, Lemma A.1]).

Note that $[\mathbf{V}_{\text{coercive}}]$ holds when $[\mathbf{V}_{\text{sing1}}]$ is satisfied. We have assumed that $d \geq 2$ in $[\mathbf{V}_{\text{sing1}}]$ for convenience: all the results stated under the Assumption $[\mathbf{V}_{\text{sing1}}]$ extend trivially to the case when $d = 1$ provided to choose in this case \mathbf{O}_V as a connected component of $\{V < +\infty\}$.

Proposition 1.6. *Assume that V satisfies $[\mathbf{V}_{\text{coercive}}]$. Then, for all $\mathbf{x}_0 \in \mathcal{E}$, there exists a unique strong solution $(X_t = (x_t, v_t, z_t), t \geq 0)$ to (1.4) such that $X_0 = \mathbf{x}_0$ and such that a.s. $X_t \in \mathcal{E} = \mathbf{O}_V \times \mathbf{R}^{dN} \times \mathbf{R}^{dN}$ for all $t \geq 0$. In addition, $(X_t(\mathbf{x}_0), t \geq 0)$ is a strong Markov process.*

Proof. Proposition 1.6 follows from the fact that $\mathcal{L}_{\text{GL}}\mathbf{H}_{\text{GL}} \leq c\mathbf{H}_{\text{GL}}$ over \mathcal{E} for some $c > 0$. We also mention that this inequality implies the key inequality $\mathbf{P}_x[\sigma_{\mathcal{H}_R} \leq t] \leq \frac{e^{ct}}{R} \mathbf{H}_{\text{GL}}(\mathbf{x})$ valid for all $\mathbf{x} \in \mathcal{H}_R$ and $t \geq 0$ ($\sigma_{\mathcal{H}_R} = \inf\{t \geq 0, X_t \notin \mathcal{H}_R\}$ is the first exit time from the open and bounded set $\mathcal{H}_R := \{\mathbf{x} \in \mathbf{R}^{3dN}, \mathbf{H}_{\text{GL}}(\mathbf{x}) < R\} \subset \mathcal{E}$). \square

The main result of this section is the extension of Theorem 1.4 to the case of singular potentials V :

Theorem 1.7. *Assume $[\mathbf{V}_{\text{sing1}}]$. Let \mathcal{O} be a subdomain of \mathbf{O}_V such that $\mathbf{O}_V \setminus \overline{\mathcal{O}}$ is nonempty, and set $\mathcal{D} = \mathcal{O} \times \mathbf{R}^d \times \mathbf{R}^d$. Let also $\delta \in (0, 1]$. Then, for all $p \in (1, +\infty)$, Items i)–iii) in Theorem 1.4 are valid verbatim for the killed semigroup $(P_t^{\mathcal{D}}, t \geq 0)$ of the process $(X_t, t \geq 0)$ solution to (1.4) over $\mathcal{E} = \mathbf{O}_V \times \mathbf{R}^{dN} \times \mathbf{R}^{dN}$ (see Proposition 1.6) with the Lyapunov function $\mathbf{W}_\delta : \mathcal{E} \rightarrow [1, +\infty)$ defined in (3.3) (and which satisfies the upper bound (3.4)).*

The proof of Theorem 1.7 is made in Section 3.

Remark 1.8. *Let us mention that when $\gamma > 0$ (resp. $\gamma = 0$), with minor changes in the proof of (C3) in Section 3, one deduces that Theorem 1.7 is still valid when V_c satisfies $[\mathbf{V}_{\text{poly-}x^k}]$ (resp. when V_c satisfies $[\mathbf{V}_{\text{poly-}x^k}]$ with $k \in (1, 2]$), and for $\delta \in ((1 - \beta)/k, 1]$, see (2.26) and (2.28) for the definition of β .*

1.3. Quasi-stationary distribution for the Nosé-Hoover process.

1.3.1. *Main result.* In this section, we consider a system of $N \geq 2$ particles with positions $x_t = (x_t^1, \dots, x_t^N) \in \mathbf{R}^{dN}$ and velocities $v_t = (v_t^1, \dots, v_t^N) \in \mathbf{R}^{dN}$ evolving according to the Nosé-Hoover process (1.5) where V satisfies $[\mathbf{V}_{\text{coercive}}]$. Recall that the state space is

$$\mathcal{E} = \mathbf{O}_V \times \mathbf{R}^{dN} \times \mathbf{R}, \quad (1.12)$$

The Hamiltonian function of the process (1.5) is denoted by

$$\mathbf{H}_{\text{NH}} : (x, v, y) \in \mathcal{E} \mapsto V(x) + \frac{1}{2}|v|^2 + \frac{1}{2}|y|^2, \quad (1.13)$$

and its infinitesimal generator by

$$\mathcal{L}_{\text{NH}} = v \cdot \nabla_x - (y + \gamma)v \cdot \nabla_v - \nabla V \cdot \nabla_v + \gamma \Delta_v + (|v|^2 - dN)\partial_y. \quad (1.14)$$

Proposition 1.9. *Assume that V satisfies $[\mathbf{V}_{\text{coercive}}]$. For all $\mathbf{x}_0 \in \mathcal{E}$, there exists a unique strong solution $(X_t = (x_t, v_t, y_t), t \geq 0)$ to (1.5) such that $X_0 = \mathbf{x}_0$. In addition, a.s. $X_t(\mathbf{x}_0) \in \mathcal{E}$ for all $t \geq 0$, and $(X_t(\mathbf{x}_0), t \geq 0)$ is a strong Markov process.*

Proof. Since for some $c > 0$, $\mathcal{L}_{\text{NH}}\mathbf{H}_{\text{NH}} \leq c\mathbf{H}_{\text{NH}}$ over \mathcal{E} , the proof is the same as Proposition 1.3, and thus omitted. Again, one has $\mathbf{P}_x[\sigma_{\mathcal{H}_R} \leq t] \leq \frac{e^{ct}}{R} \mathbf{H}_{\text{NH}}(\mathbf{x})$ for all $\mathbf{x} \in \mathcal{H}_R$ and $t \geq 0$, where $\sigma_{\mathcal{H}_R} = \inf\{t \geq 0, X_t \notin \mathcal{H}_R\}$ is the first exit time from the open and bounded subset $\mathcal{H}_R := \{\mathbf{x} \in \mathbf{R}^{2dN+1}, \mathbf{H}_{\text{NH}}(\mathbf{x}) < R\} \subset \mathcal{E}$. \square

As already explained in the introduction, to prove existence and uniqueness of quasi-stationary distributions in weighted spaces (see Theorem 1.11 below), the starting point is Theorem 4.6 below. Assumptions (C1), (C2), (C4), and (C5') (defined at the beginning of Section 4.3) will be proved when $[\mathbf{V}_{\text{coercive}}]$ holds. To prove (C3), we will rely on the work [32]. For that reason, we impose similar extra assumptions on the potential V :

Assumption $[\mathbf{V}_{\text{sing2}}]$. *The condition $[\mathbf{V}_{\text{coercive}}]$ holds with in addition: $V \in \mathcal{C}^2(\mathbf{O}_V)$, and for some $\zeta \in (1, 2)$ and $\delta \in (1/2, 1]$:*

$$\frac{|\text{Hess}V(x)|}{|\nabla V(x)|^\zeta} \rightarrow 0 \text{ and } \frac{|\nabla V(x)|^{2-\zeta}}{V(x)^{1-\delta}} \rightarrow +\infty \text{ when } V(x) \rightarrow +\infty. \quad (1.15)$$

Note that if there exists such a $\zeta \in (1, 2)$, then $\delta = 1$ always satisfies the second condition in (1.15). As it will be clear, the better δ 's are those closed to $1/2$, since much smaller Lyapunov functions can be constructed in this case.

Assumption **[Vcoercive]** differs from Assumption **normal** in [32] since: (i) V is much less regular (ii) we have an extra condition in (1.15) (namely the one involving $\delta > 0$), and (iii) because we do not assume that $\int_{\mathcal{E}} e^{-H_{\text{NH}}(\mathbf{x})} d\mathbf{x} < +\infty$ (since this will be automatically satisfied, see Remark 1.10). The last (extra) condition involving $\delta > 0$ in (1.15) will be needed in order to build smaller Lyapunov function than in [32]. Indeed, with such a $\delta > 0$, we will build Lyapunov function \mathbf{W} such that $\mathbf{W} \leq e^{c^\delta H_{\text{NH}}^\delta}$ on \mathcal{E} for some $c > 0$ independent of $\delta > 0$.

Remark 1.10. *It will be shown in this work that the nonkilled process $(P_t, t \geq 0)$ is strong Feller and satisfies the topological transitivity [77, Eq. (2.2)]. In addition, under **[Vcoercive]**, there exists a Lyapunov function \mathbf{W} over \mathcal{E} such that $\mathcal{L}_{\text{NH}}\mathbf{W} \leq -c + b\mathbf{1}_K$ (see [32]). Therefore, since the measure $\mu_{\text{Gibbs}}(d\mathbf{x}) = e^{-H_{\text{NH}}(\mathbf{x})} d\mathbf{x}$ is invariant, $\int_{\mathcal{E}} e^{-H_{\text{NH}}(\mathbf{x})} d\mathbf{x}$ is finite.*

The main result of this section is the following and provides existence, uniqueness of the quasi-stationary distribution of the Nosé-Hoover process (1.5) in a domain $\mathcal{D} = \mathcal{O} \times \mathbf{R}^{dN} \times \mathbf{R}$ (as well as the exponential convergence towards this quasi-stationary distribution).

Theorem 1.11. *Assume that V satisfies **[Vsing2]**. Let $\delta \in (1/2, 1]$ be as in the last condition in (1.15). Let $\mathcal{D} = \mathcal{O} \times \mathbf{R}^{dN} \times \mathbf{R}$ where \mathcal{O} is a subdomain of \mathbf{O}_V such that $\mathbf{O}_V \setminus \overline{\mathcal{O}}$ is nonempty. Then, for all $p \in (1, +\infty)$, Items i)→iii) in Theorem 1.4 are valid verbatim for the killed semigroup $(P_t^{\mathcal{D}}, t \geq 0)$ of the process $(X_t, t \geq 0)$ solution to (1.5) over $\mathcal{E} = \mathbf{O}_V \times \mathbf{R}^{dN} \times \mathbf{R}$ (see Proposition 1.9), with the Lyapunov function $\mathbf{W}_\delta : \mathcal{E} \rightarrow [1, +\infty)$ defined in (4.17) (and which satisfies the upper bound (4.18)).*

Theorem 1.11 is proved in Section 4.

1.3.2. *On Assumption **[Vsing2]**.* In this section, we provide some examples of singular potential functions used in molecular dynamics which satisfy **[Vsing2]**. To this end, let us consider a potential V of the form (1.11) where:

- The perturbation potential $V_{\mathbf{p}} \in \mathcal{C}_c^2(\mathbf{O}_V)$.
- The confining potential $V_{\mathbf{c}}$ is \mathcal{C}^2 over \mathbf{R}^d and behaves at infinity as $|x|^k$ with $k > 1$.
- Either $V_{\mathbf{I}} \equiv 0$ over \mathbf{R}^{dN} (in this case, $\mathbf{O}_V = \mathbf{R}^{dN}$) or $V_{\mathbf{I}}$ satisfies **[Vint]** with $\Phi \in \mathcal{C}^2(\mathbf{R}^d \setminus \{0\})$ (in this case, \mathbf{O}_V is given by $\{x^i \neq x^j\}$).

As already seen, Assumption **[Vcoercive]** is satisfied. Since in addition $(k-2)/(k-1) < 1$ and $1 < (\beta+2)/(\beta+1) < 2$, the first condition in (1.15) is also always satisfied for any $\zeta \in (1 + \frac{1}{\beta+1}, 2)$ (use also [33, Lemma A.1]). The last condition in (1.15) writes $\delta > \max[1/2, 1 - \frac{k-1}{k}(2-\zeta), 1 - \frac{\beta+1}{\beta}(2-\zeta)]$. Note that $2 - \zeta \in (0, \frac{\beta}{\beta+1})$. The best choice of ζ is to take it small enough such that $2 - \zeta$ is closed (from below) to $\frac{\beta}{\beta+1}$. In conclusion, **[Vsing2]** holds in this case if

$$\max \left[1/2, 1 - \frac{k-1}{k} \frac{\beta}{\beta+1} \right] < \delta \leq 1.$$

If $\beta \geq 1$, by choosing the external potential $V_{\mathbf{c}}$ such that $k \gg 1$, this previous condition simply becomes empty, i.e. one can choose any $\delta \in (1/2, 1]$.

2. GENERALIZED LANGEVIN PROCESS: PROOF OF THEOREM 1.4

This section is dedicated to the proof of Theorem 1.4 (see also Subsection 2.4 for the proof of Theorem 1.5). We recall that we will rely on [28, Theorem 2.2] and, the strategy thus consists to show that **(C1)**→**(C5)** hold.

In all this section, we assume that **[Vloc]** holds.

2.1. On the conditions (C1), (C2), and (C4). Assumption (C2) is proved in Section 2.1.2, and (C1) and (C4) are proved in Section 2.1.3 (see Proposition 2.3, Theorem 2.6, and Proposition 2.7). We first provide in Section 2.1.1 explanations of the method we use in this work to check the regularity conditions (C1), (C2), and (C4) for the process (1.4) as well as for the process (1.5).

2.1.1. The energy splitting approach to prove the regularity conditions. In this section, we explain the strategy developed in this work to prove (C1), (C2), and (C4) in a weak regularity setting.

On condition (C1). We first observe that if $V \in \mathcal{C}^\infty(\mathbf{R})$, using the Hörmander's theory, it is straightforward to deduce (C1). When ∇V is only locally Lipschitz, one must argue differently. When $\gamma > 0$, thanks to the global Girsanov formula (2.5), we can make the non smooth term ∇V appear only in the so-called Doléans-Dade exponential. With this formula, the proof of (C1) relies on tools from the theory of SDEs. When $\gamma = 0$, we cannot argue as previously. This is because there is no Brownian motion anymore in the velocity variable v_t in (1.4). As explained in the introduction above, we will thus adopt a different approach to prove (C1) (and also (C4)).

This approach is based on a rather natural strategy which can be summarized as the study of the behavior of the process at low and at high energy \mathbf{H}_{GL} w.r.t. initial conditions in the compact sets. To explain this approach, the starting point consists in splitting the measure $\mathbf{P}_x[X_t \in \cdot]$ as follows:

$$\mathbf{P}_x[X_t \in \cdot] = \mathbf{P}_x[X_t \in \cdot, \sigma_{\mathcal{H}_R} \leq t] + \mathbf{P}_x[X_t \in \cdot, t < \sigma_{\mathcal{H}_R}] =: \rho_x^R(\cdot) + \theta_x^R(\cdot). \quad (2.1)$$

The asymptotic behavior of the function $R \mapsto \rho_x^R(\cdot)$ as $R \rightarrow +\infty$ uniformly w.r.t the initial conditions in the compact sets provides the behavior of the process w.r.t high energies \mathbf{H}_{GL} , while the continuity property of $x \mapsto \theta_x^R(\cdot)$ at fixed $R > 0$ describes the behavior of the process at low energy w.r.t the initial conditions. The approach then relies on the observation that (C1) holds if

$$\lim_{R \rightarrow +\infty} \rho_x^R(\cdot) \rightarrow 0 \text{ uniformly w.r.t. } x \text{ in the compact sets} \quad (2.2)$$

and if for all $R > 0$,

$$x \mapsto \theta_x^R(\cdot) \text{ is continuous for the } \tau\text{-topology over } \mathcal{H}_R, \quad (2.3)$$

i.e. for the topology corresponding to convergence against test functions $f \in b\mathcal{B}(\mathcal{H}_R)$. Equation (2.2) is in our setting a consequence of (1.10) which we recall, follows from the fact that $\mathcal{L}_{\text{GL}}\mathbf{H}_{\text{GL}} \leq c\mathbf{H}_{\text{GL}}$. The behavior of the process at low energy (namely (2.3)) is trickier to deduce. It will be obtained combining mainly two general ingredients: the powerful convergence result Proposition 1.2 which, we recall, requires in particular uniform integrability of the transition probabilities, and the uniform continuity of the distribution functions near 0^+ of exit times from \mathbf{R}^{3d} -balls uniformly w.r.t the initial conditions (see Lemma 2.5). The Markov property of the process (1.4) will be also fully exploited.

On condition (C4). The proof of the continuity of the mapping $x \mapsto \mathbf{P}_x[X_t \in \cdot, t < \sigma_{\mathcal{D}}]$ (i.e. the proof of (C4)), where $\mathcal{D} = \mathcal{O} \times \mathbf{R}^m$, requires extra analysis since it involves to study the continuity property of $x \mapsto \sigma_{\mathcal{D}}(x)$. The techniques developed for the kinetic Langevin process (1.1) in [28, 29] (see also [47, 48]) to prove (C4) require $\partial\mathcal{O} \cap \mathbf{O}_V$ to be \mathcal{C}^2 . These techniques cannot longer be used without regularity assumption on $\partial\mathcal{O}$. To prove (C4), we will use the energy splitting approach (so-called because based on the energy splitting Equation (2.1)) described previously. However, we mention that to check (C4), we have to study the distribution functions near 0^+ of exit times from \mathbf{R}^d -balls uniformly w.r.t the initial conditions, which is the purpose of Lemma 2.4.

We mention that the energy splitting approach is also used at many other places in this work, and in particular it is the starting point for the proofs of:

- Lemma 2.4 as well as in the proof of (C2) (see the proof of Proposition 2.2).
- Conditions (C1), (C2), and (C4) for both the generalized Langevin process (1.4) and the Nosé-Hoover process (1.5) when V is a singular potential (see the proofs of Proposition 3.1, Theorem 4.1, and Proposition 4.2).

Remark 2.1. Finally, we mention that the energy splitting approach can be also applied to solutions of other SDEs as soon as there is a Lyapunov function V such that $\mathcal{L}V \leq cV$ ($c > 0$, and \mathcal{L} being the extended generator of the process). What replaces H in this case is the energy V .

2.1.2. *On Assumption (C2).* In this section, we check Assumption (C2).

Proposition 2.2. Assume $[V_{\text{loc}}]$. Let $t \geq 0$ and $(x_n)_n$ in \mathbf{R}^{3d} such that $x_n \rightarrow x \in \mathbf{R}^{3d}$ as $n \rightarrow +\infty$. Then, for all $\epsilon > 0$, $\mathbf{P}[\sup_{s \in [0, t]} |X_s(x_n) - X_s(x)| \geq \epsilon] \rightarrow 0$ as $n \rightarrow +\infty$. In particular, Assumption (C2) is satisfied.

Proof. We denote by \mathbf{a} the drift of the equation (1.4), namely for $\mathbf{x} = (x, v, z) \in \mathbf{R}^{3d}$,

$$\mathbf{a}(\mathbf{x}) = \begin{pmatrix} v \\ -\nabla V(x) - \gamma v + \lambda z \\ -\alpha z - \lambda v \end{pmatrix}.$$

Note that \mathbf{a} is a locally Lipschitz vector field over \mathbf{R}^{3d} . Let $R_0 > 0$ such that $x_n, x \in \mathcal{H}_R = \{x, H_{\text{GL}}(x) < R\}$ for all $R \geq R_0$ and $n \geq 0$. In the following we assume that $R \geq R_0$. By Gronwall's inequality, we have for all $R \geq R_0$, when $t < \sigma_{\mathcal{H}_R}(x) \wedge \sigma_{\mathcal{H}_R}(x_n)$,

$$\sup_{s \in [0, t]} |X_s(x) - X_s(x_n)| \leq |x - x_n| e^{\mathbf{a}_R t},$$

for some $\mathbf{a}_R > 0$. Thus, one has for all $\epsilon > 0$ and $R \geq R_0$, as $n \rightarrow \infty$,

$$\mathbf{p}_n(R) := \mathbf{P} \left[\sup_{s \in [0, t]} |X_s(x) - X_s(x_n)| \geq \epsilon, t < \sigma_{\mathcal{H}_R}(x) \wedge \sigma_{\mathcal{H}_R}(x_n) \right] \rightarrow 0.$$

Consequently, it holds:

$$\begin{aligned} & \mathbf{P} \left[\sup_{s \in [0, t]} |X_s(x) - X_s(x_n)| \geq \epsilon \right] \\ &= \mathbf{p}_n(R) + \mathbf{P} \left[\sup_{s \in [0, t]} |X_s(x) - X_s(x_n)| \geq \epsilon, t \geq \sigma_{\mathcal{H}_R}(x) \wedge \sigma_{\mathcal{H}_R}(x_n) \right] \\ &\leq \mathbf{p}_n(R) + \mathbf{P} [t \geq \sigma_{\mathcal{H}_R}(x) \wedge \sigma_{\mathcal{H}_R}(x_n)] \\ &\leq \mathbf{p}_n(R) + \mathbf{P} [t \geq \sigma_{\mathcal{H}_R}(x)] + \mathbf{P} [t \geq \sigma_{\mathcal{H}_R}(x_n)] \\ &\leq \mathbf{p}_n(R) + 2R_0 \frac{e^{ct}}{R}, \end{aligned}$$

where we have used (1.10) to get the last inequality together with the fact that $H_{\text{GL}}(x_n) < R_0$ and $H_{\text{GL}}(x) < R_0$. Let us now consider $\delta > 0$ and $\epsilon > 0$. Pick $R_\delta > 0$ such that $2R_0 \frac{e^{ct}}{R_\delta} \leq \delta/2$. For this fixed R_δ , $\mathbf{p}_n(R_\delta) \rightarrow 0$ as $n \rightarrow +\infty$, and thus, there exists $N_\delta \geq 1$ such that for all $n \geq N_\delta$, $\mathbf{p}_n(R_\delta) \leq \delta/2$. The proof of the proposition is complete. \square

2.1.3. *On Assumptions (C1) and (C4).* In this section, we prove that (C1) and (C4) are satisfied for the process (1.4) when $[V_{\text{loc}}]$ holds.

On Assumption (C1). In this section, we prove (C1).

Assumption (C1) when $\gamma > 0$.

Proposition 2.3. Assume $[V_{\text{loc}}]$ and $\gamma > 0$. Then, the nonkilled semigroup P_t of the solution to the generalized Langevin equation (1.4) is strong Feller for every $t > 0$.

The proof of Proposition 2.3 we give below actually only requires that V is coercive and is differentiable, and that ∇V is just continuous (and in this case, one rather considers the weak solution to (1.4)).

Proof. Let $(X_t^0 = (x_t^0, v_t^0, z_t^0), t \geq 0)$ in \mathbf{R}^{3d} be the strong solution to the stochastic differential equation

$$dx_t^0 = v_t^0 dt, \quad dv_t^0 = \sqrt{2\gamma} dW_t, \quad dz_t^0 = \sqrt{2\alpha} dB_t. \quad (2.4)$$

We denote by \mathbf{F} the following vector field over \mathbf{R}^{3d} and by Σ the following square constant matrix of size $2d$:

$$\mathbf{F}(\mathbf{x}) = \begin{pmatrix} -\nabla V(x) - \gamma v + \lambda z \\ -\alpha z - \lambda v \end{pmatrix} \quad \text{and} \quad \Sigma = \begin{pmatrix} \sqrt{2\gamma} I_{\mathbf{R}^d} & 0 \\ 0 & \sqrt{2\alpha} I_{\mathbf{R}^d} \end{pmatrix}.$$

Arguing as in [77, Lemma 1.1], the following Girsanov's formula holds for all $T > 0$,

$$\frac{d\mathbf{P}_x}{d\mathbf{P}_x^0} \Big|_{\mathcal{F}_T} = \mathcal{M}_T(\mathbf{x}), \quad (2.5)$$

where \mathbf{P}_x (resp. \mathbf{P}_x^0) is the law of $(X_t(\mathbf{x}), t \geq 0)$ (resp. of $(X_t^0(\mathbf{x}), t \geq 0)$), and for $t \geq 0$,

$$\mathcal{M}_t(\mathbf{x}) = \exp \left[\int_0^t \Sigma^{-1} \mathbf{F}(X_s^0(\mathbf{x})) \cdot d\mathbf{w}_s - \frac{1}{2} \int_0^t |\Sigma^{-1} \mathbf{F}(X_s^0(\mathbf{x}))|^2 ds \right],$$

is the Doléans-Dade exponential (true) martingale, and $\mathbf{w}_s = (B_s, W_s)^T$.

Fix $t > 0$. By (2.5), P_t is strong Feller if $\mathbf{z} \in \mathbf{R}^{3d} \mapsto \mathbf{E}_z[f(X_t^0) \mathcal{M}_t]$ is continuous, which we shall prove now. Note that a.s. $\sup_{s \in [0, t]} |X_s^0(\mathbf{z}) - X_s^0(\mathbf{x})| \rightarrow 0$ as $\mathbf{z} \rightarrow \mathbf{x} \in \mathbf{R}^{3d}$. Note also that $(X_t^0, t \geq 0)$ has a smooth density w.r.t. the Lebesgue measure. Then, using Proposition 1.2, we deduce that for any $f \in b\mathcal{B}(\mathbf{R}^{3d})$, $\mathbf{z} \in \mathbf{R}^{3d} \mapsto f(X_t^0(\mathbf{z}))$ is continuous in \mathbf{P} -probability.

On the other hand, $\mathbf{z} \in \mathbf{R}^{3d} \mapsto \mathcal{M}_t(\mathbf{z})$ is continuous in \mathbf{P} -probability. Since \mathbf{F} is unbounded and not globally Lipschitz, we provide the proof of this claim. Set for $R \geq 1$,

$$\sigma_{\mathbf{B}(0, R)}^0(\mathbf{z}) := \inf\{s \geq 0, X_s^0(\mathbf{z}) \notin \mathbf{B}(0, R)\},$$

where $\mathbf{B}(0, R) := \{y \in \mathbf{R}^{3d}, |y| < R\}$. If $|\mathbf{z}| \leq \sqrt{R}$, $\mathbf{P}_z[\sigma_{\mathbf{B}(0, R)}^0 \leq t] \leq \mathbf{h}(R) := \mathbf{P}[\sup_{s \in [0, t]} |\Sigma \mathbf{w}_s| \geq R - \sqrt{R}] + \mathbf{P}[\sqrt{2\gamma} \int_0^t |W_s| ds \geq R - t\sqrt{R} - \sqrt{R}] \rightarrow 0$ as $R \rightarrow +\infty$. Let $\mathbf{z}_n \rightarrow \mathbf{z} \in \mathbf{R}^{3d}$, and $R_z \geq 1$ such that $|\mathbf{z}_n| + |\mathbf{z}| \leq \sqrt{R_z}$, $\forall n \geq 0$. Pick $c > 0$. Let $\epsilon > 0$ and $R_\epsilon > R_z$ such that $\mathbf{h}(R_\epsilon) \leq \epsilon/4$. Consider also a continuous bounded vector field $\mathbf{F}_{R_\epsilon} : \mathbf{R}^{3d} \rightarrow \mathbf{R}^{2d}$ such that $\mathbf{F}_{R_\epsilon} = \mathbf{F}$ on $\mathbf{B}(0, R_\epsilon + 1)$. Set $\delta_n(\mathbf{F}) := |\int_0^t \Sigma^{-1} [\mathbf{F}(q_s^0(\mathbf{z}_n)) - \mathbf{F}(q_s^0(\mathbf{z}))] \cdot d\mathbf{w}_s|$. Then, for all $n \geq 0$, the quantity $\mathbf{P}[\delta_n(\mathbf{F}) > c]$ is bounded by

$$\begin{aligned} & \mathbf{P}[\sigma_{\mathbf{B}(0, R_\epsilon)}^0(\mathbf{z}_n) \wedge \sigma_{\mathbf{B}(0, R_\epsilon)}^0(\mathbf{z}) \leq t] + \mathbf{P}[\delta_n(\mathbf{F}) > c, t < \sigma_{\mathbf{B}(0, R_\epsilon)}^0(\mathbf{z}) \wedge \sigma_{\mathbf{B}(0, R_\epsilon)}^0(\mathbf{z}_n)] \\ & \leq \mathbf{P}[\sigma_{\mathbf{B}(0, R_\epsilon)}^0(\mathbf{z}_n) \leq t] + \mathbf{P}[\sigma_{\mathbf{B}(0, R_\epsilon)}^0(\mathbf{z}) \leq t] + \mathbf{P}[\delta_n(\mathbf{F}_{R_\epsilon}) > c, t < \sigma_{\mathbf{B}(0, R_\epsilon)}^0(\mathbf{z}) \wedge \sigma_{\mathbf{B}(0, R_\epsilon)}^0(\mathbf{z}_n)] \\ & \leq \frac{\epsilon}{2} + \mathbf{P}[\delta_n(\mathbf{F}_{R_\epsilon}) > c]. \end{aligned}$$

Since $\mathbf{P}[\delta_n(\mathbf{F}_{R_\epsilon}) > c] \rightarrow 0$ as $n \rightarrow +\infty$ by well-known convergence properties of stochastic integrals, we finally get that there exists $N_\epsilon \geq 0$, for all $n \geq N_\epsilon$, $\mathbf{P}[\delta_n(\mathbf{F}) > c] \leq \epsilon$. With similar arguments, we also prove that the mapping $\mathbf{x} \in \mathbf{R}^{3d} \mapsto \int_0^t |F(q_s^0(\mathbf{x}))|^2 ds$ is continuous in \mathbf{P} -probability. The claim then follows applying the continuous mapping theorem.

Since in addition, $\mathbf{E}[\mathcal{M}_t(\mathbf{x})] = 1$ for all \mathbf{x} , using the Vitali convergence theorem, $\mathbf{z} \in \mathbf{R}^{3d} \mapsto \mathbf{E}_z[f(X_t^0) \mathcal{M}_t]$ is continuous. The proof of **(C1)** is complete when $\gamma > 0$. \square

Assumption **(C1)** when $\gamma = 0$.

For $\mathbf{x} = (x, v, z) \in \mathbf{R}^{3d}$, we denote by

$$\sigma_{\mathcal{B}(x, \delta)}(\mathbf{x}) = \inf\{t \geq 0, x_t(\mathbf{x}) \notin \mathcal{B}(x, \delta)\}, \quad (2.6)$$

the first exit time for the process $(x_t(\mathbf{x}), t \geq 0)$ from the open ball $\mathcal{B}(x, \delta)$ in \mathbf{R}^d centered at $x \in \mathbf{R}^d$ and of radius $\delta > 0$. When there is no confusion, we simply write it $\sigma_{\mathcal{B}(x, \delta)}$.

We start with two crucial lemmata which hold for any $\gamma \geq 0$ and which will be fundamental to prove **(C1)** when $\gamma = 0$ and **(C4)** when $\gamma \geq 0$.

Lemma 2.4. Assume $[\mathbf{V}_{\text{loc}}]$ and $\gamma \geq 0$. It holds for all compact subset K of \mathbf{R}^{3d} and $\delta > 0$,

$$\lim_{s \rightarrow 0^+} \sup_{\mathbf{x}=(x,v,z) \in K} \mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(x,\delta)} \leq s] = 0.$$

We will perform the proof when $\gamma = 0$ but, it is straightforward to adapt the proof to the case $\gamma > 0$.

Proof. Assume $\gamma = 0$. Fix $\delta > 0$ and let $R_K > 0$ such that $K \subset \mathcal{H}_{R_K}$. Let $\mathbf{x} = (x, v, z) \in K$ and $R \geq R_K$. We have using (1.10), for all $s \in [0, 1]$,

$$\mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(x,\delta)} \leq s] \leq \mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(x,\delta)} \leq s, s < \sigma_{\mathcal{H}_R}] + \frac{e^c}{R} \sup_{y \in K} \mathbf{H}_{\text{GL}}(y).$$

In addition, it holds

$$\begin{aligned} \mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(x,\delta)} \leq s, s < \sigma_{\mathcal{H}_R}] &\leq \mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(x,\delta)} \leq s, |x_s - x| < \delta/2, s < \sigma_{\mathcal{H}_R}] \\ &\quad + \mathbf{P}_{\mathbf{x}}[|x_s - x| \geq \delta/2, s < \sigma_{\mathcal{H}_R}]. \end{aligned}$$

Note that when $X_0 = \mathbf{x}$, $\sigma_{\mathcal{B}(x,\delta)} \leq s$, and $|x_s - x| < \delta/2$, it holds $|x_s - x_{\sigma_{\mathcal{B}(x,\delta)}}| \geq \delta/2$. Then, by the strong Markov property:

$$\begin{aligned} &\mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(x,\delta)} \leq s, |x_s - x| < \delta/2, s < \sigma_{\mathcal{H}_R}] \\ &\leq \mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(x,\delta)} \leq s, |x_s - x_{\sigma_{\mathcal{B}(x,\delta)}}| \geq \delta/2, s < \sigma_{\mathcal{H}_R}] \\ &= \mathbf{P}_{\mathbf{x}}[\{\sigma_{\mathcal{B}(x,\delta)} \leq s\} \cap \{|x_s - x_{\sigma_{\mathcal{B}(x,\delta)}}| \geq \delta/2\} \cap \{s < \sigma_{\mathcal{H}_R}\} \cap \{X_u \in \mathcal{H}_R, \forall u \in [0, \sigma_{\mathcal{B}(x,\delta)}]\}] \\ &= \mathbf{E}_{\mathbf{x}} \left[\mathbf{1}_{\sigma_{\mathcal{B}(x,\delta)}(\mathbf{x}) \leq s} \mathbf{1}_{X_u \in \mathcal{H}_R, \forall u \in [0, \sigma_{\mathcal{B}(x,\delta)}]} \right. \\ &\quad \left. \times \mathbf{P}_{X_{\sigma_{\mathcal{B}(x,\delta)}(\mathbf{x})}(\mathbf{x})} [|x_{s-\sigma_{\mathcal{B}(x,\delta)}(\mathbf{x})} - x_0| \geq \delta/2, s - \sigma_{\mathcal{B}(x,\delta)}(\mathbf{x}) < \sigma_{\mathcal{H}_R}] \right] := \mathbf{p}(\mathbf{x}, s, R). \end{aligned}$$

Let us now consider $\epsilon > 0$. We choose $R_{\epsilon,K} = 3e^c \sup_{y \in K} \mathbf{H}_{\text{GL}}(y)/\epsilon + R_K$. Then, using (1.10), one has for all $\mathbf{x} \in K$ and $s \in [0, 1]$,

$$\mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(x,\delta)} \leq s] \leq \mathbf{p}(\mathbf{x}, s, R_{\epsilon,K}) + \mathbf{P}_{\mathbf{x}}[|x_s - x| \geq \delta/2, s < \sigma_{\mathcal{H}_{R_{\epsilon,K}}}] + \frac{\epsilon}{3}. \quad (2.7)$$

Let us now study the term $\mathbf{p}(\mathbf{x}, s, R_{\epsilon,K})$. To this end, let $s \in [0, 1]$ and let us consider an initial condition $\mathbf{z} = (x_z, v_z, z_z)$ such that $x_z \in \partial\mathcal{B}(x, \delta)$, $\mathbf{z} \in \mathcal{H}_{R_{\epsilon,K}}$, and $u \in [0, s]$. We now study the term $\mathbf{P}_{\mathbf{z}}[|x_{s-u} - x_z| \geq \delta/2, s - u < \sigma_{\mathcal{H}_{R_{\epsilon,K}}}]$.

Note that $x_{s-u} = x_z + \int_0^{s-u} v_t dt$, and thus,

$$\begin{aligned} x_{s-u} - x_z &= \int_0^{s-u} \left[v_z - \int_0^t \nabla V(x_a) da \right] dt \\ &\quad + \int_0^{s-u} \left[\int_0^t \lambda(z_z + \int_0^a [-\alpha z_h - \lambda v_h] dh + \sqrt{2\alpha} B_a) da \right] dt. \end{aligned}$$

Assume now that $s - u < \sigma_{\mathcal{H}_{R_{\epsilon,K}}}(\mathbf{z})$, i.e.

$$X_h(\mathbf{z}) \in \mathcal{H}_{R_{\epsilon,K}} \text{ for all } h \in [0, s - u]. \quad (2.8)$$

Let $c_{\epsilon,K} > 0$ be such that for all $\mathbf{x} = (x, v, z) \in \mathcal{H}_{R_{\epsilon,K}}$, $|\nabla V(x)| + |\mathbf{x}| \leq c_{\epsilon,K}$. We then have $|\mathbf{z}| \leq c_{\epsilon,K}$ and, from (2.8), $|\nabla V(x_h)| + |X_h(\mathbf{z})| \leq c_{\epsilon,K}$ for all $h \in [0, s - u]$. In what follows $c_{\epsilon,K} > 0$ is a constant which only depends on $\epsilon > 0$ and K , which can change from occurrence to another. Hence, when

$X_0 = \mathbf{z}$, $|x_{s-u} - x_{\mathbf{z}}| \geq \frac{\delta}{2}$, and $s - u < \sigma_{\mathcal{H}_{R_{\epsilon,K}}}(\mathbf{z})$, it holds since $0 \leq s - u \leq s \leq 1$:

$$\begin{aligned} \frac{\delta}{2} &\leq |x_{s-u} - x_{\mathbf{z}}| \leq \int_0^{s-u} \left[|v_{\mathbf{z}}| + \int_0^t |\nabla V(x_a)| da \right] dt \\ &\quad + \int_0^{s-u} \left[\int_0^t \lambda(|z_{\mathbf{z}}| + \int_0^a [\alpha|z_h| + \lambda|v_h|] dh + \sqrt{2\alpha}|B_a|) da \right] dt \\ &\leq c_{\epsilon,K}s + \sqrt{2\alpha} \int_0^s \int_0^t |B_a| da dt, \end{aligned}$$

and consequently $\sqrt{2\alpha} \int_0^s \int_0^t |B_a| da dt \geq \frac{\delta}{2} - c_{\epsilon,K}s$. Set $s_{\epsilon,K,\delta} = \delta/(4c_{\epsilon,K})$. For $s \in [0, s_{\epsilon,K,\delta}]$, one has by Markov's inequality,

$$\mathbf{P}_{\mathbf{z}}[|x_{s-u} - x_{\mathbf{z}}| \geq \delta/2, s - u < \sigma_{\mathcal{H}_{R_{\epsilon,K}}}] \leq \mathbf{P}\left[\sqrt{2\alpha} \int_0^s \int_0^t |B_u| du dt \geq \frac{\delta}{4}\right] \leq \mathbf{m}_s,$$

where $\mathbf{m}_s = 2s^2\sqrt{2\alpha}/\delta$. Hence, we deduce that for any $s \in [0, s_{\epsilon,K,\delta}]$,

$$\mathbf{p}(\mathbf{x}, s, R_{\epsilon,K}) \leq \mathbf{m}_s.$$

With the same arguments, up to choosing $s_{\epsilon,K,\delta} > 0$ smaller, for every $s \in [0, s_{\epsilon,K,\delta}]$, it holds $\sup_{\mathbf{x} \in K} \mathbf{P}_{\mathbf{x}}[|x_s - x| \geq \delta/2, s < \sigma_{\mathcal{H}_{R_{\epsilon,K}}}] \leq \mathbf{m}_s$. Coming back to (2.7), we have thus proved that for all compact set $K \subset \mathbf{R}^{3d}$, $\delta > 0$, $\epsilon > 0$, there exists $s_{\epsilon,K,\delta} > 0$, for all $s \in [0, s_{\epsilon,K,\delta}]$, and all $\mathbf{x} \in K$, $\mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(\mathbf{x},\delta)} \leq s] \leq \epsilon$. The proof of Lemma 2.4 is complete. \square

Let $\mathbf{b} : \mathbf{R}^d \rightarrow \mathbf{R}^d$ be a globally Lipschitz vector field. Introduce the unique strong solution $(\bar{X}_t = (\bar{x}_t, \bar{v}_t, \bar{z}_t), t \geq 0)$ to (1.4) when ∇V replaced by \mathbf{b} , i.e. the solution to:

$$\begin{cases} d\bar{x}_t &= \bar{v}_t dt \\ d\bar{v}_t &= \mathbf{b}(\bar{x}_t) dt - \gamma \bar{v}_t dt + \lambda \bar{z}_t dt + \sqrt{2\gamma} dW_t \\ d\bar{z}_t &= -\alpha \bar{z}_t dt - \lambda \bar{v}_t dt + \sqrt{2\alpha} dB_t. \end{cases} \quad (2.9)$$

For $\mathbf{x} \in \mathbf{R}^{3d}$, we now denote by

$$\bar{\sigma}_{\mathbf{B}(\mathbf{x},\delta)}(\mathbf{x}) = \inf\{t \geq 0, \bar{X}_t(\mathbf{x}) \notin \mathbf{B}(\mathbf{x}, \delta)\},$$

the first exit time for the process $(\bar{X}_t(\mathbf{x}), t \geq 0)$ from the ball $\mathbf{B}(\mathbf{x}, \delta) = \{\mathbf{y} \in \mathbf{R}^{3d}, |\mathbf{y} - \mathbf{x}| < \delta\}$. We have the following result which will be used in the proof **(C1)**.

Lemma 2.5. *Assume $[\mathbf{V}_{\text{loc}}]$ and $\gamma \geq 0$. Then, it holds for all compact subset K of \mathbf{R}^{3d} and $\delta > 0$,*

$$\lim_{s \rightarrow 0^+} \sup_{\mathbf{x}_0 \in K} \mathbf{P}_{\mathbf{x}_0}[\bar{\sigma}_{\mathbf{B}(\mathbf{x}_0,\delta)} \leq s] = 0.$$

Proof. Let $r > 0$ be such that the δ -neighborhood K_δ of K is included in $\mathbf{B}(0, r)$. Since the drift in (2.9) is globally Lipschitz, there exists $c > 0$, for all $s \in [0, 1]$ and $\mathbf{x} \in \mathbf{B}(0, r)$, $|\bar{X}_s(\mathbf{x})| \leq r + c(1 + \int_0^s |\bar{X}_u(\mathbf{x})| du) + cY$, where $Y := \sup_{u \in [0,1]} (|B_u| + |W_u|)$. Hence, by Grönwall's inequality, $|\bar{X}_s(\mathbf{x})| \leq C(1 + Y)$. We have $\mathbf{P}_{\mathbf{x}_0}[\bar{\sigma}_{\mathbf{B}(\mathbf{x}_0,\delta)} \leq s] \leq \mathbf{P}_{\mathbf{x}_0}[\bar{\sigma}_{\mathbf{B}(\mathbf{x}_0,\delta)} \leq s, |\bar{X}_s - \bar{X}_0| < \delta/2] + \mathbf{P}_{\mathbf{z}}[|\bar{X}_s - \bar{X}_0| \geq \delta/2]$, and

$$\begin{aligned} &\mathbf{P}_{\mathbf{x}_0}[\bar{\sigma}_{\mathbf{B}(\mathbf{x}_0,\delta)} \leq s, |\bar{X}_s - \bar{X}_0| < \delta/2] \\ &\leq \mathbf{E}_{\mathbf{x}_0} \left[\mathbf{1}_{\bar{\sigma}_{\mathbf{B}(\mathbf{x}_0,\delta)}(\mathbf{x}_0) \leq s} \mathbf{P}_{\bar{X}_{\bar{\sigma}_{\mathbf{B}(\mathbf{x}_0,\delta)}(\mathbf{x}_0)}(\mathbf{x}_0)} [|\bar{X}_{s-\bar{\sigma}_{\mathbf{B}(\mathbf{x}_0,\delta)}(\mathbf{x}_0)} - \bar{X}_0| \geq \delta/2] \right]. \end{aligned}$$

Let $\mathbf{x}_0 \in K$, $\mathbf{x} = (x, v, z) \in \partial\mathbf{B}(\mathbf{x}_0, \delta)$ ($\Rightarrow \mathbf{x} \in K_\delta$), and $u \in [0, s]$. It holds $\mathbf{P}_{\mathbf{x}}[|\bar{X}_{s-u} - \mathbf{x}| \geq \delta/2] \leq \mathbf{P}_{\mathbf{x}}[|\bar{x}_{s-u} - x| \geq \delta/2] + \mathbf{P}_{\mathbf{x}}[|\bar{v}_{s-u} - v| \geq \delta/2] + \mathbf{P}_{\mathbf{x}}[|\bar{z}_{s-u} - z| \geq \delta/2]$. Moreover, there exists $C > 0$, $\mathbf{P}_{\mathbf{x}}[|\bar{z}_{s-u} - z| \geq \delta/2] \leq \mathbf{d}_s := \mathbf{P}[\sqrt{2\alpha} \sup_{t \in [0,s]} |B_t| + Cs(Y + 1) \geq \delta/2] \rightarrow 0$ when $s \rightarrow 0^+$. The other terms are treated similarly to deduce the expected result. \square

We are now ready to prove the following result.

Theorem 2.6. *Assume $[\mathbf{V}_{\text{loc}}]$. Let $\gamma = 0$. Then, for every $t > 0$, the nonkilled semigroup P_t of the generalized Langevin process (1.4) is strong Feller over \mathbf{R}^{3d} .*

Proof. Let $f \in b\mathcal{B}(\mathbf{R}^{3d})$ and $t > 0$ be fixed. We want to prove that $\mathbf{z} \mapsto \mathbf{E}_{\mathbf{z}}[f(X_t)]$ is continuous over \mathbf{R}^{3d} .

We write for $\mathbf{x} \in \mathbf{R}^{3d}$ and $R > 0$ (see (2.1)):

$$\mathbf{E}_{\mathbf{x}}[f(X_t)] = \mathbf{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{H}_R}}] + \mathbf{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t \geq \sigma_{\mathcal{H}_R}}].$$

Since the open set $\mathcal{V}_R = \{y \in \mathbf{R}^d, V(y) < R\}$ is relatively compact and ∇V is locally Lipschitz, we can consider² a globally Lipschitz vector field $\mathbf{b}_R : \mathbf{R}^d \rightarrow \mathbf{R}^d$ such that $\mathbf{b}_R = -\nabla V$ in a neighborhood of $\overline{\mathcal{V}_R}$. Let us then introduce the unique strong solution $(\bar{X}_t^R = (\bar{x}_t^R, \bar{v}_t^R, \bar{z}_t^R), t \geq 0)$ to (2.9) when \mathbf{b} replaced by \mathbf{b}_R and $\gamma = 0$. Note that $(x, v, z) \in \mathcal{H}_R \Rightarrow x \in \mathcal{V}_R$. Therefore, the processes $(X_t, t \geq 0)$ and $(\bar{X}_t^R, t \geq 0)$ coincides in law up to their first exit time from \mathcal{H}_R , and thus, denoting by $\bar{\sigma}_{\mathcal{H}_R} := \inf\{t \geq 0, \bar{X}_t^R \notin \mathcal{H}_R\}$, we deduce that:

$$\mathbf{E}_{\mathbf{x}}[f(X_t)] = \mathbf{E}_{\mathbf{x}}[f(\bar{X}_t^R)\mathbf{1}_{t < \bar{\sigma}_{\mathcal{H}_R}}] + \mathbf{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t \geq \bar{\sigma}_{\mathcal{H}_R}}]. \quad (2.10)$$

Let us now assume that $\mathbf{x}_n \rightarrow \mathbf{x} \in \mathbf{R}^{3d}$. Let $R_0 > 0$ such that $\mathbf{x}_n, \mathbf{x} \in \mathcal{H}_{R_0}$.

Let us now prove (2.3), i.e. that for all $R > 0$, as $n \rightarrow +\infty$,

$$\mathbf{E}_{\mathbf{x}_n}[f(\bar{X}_t^R)\mathbf{1}_{t < \bar{\sigma}_{\mathcal{H}_R}}] \rightarrow \mathbf{E}_{\mathbf{x}}[f(\bar{X}_t^R)\mathbf{1}_{t < \bar{\sigma}_{\mathcal{H}_R}}]. \quad (2.11)$$

To prove (2.11), we first prove that the nonkilled semigroup of $(\bar{X}_t^R, t \geq 0)$ is strong Feller, i.e. that

$$\text{for all } R > 0, \mathbf{z} \in \mathbf{R}^{3d} \mapsto \mathbf{E}_{\mathbf{z}}[f(\bar{X}_t^R)] \text{ is continuous.} \quad (2.12)$$

Note that since \mathbf{b}_R is globally Lipschitz, it holds as $n \rightarrow +\infty$:

$$\sup_{s \in [0, t]} |\bar{X}_s^R(\mathbf{x}_n) - \bar{X}_s^R(\mathbf{x})| \rightarrow 0 \text{ in } \mathbf{P}\text{-probability.} \quad (2.13)$$

Using again that \mathbf{b}_R is globally Lipschitz over \mathbf{R}^d , we can use [18, Theorem 1.1] to deduce that for all $\mathbf{z} \in \mathbf{R}^{3d}$, $\bar{X}_t^R(\mathbf{z})$ admits a density $\bar{p}_t^R(\mathbf{z}, \mathbf{y})$ (w.r.t. the Lebesgue measure $d\mathbf{y}$ over \mathbf{R}^{3d}) which moreover satisfies the following Gaussian upper bound:

$$\bar{p}_t^R(\mathbf{z}, \mathbf{y}) \leq C_t^R \exp(-c_t^R |\boldsymbol{\theta}_t^R(\mathbf{z}) - \mathbf{y}|^2), \quad (2.14)$$

for some $C_t^R, c_t^R > 0$ independent of $\mathbf{z}, \mathbf{y} \in \mathbf{R}^{3d}$, and where $(\boldsymbol{\theta}_t^R(\mathbf{z}) = (\mathbf{x}_t^R(\mathbf{z}), \mathbf{v}_t^R(\mathbf{z}), \mathbf{z}_t^R(\mathbf{z})), t \geq 0)$ is the solution for $t \geq 0$ of the deterministic equation:

$$\dot{\mathbf{x}}_t^R = \mathbf{v}_t^R, \dot{\mathbf{v}}_t^R = \mathbf{b}_R(\mathbf{x}_t^R) + \lambda \mathbf{z}_t^R, \dot{\mathbf{z}}_t^R = -\alpha \mathbf{z}_t^R - \lambda \mathbf{v}_t^R,$$

with initial condition $\boldsymbol{\theta}_0^R(\mathbf{z}) = \mathbf{z}$.

On the other hand, since $(\mathbf{x}_n)_n$ is bounded and $\mathbf{z} \mapsto \boldsymbol{\theta}_t^R(\mathbf{z})$ is continuous (because \mathbf{b}_R is globally Lipschitz), it follows that there exists $K > 0$ such that for all n , $|\boldsymbol{\theta}_t^R(\mathbf{x}_n)| \leq K$. Thus

$$\bar{p}_t^R(\mathbf{x}_n, \mathbf{y}) \leq C_t^\epsilon \exp(c_t^\epsilon K^2) \exp(2c_t^\epsilon K |\mathbf{y}|) \exp(-c_t^\epsilon |\mathbf{y}|^2). \quad (2.15)$$

Let $\mu(d\mathbf{y}) = \kappa \exp(-|\mathbf{y}|)d\mathbf{y}$ (where $\kappa^{-1} = \int \exp(-|\mathbf{y}|)d\mathbf{y}$), and set $\bar{q}_t^R(\mathbf{z}, \mathbf{y}) = \kappa^{-1} \exp(|\mathbf{y}|)\bar{p}_t^R(\mathbf{z}, \mathbf{y})$. It then follows from (2.15) that as $r \rightarrow +\infty$,

$$\sup_n \int_{|\mathbf{y}| \geq r} \bar{q}_t^R(\mathbf{x}_n, \mathbf{y}) \mu(d\mathbf{y}) \rightarrow 0.$$

Consequently, for any $f \in b\mathcal{B}(\mathbf{R}^{3d})$, by Proposition 1.2, as $n \rightarrow +\infty$, $f(\bar{X}_t^R(\mathbf{x}_n)) \rightarrow f(\bar{X}_t^R(\mathbf{x}))$ in probability, and then, because f is bounded, this convergence also holds in any r th mean ($r \geq 1$). This proves (2.12).

²See e.g. [52].

We are now in position to prove Equation (2.11). The proof is inspired from the one of [15, Theorem 2.2]. Let $R > 0$, K be a compact subset of \mathcal{H}_R , $t > 0$, and $\delta := \text{dist}(K, \partial\mathcal{H}_R) > 0$. Let also $0 \leq s \leq t$, $\mathbf{z} \in \mathcal{H}_R$, and $f \in b\mathcal{B}(\mathcal{H}_R)$. Then, by the Markov property, it holds

$$\mathbf{E}_{\mathbf{z}}[f(\bar{X}_t^R)\mathbf{1}_{t < \bar{\sigma}_{\mathcal{H}_R}}] = \mathbf{E}_{\mathbf{z}}[\mathbf{1}_{s < \bar{\sigma}_{\mathcal{H}_R}}\psi_s(\bar{X}_s^R)],$$

where $\psi_s(\mathbf{z}) = \mathbf{E}_{\mathbf{z}}[\mathbf{1}_{t-s < \bar{\sigma}_{\mathcal{H}_R}}f(\bar{X}_{t-s}^R)]$. Therefore:

$$\sup_{\mathbf{z} \in K} |\mathbf{E}_{\mathbf{z}}[f(\bar{X}_t^R)\mathbf{1}_{t < \bar{\sigma}_{\mathcal{H}_R}}] - \mathbf{E}_{\mathbf{z}}[\psi_s(\bar{X}_t^R)]| \leq \|f\|_{\infty} \sup_{\mathbf{z} \in K} \mathbf{P}_{\mathbf{z}}[\bar{\sigma}_{\mathcal{H}_R} \leq s] \leq \|f\|_{\infty} \sup_{\mathbf{z} \in K} \mathbf{P}_{\mathbf{z}}[\bar{\sigma}_{\mathbf{B}(\mathbf{z}, \delta)}^R \leq s].$$

which tends to 0 as $s \rightarrow 0^+$, thanks to Lemma 2.5, where

$$\bar{\sigma}_{\mathbf{B}(\mathbf{z}, \delta)}^R(\mathbf{x}) = \inf\{t \geq 0, \bar{X}_t^R(\mathbf{x}) \notin \mathbf{B}(\mathbf{x}, \delta)\}.$$

Hence, using (2.12), one deduces that $\mathbf{z} \in \mathcal{H}_R \mapsto \mathbf{E}_{\mathbf{z}}[f(\bar{X}_t^R)\mathbf{1}_{t < \bar{\sigma}_{\mathcal{H}_R}}]$ is continuous.

We now conclude the proof of Theorem 2.6. Consider $\epsilon > 0$. Thanks to (1.10) and because \mathbf{H}_{GL} is locally bounded, there exists $R_{\epsilon} \geq R_0$ such that

$$|\mathbf{E}_{\mathbf{x}}[f(X_t)\mathbf{1}_{t \geq \sigma_{\mathcal{H}_{R_{\epsilon}}}}]| + \sup_{n \geq 0} |\mathbf{E}_{\mathbf{x}_n}[f(X_t)\mathbf{1}_{t \geq \sigma_{\mathcal{H}_{R_{\epsilon}}}}]| \leq \epsilon/2. \quad (2.16)$$

Using (2.11), there exists $N_{\epsilon} \in \mathbf{N}$ such that for all $n \geq N_{\epsilon}$,

$$|\mathbf{E}_{\mathbf{x}_n}[f(\bar{X}_t^{R_{\epsilon}})\mathbf{1}_{t < \bar{\sigma}_{\mathcal{H}_{R_{\epsilon}}}}] - \mathbf{E}_{\mathbf{x}}[f(\bar{X}_t^{R_{\epsilon}})\mathbf{1}_{t < \bar{\sigma}_{\mathcal{H}_{R_{\epsilon}}}}]| \leq \epsilon/2.$$

Using (2.10) and (2.16), for all $n \geq N_{\epsilon}$, $|\mathbf{E}_{\mathbf{x}_n}[f(X_t)] - \mathbf{E}_{\mathbf{x}}[f(X_t)]| \leq \epsilon$. This concludes the proof of Theorem 2.6. \square

On Assumption (C4). Let us consider a subdomain \mathcal{D} of \mathbf{R}^{3d} of the form

$$\mathcal{D} = \mathcal{O} \times \mathbf{R}^d \times \mathbf{R}^d,$$

where \mathcal{O} is a subdomain of \mathbf{R}^d . Thanks to Lemma 2.4, we can check (C4).

Proposition 2.7. *Assume [V_{loc}]. Then, for all $t > 0$ and $\gamma \geq 0$, $P_t^{\mathcal{D}}$ is strong Feller. In particular (C4) holds.*

Proof. Pick a compact subset K of \mathcal{O} and $t > 0$. Set $\delta := \text{dist}(K, \partial\mathcal{D}) > 0$ (where $\partial\mathcal{D} = \partial\mathcal{O} \times \mathbf{R}^d \times \mathbf{R}^d$). One has for $0 \leq s \leq t$, $\mathbf{x} \in \mathcal{D}$, and $f \in b\mathcal{B}(\mathcal{D})$, $P_t^{\mathcal{D}}f(\mathbf{x}) = \mathbf{E}_{\mathbf{x}}[\mathbf{1}_{s < \sigma_{\mathcal{D}}}g_s(X_s)]$, where $g_s(\mathbf{z}) = \mathbf{E}_{\mathbf{z}}[\mathbf{1}_{t-s < \sigma_{\mathcal{D}}}f(X_{t-s})]$. By (C1), $P_s g_s$ is continuous over \mathbf{R}^{3d} . In addition, it holds: $\sup_{\mathbf{x} \in K} |P_t^{\mathcal{D}}f(\mathbf{x}) - P_s g_s(\mathbf{x})| \leq \|f\|_{\infty} \sup_{\mathbf{x} \in K} \mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{D}} \leq s] \leq \|f\|_{\infty} \sup_{\mathbf{x} \in K} \mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(\mathbf{x}, \delta)} \leq s] \rightarrow 0$ as $s \rightarrow 0^+$, thanks to Lemma 2.4. Thus $P_t^{\mathcal{D}}f$ is continuous. \square

2.2. On Assumption (C5). In this section, we check (C5). To do so, the well-known starting point is the knowledge of the support of the law of the trajectories of the Brownian motion. To check (C5), we thus construct suitable control curves. The details of the proof of (C5) will be given since ∇V is only locally Lipschitz. In all this section, $\mathcal{D} = \mathcal{O} \times \mathbf{R}^d \times \mathbf{R}^d$ and \mathcal{O} is a subdomain of \mathbf{R}^d such that $\mathbf{R}^d \setminus \bar{\mathcal{O}}$ is nonempty.

2.2.1. The case when $\gamma = 0$. To prove Assumption (C5), we will construct, for any $T > 0$ and any two points $\mathbf{x}_0, \mathbf{x}_T \in \mathcal{D}$, a so-called control curve $\mathbf{l} \in [0, T] \rightarrow \mathcal{O}$ joining \mathbf{x}_0 to \mathbf{x}_T (this will be done using local polynomial interpolations). Note here that we need to impose that the range of the control curve γ lies in \mathcal{O} to ensure the condition that $t < \sigma_{\mathcal{D}}(\mathbf{x}_0)$ when $X_{[0, T]}(\mathbf{x}_0)$ is sufficiently close to γ on $[0, T]$ (for the supremum norm over $[0, T]$).

We start with the following lemma.

Lemma 2.8. *Let us consider $t_* > 0$, $\mathbf{x}_0 = (x_0, y_0, z_0) \in \mathbf{R}^{3d}$ and $\mathbf{x}_1 = (x_1, v_1, z_1) \in \mathbf{R}^{3d}$. Then, there exists a smooth curve $\ell : [0, t_*] \rightarrow \mathbf{R}^d$ such that $\ell(0) = x_0$, $\dot{\ell}(0) = v_0$, $\ddot{\ell}(0) = z_0$, $\ell(t_*) = x_1$, $\dot{\ell}(t_*) = v_1$, $\ddot{\ell}(t_*) = z_1$, and*

$$\sup_{s \in [0, t_*]} |\ell(s) - x_0| \leq C|x_0 - x_1| + C(|v_0| + |v_1|)t_* + C(|z_0| + |z_1|)t_*^2,$$

where $C > 0$ is a universal constant.

In the following, we say that such a curve γ joins \mathbf{x}_0 to \mathbf{x}_T .

Proof. Choose $\ell(s) = \sum_{k=0}^5 c_k s^k$ where $c_0 = x_0$, $c_1 = v_1$, $c_2 = z_0/2$, $c_3 = -10x_0/t_*^3 - 6v_0/t_*^2 - 3z_0/(2t_*) + 10x_1/t_*^3 - 4v_1/t_*^2 + z_1/(2t_*)$, $c_4 = 15x_0/t_*^4 + 8v_0/t_*^3 + 3z_0/(2t_*^2) - 15x_1/t_*^4 + 7v_1/t_*^3 - z_1/t_*^2$, $c_5 = -6x_0/t_*^5 - 3v_0/t_*^4 - z_0/(2t_*^3) + 6x_1/t_*^5 - 3v_1/t_*^4 + z_1/(2t_*^3)$. \square

Lemma 2.9. *Let us consider $T > 0$, $\mathbf{x}_0 = (x_0, y_0, z_0) \in \mathcal{D}$, and $\mathbf{x}_T = (x_T, v_T, z_T) \in \mathcal{D}$. Then, there exists a \mathcal{C}^2 and piecewise \mathcal{C}^3 curve $\mathfrak{l} : [0, T] \rightarrow \mathbf{R}^d$, such that $\mathfrak{l}(0) = x_0$, $\dot{\mathfrak{l}}(0) = v_0$, $\ddot{\mathfrak{l}}(0) = z_0$, $\mathfrak{l}(T) = x_T$, $\dot{\mathfrak{l}}(T) = v_T$, $\ddot{\mathfrak{l}}(T) = z_T$, and*

$$\text{Ran}(\mathfrak{l}) \subset \mathcal{O}.$$

Proof. The set \mathcal{O} is path-connected since it is connected and open in \mathbf{R}^d . Let $\Psi : [0, T] \rightarrow \mathcal{O}$ be an injective curve such that $\Psi(0) = x_0$ and $\Psi(T) = x_T$. Let $\delta > 0$ be such that the closure of the δ -neighborhood \mathcal{U}_δ of $\text{Ran}(\Psi)$ is included in \mathcal{O} .

Let $\epsilon > 0$. Take a subdivision of $\text{Ran}(\Psi)$ containing $N_\epsilon + 1 \in \mathbf{N}^*$ points $\{x_0, x_1^\epsilon, \dots, x_{N_\epsilon-1}^\epsilon, x_T\}$ with $|x_j^\epsilon - x_{j+1}^\epsilon| \leq \epsilon$, $j \in \{0, \dots, N_\epsilon - 1\}$ (with $x_0^\epsilon := x_0$ and $x_{N_\epsilon}^\epsilon := x_T$).

Note that $N_\epsilon \rightarrow +\infty$ as $\epsilon \rightarrow 0^+$. Set now $t_*^\epsilon = T/N_\epsilon$. Pick two unimportant points $v, z \in \mathbf{R}^d$. By Lemma 2.8, we can consider N_ϵ curves $\ell_0^\epsilon : [0, t_*^\epsilon] \rightarrow \mathbf{R}^d$ joining x_0 to $x_1^\epsilon = (x_1^\epsilon, v, z)$, $\ell_1^\epsilon : [0, t_*^\epsilon] \rightarrow \mathbf{R}^d$ joining x_1^ϵ to $x_2^\epsilon = (x_2^\epsilon, v, z)$, \dots , $\ell_{N_\epsilon-1}^\epsilon : [0, t_*^\epsilon] \rightarrow \mathbf{R}^d$ joining $x_{N_\epsilon-1}^\epsilon = (x_{N_\epsilon-1}^\epsilon, v, z)$ to x_T . The curve \mathfrak{l}^ϵ is then defined on $[0, T]$ by:

$$\text{for all } t \in [0, T], \mathfrak{l}^\epsilon(t) = \ell_j^\epsilon(t - jt_*^\epsilon) \text{ if } jt_*^\epsilon \leq t < (j+1)t_*^\epsilon, j \in \{0, \dots, N_\epsilon - 1\},$$

and $\mathfrak{l}^\epsilon(T) = x_T$. Note that by Lemma 2.8, if ϵ is small enough (say $\epsilon < \epsilon_0$), for all $j \in \{0, \dots, N_\epsilon - 1\}$, $\text{Ran}(\ell_j^\epsilon) \subset \mathcal{U}_\delta$, so that $\text{Ran}(\mathfrak{l}^\epsilon) \subset \mathcal{O}$. The proof of the lemma is complete choosing any \mathfrak{l}^ϵ , with $0 < \epsilon < \epsilon_0$. \square

We are now ready to prove that Assumption **(C5)** is satisfied when $\gamma = 0$.

Proposition 2.10. *Assume $\gamma = 0$ and **[Vloc]**. Then, for any $T > 0$, $\mathbf{x}_0 = (x_0, v_0, z_0) \in \mathcal{D}$ and any nonempty open subset \mathbf{O} of \mathcal{D} , it holds:*

$$\mathbf{P}_{\mathbf{x}_0}[X_T \in \mathbf{O}, T < \sigma_{\mathcal{D}}] > 0. \quad (2.17)$$

Moreover, **(C5)** holds.

Proof. Pick $\mathbf{x}_T \in \mathbf{O}$. Using Lemma 2.9, one can consider a \mathcal{C}^2 and piecewise \mathcal{C}^3 curve $\mathfrak{l} : [0, T] \rightarrow \mathcal{O}$ such that $\mathfrak{l}(0) = x_0$, $\dot{\mathfrak{l}}(0) = v_0$, $\ddot{\mathfrak{l}}(0) = \lambda z_0 - \nabla V(x_0)$, $\mathfrak{l}(T) = x_T$, $\dot{\mathfrak{l}}(T) = v_T$, $\ddot{\mathfrak{l}}(T) = \lambda z_T - \nabla V(x_T)$. Let us then define the function $\mathfrak{h} : [0, T] \rightarrow \mathbf{R}^d$ by

$$\mathfrak{h}(t) = \frac{1}{\lambda\sqrt{2\alpha}} \frac{d}{dt} [\ddot{\mathfrak{l}} + \nabla V(\mathfrak{l})](t), \quad t \in [0, T].$$

Note that $\mathfrak{h} \in \mathcal{L}^\infty([0, T], \mathbf{R}^d)$ since $t \mapsto [\ddot{\mathfrak{l}} + \nabla V(\mathfrak{l})](t)$ belongs to the Sobolev space $\mathcal{W}^{1,\infty}([0, T], \mathbf{R}^d)$. Recall that the support (for the supremum norm over $[0, T]$) of the law of the trajectory of the standard Brownian motion on $[0, T]$ is the closure of the set

$$\mathcal{L}_0^2([0, T], \mathbf{R}^d) = \left\{ u : [0, T] \rightarrow \mathbf{R}^d, \int_0^T u^2(s) ds < +\infty \text{ and } u(0) = 0 \right\}. \quad (2.18)$$

Therefore, for all $\eta > 0$, $\mathbf{P}[\mathcal{A}_\eta] > 0$, where $\mathcal{A}_\eta := \{\sup_{t \in [0, T]} |B_t - \int_0^t h(s) ds| < \eta\}$. Let us consider an open bounded neighborhood \mathcal{V}_l of $\text{Ran}(l)$ in \mathbf{R}^d such that $\overline{\mathcal{V}_l} \subset \mathcal{O}$ (note that in particular $\mathbf{x}_0, \mathbf{x}_T \in \mathcal{V}_l$). For all $\epsilon > 0$ small enough (say $\epsilon \in (0, \epsilon_l)$, $\epsilon_l > 0$), the following two conditions are satisfied:

- a. For any $\mathbf{c} : [0, T] \rightarrow \mathbf{R}^d$ such that $\sup_{s \in [0, T]} |\mathbf{c}(s) - l(s)| \leq \epsilon$, $\text{Ran}(\mathbf{c}) \subset \mathcal{V}_l$.
- b. For any $\mathbf{x} \in \mathbf{R}^{3d}$ such that $\mathbf{x} \in \mathbf{B}(\mathbf{x}_T, \epsilon)$, $\mathbf{x} \in \mathbf{O}$.

Denote by $\mathcal{D}_l = \mathcal{V}_l \times \mathbf{R}^d \times \mathbf{R}^d \subset \mathcal{D}$. Let us consider a globally Lipschitz vector field $\mathbf{b}_l : \mathbf{R}^d \rightarrow \mathbf{R}^d$ such that $\mathbf{b}_l = -\nabla V$ in a neighborhood of $\overline{\mathcal{V}_l}$. Recall $(\bar{X}_t^l = (\bar{x}_t^l, \bar{v}_t^l, \bar{z}_t^l), t \geq 0)$ is the solution to (2.9) when $\mathbf{b} = \mathbf{b}_l$. Note that $\mathbf{P}_{\mathbf{x}_0}[X_T \in \mathbf{O}, T < \sigma_{\mathcal{D}}] \geq \mathbf{P}_{\mathbf{x}_0}[X_T \in \mathbf{O}, T < \sigma_{\mathcal{D}_l}] = \mathbf{P}_{\mathbf{x}_0}[X_T^l \in \mathbf{O}, T < \bar{\sigma}_{\mathcal{D}_l}]$ (where $\bar{\sigma}_{\mathcal{D}_l}$ is the first exit time of the process \bar{X}^l from \mathcal{D}_l). To prove (2.17), it is therefore enough to show that $\mathbf{P}_{\mathbf{x}_0}[X_T^l \in \mathbf{O}, T < \bar{\sigma}_{\mathcal{D}_l}] > 0$, which is the purpose of what follows.

Let $(\bar{X}_t^\circ = (x_t^\circ, v_t^\circ, z_t^\circ) \in \mathbf{R}^{3d}, t \geq 0)$ be the solution to

$$dx_t^\circ = v_t^\circ dt, \quad dv_t^\circ = \mathbf{b}_l(x_t^\circ) dt + \lambda z_t^\circ dt, \quad dz_t^\circ = \sqrt{2\alpha} dB_t. \quad (2.19)$$

Define $f_t(\mathbf{x}) = -\alpha z_t^\circ(\mathbf{x}) - \lambda v_t^\circ(\mathbf{x})$, $t \geq 0$. Recall that since \mathbf{b}_l is globally Lipschitz (see the beginning of the proof of Lemma 2.5), for all $\mathbf{x} \in \mathbf{R}^{3d}$ and $T > 0$, there exists $C > 0$, $\sup_{s \in [0, T]} |\bar{X}_s^\circ| \leq C(1 + Y_T)$ where $Y_T := \sup_{s \in [0, T]} |B_s|$. Hence, for $\epsilon > 0$ small enough, $\mathbf{E}[e^{\epsilon |f_t(\mathbf{x})|^2}] \leq C\mathbf{E}[e^{C\epsilon Y_T^2}] < +\infty$. Therefore, one can use [25, Theorem 3.1 in Section 7] and [25, Theorem 1.1 in Section 7], to deduce that the law of $(\bar{X}_t^\circ, t \in [0, T])$ is equivalent to the law of $(\bar{X}_t^\circ, t \in [0, T])$. Let us thus prove that $\mathbf{P}_{\mathbf{x}_0}[\bar{X}_T^\circ \in \mathbf{O}, T < \bar{\sigma}_{\mathcal{D}_l}^\circ] > 0$ (where $\bar{\sigma}_{\mathcal{D}_l}^\circ := \inf\{t \geq 0, \bar{X}_t^\circ \notin \mathcal{D}_l\}$).

Set $\mathbf{n}(t) = (l(t), \dot{l}(t), \lambda^{-1}(\ddot{l}(t) + \nabla V(l(t))))$, for $t \in [0, T]$. Note that for $t \in [0, T]$, $\mathbf{h}(t) = \frac{1}{\lambda\sqrt{2\alpha}} \frac{d}{dt} [\ddot{l} - \mathbf{b}_l(l)](t)$. Then, using that \mathbf{b}_l is globally Lipschitz and that $\mathbf{n}(0) = \mathbf{x}_0$, it is straightforward to get that $\sup_{s \in [0, T]} |\bar{X}_s^\circ - \mathbf{n}(t)| \leq C_T \eta$ on \mathcal{A}_η . Choose $\eta > 0$ such that $C\eta < \epsilon_l$. By Item a above, $T < \bar{\sigma}_{\mathcal{D}_l}^\circ$. In addition, since $\mathbf{n}(T) = \mathbf{x}_T$, by Item b above, $\bar{X}_T^\circ \in \mathbf{O}$. Therefore, $\mathbf{P}_{\mathbf{x}_0}[\bar{X}_T^\circ \in \mathbf{O}, T < \bar{\sigma}_{\mathcal{D}_l}^\circ] > 0$. This ends the proof of (2.17).

Since $\mathbf{R}^d \setminus \overline{\mathcal{O}} \neq \emptyset$, we also prove with similar arguments that for all $\mathbf{z} \in \mathcal{D}$, $\mathbf{P}_{\mathbf{z}}[\sigma_{\mathcal{D}} < +\infty] > 0$. This ends the proof of Proposition 2.10. \square

2.2.2. *The case when $\gamma > 0$.* In this section we prove the following result.

Proposition 2.11. *Assume $\gamma > 0$ and $[\mathbf{V}_{\text{loc}}]$. Then, (C5) holds.*

Proof. In view of (2.5), it is enough to prove (C5) for the process $(X_t^0, t \geq 0)$ defined in (2.4). Let $T > 0$, $\mathbf{x}_0 = (x_0, v_0, z_0) \in \mathcal{D}$, \mathbf{O} be a nonempty open subset of \mathcal{D} , and $\mathbf{x}_T = (x_T, v_T, z_T) \in \mathbf{O}$. Let also $\mathbf{e} : [0, T] \rightarrow \mathbf{R}^d$ be \mathcal{C}^1 and piecewise \mathcal{C}^2 such that $\mathbf{e}(0) = x_0$, $\dot{\mathbf{e}}(0) = v_0$, $\mathbf{e}(T) = x_T$, $\dot{\mathbf{e}}(T) = v_T$, and $\text{Ran}(\mathbf{e}) \subset \mathcal{O}$. Let $\mathbf{u} : [0, T] \rightarrow \mathbf{R}^d$ be a smooth curve with $\mathbf{u}(0) = z_0$ and $\mathbf{u}(T) = z_T$. Define $\mathbf{m}(t) = (\mathbf{e}(t), \dot{\mathbf{e}}(t), \mathbf{u}(t))$ (note that $\mathbf{m}(0) = \mathbf{x}_0$ and $\mathbf{m}(T) = \mathbf{x}_T$). For any $\eta > 0$, the event $\mathcal{A}_\eta := \{\sup_{t \in [0, T]} |\sqrt{2\gamma} W_t - \int_0^t \ddot{\mathbf{e}}| < \eta\} \cap \{\sup_{t \in [0, T]} |\sqrt{2\alpha} B_t - \int_0^t \dot{\mathbf{u}}| < \eta\}$ has positive probability (see (2.18)). A straightforward computation shows that when $X_0^0 = \mathbf{x}_0$, $\mathcal{A}_{\epsilon/C_T} \subset \{\sup_{s \in [0, T]} |X_s^0 - \mathbf{m}(s)| < \epsilon\}$ for some $C_T > 0$. Hence, $\mathbf{P}_{\mathbf{x}_0}[\sup_{s \in [0, T]} |X_s^0 - \mathbf{m}(s)| < \epsilon] > 0$. This concludes the proof of Proposition 2.11. \square

2.3. **On Assumption (C3).** In this section, we construct two Lyapunov functions $W_\delta : \mathbf{R}^{3d} \rightarrow [1, +\infty)$ satisfying Assumption (C3), where $\delta > 0$ is a parameter to be chosen later.

Assume $[\mathbf{V}_{\text{poly-}x^k}]$. We define the vector field \mathbf{L} as follows. Let $\chi : \mathbf{R}^d \rightarrow [0, 1]$ be a smooth function such that $\chi(x) = 0$ if $|x| \leq 1$ and $\chi(x) = 1$ if $|x| \geq 2$. We define $\mathbf{J}(x) = x|x|^{\beta-1}\chi(x)$, $\beta \in [0, 1]$. Note that \mathbf{J} is \mathcal{C}^1 and the first derivatives of \mathbf{J} are bounded over \mathbf{R}^d (because $\beta \leq 1$), say by $C_J := \sup_{\mathbf{R}^d} |\text{Jac}(\mathbf{J})|_2 > 0$ (where $|\mathbf{M}|_2 := \sup\{|\mathbf{M}y|, |y| = 1\}$, $\mathbf{M} \in \mathcal{M}_d(\mathbf{R})$). One then sets:

$$\mathbf{L} = \kappa \mathbf{J}, \quad \kappa := \frac{\lambda}{2C_J},$$

so that (and this will be used in the case $\gamma = 0$ below),

$$\mathfrak{C}_L := \sup_{\mathbf{R}^d} |\text{Jac}(L)|_2 \leq \lambda/2. \quad (2.20)$$

For all $(x, v, z) \in \mathbf{R}^{3d}$, $\mathfrak{b} \geq 0$, and $\mathfrak{h}, \mathfrak{a} > 0$, we define (see (1.8)), $F_0(x, v, z) = \mathfrak{h}H_{\text{GL}}(x, v, z) + \mathfrak{a}L(x) \cdot v + \mathfrak{b}v \cdot z$. The parameter $\beta > 0$ will be chosen such that

$$\inf_{\mathbf{R}^{3d}} F_0 \in \mathbf{R}. \quad (2.21)$$

We then set $F_{\text{GL}} = F_0 - \inf_{\mathbf{R}^{3d}} F_0 + 1$ and

$$W_\delta = \exp[F_{\text{GL}}^\delta], \quad \text{where } \frac{1-\beta}{k} < \delta \leq 1. \quad (2.22)$$

In the following, for ease of notation we simply write F for F_{GL} . Since $F^{1-\delta} \geq 1$, a straightforward computation implies that over \mathbf{R}^{3d} ,

$$\frac{\mathcal{L}_{\text{GL}}W_\delta}{W_\delta} \leq \frac{\delta}{F^{1-\delta}} \left[\mathcal{L}_{\text{GL}}F + \delta\gamma|\nabla_v F|^2 + \delta\alpha|\nabla_z F|^2 \right], \quad (2.23)$$

where $\mathcal{L}_{\text{GL}}F = v \cdot \nabla_x F + (-\gamma v - \nabla_x V + \lambda z) \cdot \nabla_v F + \gamma \Delta_v F - (\alpha z + \lambda v) \cdot \nabla_z F + \alpha \Delta_z F$. We also have $\nabla_x F(x, v, z) = \mathfrak{h} \nabla_x V + \mathfrak{a} \text{Jac}(L)(x)v$, $\nabla_v F(x, v, z) = \mathfrak{h}v + \mathfrak{a}L(x) + \mathfrak{b}z$, and $\nabla_z F(x, v, z) = \mathfrak{h}z + \mathfrak{b}v$. Consequently, one has for all $(x, v, z) \in \mathbf{R}^{3d}$:

$$\begin{aligned} \mathcal{L}_{\text{GL}}F(x, v, z) &= -\lambda\mathfrak{b}|v|^2 - \gamma\mathfrak{h}|v|^2 + \mathfrak{a}v \cdot \text{Jac}(L)(x)v - \gamma\mathfrak{a}L(x) \cdot v - \mathfrak{a}\nabla V(x) \cdot L(x) \\ &\quad - \alpha\mathfrak{h}|z|^2 + \lambda\mathfrak{b}|z|^2 + \lambda\mathfrak{a}z \cdot L(x) - \gamma\mathfrak{b}v \cdot z - \mathfrak{b}\nabla V(x) \cdot z - \alpha\mathfrak{b}z \cdot v \\ &\quad + \mathfrak{h}d(\gamma + \alpha) \end{aligned} \quad (2.24)$$

and

$$(\delta\gamma|\nabla_v F|^2 + \delta\alpha|\nabla_z F|^2)(x, v, z) = \delta\gamma|\mathfrak{h}v + \mathfrak{a}L(x) + \mathfrak{b}z|^2 + \delta\alpha|\mathfrak{h}z + \mathfrak{b}v|^2. \quad (2.25)$$

2.3.1. *The case when $\gamma > 0$.* In this section, $\gamma > 0$,

$$\mathfrak{b} = 0, \quad k > 1, \quad 0 < \beta < \min(1, k/2, k-1). \quad (2.26)$$

Let us now check (2.21). Let $p_0, q_0 > 1$ such that $1/p_0 + 1/q_0 = 1$. Then, using $[\mathbf{V}_{\text{poly-}x^k}]$, for all $(x, v, z) \in \mathbf{R}^{3d}$, one has if $|x| \geq r_V$:

$$F_0(x, v, z) \geq c_V \mathfrak{h}|x|^k + \frac{\mathfrak{h}}{2}|v|^2 + \frac{\mathfrak{h}}{2}|z|^2 - \frac{\mathfrak{a}\kappa}{p_0}|x|^{\beta p_0} - \frac{\mathfrak{a}\kappa}{q_0}|v|^{q_0}.$$

Pick $\epsilon > 0$ small enough such that $p_0 = k/\beta - \epsilon > 1$ and $q_0 = (k - \epsilon\beta)/(k - \epsilon\beta - \beta) < 2$ (which is possible since the latter quantity converges to $k/(k - \beta) < 2$ as $\epsilon \rightarrow 0^+$, by (2.26)). Note that $\beta p_0 < k$. Thus, for any $\mathfrak{h}, \mathfrak{a} > 0$, there exist $C, c > 0$, for all $(x, v, z) \in \mathbf{R}^{3d}$,

$$F_0(x, v, z) \geq c(|x|^k + |v|^2 + |z|^2) - C.$$

Thus (2.21) holds. Note also that for any $\mathfrak{h}, \mathfrak{a} > 0$, there exist $c' > 0$, for all $(x, v, z) \in \mathbf{R}^{3d}$,

$$F_0(x, v, z) \leq c'(|x|^k + |v|^2 + |z|^2 + 1). \quad (2.27)$$

Proposition 2.12. *Assume $\gamma > 0$, $[\mathbf{V}_{\text{poly-}x^k}]$, $k > 1$, and (2.26). Then, for any $\mathfrak{h}, \mathfrak{a} > 0$ small enough (these conditions are made explicit in the proof), **(C3)** is satisfied with the function W_δ defined in (2.22).*

Proof. Recall that $\mathfrak{b} = 0$. Let $(x, v, z) \in \mathbf{R}^{3d}$ with $|x| \geq \max(2, r_V)$. Using $[\mathbf{V}_{\text{poly-}x^k}]$, (2.24) and (2.25), one gets:

$$\begin{aligned} &(\mathcal{L}_{\text{GL}}F + \delta\gamma|\nabla_v F|^2 + \delta\alpha|\nabla_z F|^2)(x, v, z) \\ &\leq -\gamma\mathfrak{h}|v|^2 + \mathfrak{a}\mathfrak{C}_L|v|^2 + \gamma\mathfrak{a}\kappa|x|^\beta|v| - \mathfrak{a}\kappa c_V|x|^{k-1+\beta} \\ &\quad + 2\delta\gamma\mathfrak{h}^2|v|^2 + 2\delta\gamma\mathfrak{a}^2|L(x)|^2 + \lambda\mathfrak{a}\kappa|x|^\beta|z| - \alpha\mathfrak{h}|z|^2 + \delta\alpha\mathfrak{h}^2|z|^2 + d\mathfrak{h}(\alpha + \gamma). \end{aligned}$$

Choose $\mathfrak{h} > 0$ small enough such that $-\gamma\mathfrak{h} + 2\delta\gamma\mathfrak{h}^2 < 0$ and $-\alpha\mathfrak{h} + \delta\alpha\mathfrak{h}^2 < 0$. Then, choose $\mathfrak{a} > 0$ small enough such that $\mathfrak{C}_L\mathfrak{a} - \gamma\mathfrak{h} + 2\delta\gamma\mathfrak{h}^2 < 0$. Fix now such $\mathfrak{h}, \mathfrak{a} > 0$. Recall that $|x|^\beta|y| \leq \frac{1}{p_0}|x|^{\beta p_0} + \frac{1}{q_0}|y|^{q_0} = o(|x|^k + |y|^2)$ as $|x| + |y| \rightarrow +\infty$. In addition $|\mathbf{L}(x)|^2 = \kappa^2|x|^{2\beta}$ and $2\beta < k - 1 + \beta$ since $\beta < k - 1$ (see (2.26)). This implies that there exist $C, c > 0$ such that

$$(\mathcal{L}_{\text{GL}}\mathbf{F} + \delta\gamma|\nabla_v\mathbf{F}|^2 + \delta\alpha|\nabla_z\mathbf{F}|^2)(x, v, z) \leq -c(|v|^2 + |z|^2 + |x|^{k-1+\beta}) + C.$$

Using in addition (2.23), (2.27), and (2.26), we deduce that $\mathcal{L}_{\text{GL}}\mathbf{W}_\delta/\mathbf{W}_\delta \rightarrow -\infty$ as $|x| + |v| + |z| \rightarrow +\infty$. This concludes the proof of the proposition. \square

2.3.2. *The case when $\gamma = 0$.* In this section $\gamma = 0$,

$$\mathfrak{b} = \mathfrak{a} > 0, k \in (1, 2], \text{ and } \beta = k - 1. \quad (2.28)$$

Let us check (2.21). Let $p_1 = k/(k - 1) > 1$ and $q_1 = p_1/(p_1 - 1) = k \leq 2$. Using $[\mathbf{V}_{\text{poly-}x^k}]$, we have for all $(x, v, z) \in \mathbf{R}^d$, if $|x| \geq r_V$,

$$\mathbf{F}_0(x, v, z) \geq c_V\mathfrak{h}|x|^k + \frac{\mathfrak{h} - \mathfrak{a}}{2}|v|^2 + \frac{\mathfrak{h} - \mathfrak{a}}{2}|z|^2 - \frac{\mathfrak{a}\kappa}{p_1}|x|^k - \frac{\mathfrak{a}\kappa}{k}|v|^k.$$

Then, for $\mathfrak{h} > 0$, choose $\mathfrak{a} > 0$ small enough such that

$$\frac{\mathfrak{a}\kappa}{p_1} < c_V\mathfrak{h} \text{ and } \frac{\mathfrak{a}\kappa}{k} + \frac{\mathfrak{a}}{2} < \frac{\mathfrak{h}}{2}. \quad (2.29)$$

Then (2.21) holds. Note also that when (2.28) is satisfied, $\mathbf{F}_0(x, v, z) \leq c'(|x|^k + |v|^2 + |z|^2) + C'$.

Proposition 2.13. *Assume $\gamma = 0$, $[\mathbf{V}_{\text{poly-}x^k}]$, $k \in (1, 2]$, and (2.28). Then, for any $\mathfrak{h}, \mathfrak{a} > 0$ small enough (these conditions are made explicit in the proof), **(C3)** is satisfied with the function \mathbf{W}_δ defined in (2.22).*

Proof. Recall $\mathfrak{b} = \mathfrak{a}$. In the following, $(x, v, z) \in \mathbf{R}^{3d}$, $|x| \geq \max(2, r_V)$, and $\eta = \sqrt{\mathfrak{a}}$. Using $[\mathbf{V}_{\text{poly-}x^k}]$, (2.24), and (2.25), one has:

$$\begin{aligned} & (\mathcal{L}_{\text{GL}}\mathbf{F} + \delta\gamma|\nabla_v\mathbf{F}|^2 + \delta\alpha|\nabla_z\mathbf{F}|^2)(x, v, z) \\ & \leq \alpha\mathfrak{h}d - \lambda\mathfrak{a}|v|^2 + \mathfrak{a}v \cdot \text{Jac}(\mathbf{L})(x)v - \mathfrak{a}\nabla V(x) \cdot \mathbf{L}(x) - \alpha\mathfrak{h}|z|^2 \\ & \quad + \lambda\mathfrak{a}|z|^2 + \lambda\mathfrak{a}|z||\mathbf{L}(x)| + \mathfrak{a}|\nabla V(x)||z| + \alpha\mathfrak{a}|z||v| + \delta\alpha|\mathfrak{h}z + \mathfrak{a}v|^2 \\ & \leq \alpha\mathfrak{h}d - \lambda\mathfrak{a}|v|^2 + \mathfrak{a}\mathfrak{C}_L|v|^2 - \mathfrak{a}\kappa c_V|x|^{2(k-1)} - \alpha\mathfrak{h}|z|^2 \\ & \quad + \lambda\mathfrak{a}|z|^2 + \lambda\kappa\mathfrak{a}|z||x|^{k-1} + \mathfrak{a}M_V|x|^{k-1}|z| + \alpha\mathfrak{a}|z||v| + \delta\alpha|\mathfrak{h}z + \mathfrak{a}v|^2 \\ & \leq \alpha\mathfrak{h}d - \lambda\mathfrak{a}|v|^2 + \mathfrak{a}\mathfrak{C}_L|v|^2 - \mathfrak{a}\kappa c_V|x|^{2(k-1)} - \alpha\mathfrak{h}|z|^2 + \lambda\mathfrak{a}|z|^2 + \lambda\mathfrak{a}\kappa|z|^2/2\eta + \lambda\mathfrak{a}\eta\kappa|x|^{2(k-1)}/2 \\ & \quad + \mathfrak{a}M_V\eta|x|^{2(k-1)}/2 + \mathfrak{a}M_V|z|^2/2\eta + \alpha\mathfrak{a}|z|^2/2\eta + \alpha\mathfrak{a}\eta|v|^2/2 + 2\delta\alpha\mathfrak{h}^2|z|^2 + 2\delta\alpha\mathfrak{a}^2|v|^2 \\ & \leq \alpha\mathfrak{h}d + |v|^2[-\lambda\mathfrak{a} + \mathfrak{a}\mathfrak{C}_L + 2\delta\alpha\mathfrak{a}^2 + \alpha\mathfrak{a}^{3/2}/2] + |x|^{2(k-1)}[-\kappa c_V\mathfrak{a} + \lambda\kappa\mathfrak{a}^{3/2}/2 + M_V\mathfrak{a}^{3/2}/2] \\ & \quad + |z|^2[-\alpha\mathfrak{h} + 2\delta\alpha\mathfrak{h}^2 + \lambda\kappa\sqrt{\mathfrak{a}}/2 + M_V\sqrt{\mathfrak{a}}/2 + \alpha\sqrt{\mathfrak{a}}/2 + \lambda\mathfrak{a}]. \end{aligned}$$

Let $\mathfrak{h} > 0$ such that $-\alpha\mathfrak{h} + 2\delta\alpha\mathfrak{h}^2 < 0$. Using also (2.20), it holds $-\lambda\mathfrak{a} + \mathfrak{a}\mathfrak{C}_L \leq -\lambda\mathfrak{a}/2$. We then choose $\mathfrak{a} > 0$ such that (2.29) holds, $-\lambda\mathfrak{a}/2 + 2\delta\alpha\mathfrak{a}^2 + \alpha\mathfrak{a}^{3/2}/2 < 0$, $-\kappa c_V\mathfrak{a} + \lambda\kappa\mathfrak{a}^{3/2}/2 + M_V\mathfrak{a}^{3/2}/2 < 0$, and $-\alpha\mathfrak{h} + 2\delta\alpha\mathfrak{h}^2 + \frac{\lambda\kappa}{2}\sqrt{\mathfrak{a}} + \frac{M_V}{2}\sqrt{\mathfrak{a}} + \frac{\alpha}{2}\sqrt{\mathfrak{a}} + \lambda\mathfrak{a} < 0$. With the same arguments as those used at the end of the proof of Proposition 2.12 and since $\delta > (2 - k)/k$, we obtain that $\mathcal{L}_{\text{GL}}\mathbf{W}_\delta/\mathbf{W}_\delta \rightarrow -\infty$ as $|x| + |v| + |z| \rightarrow +\infty$. This concludes the proof of the proposition. \square

2.4. Proof of Theorem 1.5. To prove Theorem 1.5, one first proves **(C3)**. This is done with a slight adaptation of the computations made in Section 2.3 and it indeed turns out that the Lyapunov functions W_δ constructed in Section 2.3 (when $\ell = 0$, see more precisely (2.22)) still satisfy **(C3)** with the generator $\mathcal{L} = \mathcal{L}_{\text{GL}} + \ell \cdot \nabla_v$ when ℓ satisfies **[bnon-gradient]**. Once **(C3)** is proved, one shows the conditions **(C2)**, **(C1)**, **(C4)**, **(C5)** (in this order) with the same arguments as those used in Section 2 (which rely on the approach introduced in Section 2.1.1) considering the coercive function W_1 as an energy of the system instead of the Hamiltonian H_{GL} (see Remark 2.1). The proof of Theorem 1.5 is then a consequence of [28, Theorem 2.2].

3. GENERALIZED LANGEVIN PROCESS WITH SINGULAR POTENTIALS: PROOF OF THEOREM 1.7

In this section, we prove Theorem 1.7. Anew, we will use [28, Theorem 2.2], and the strategy thus consists to show that **(C1)**→**(C5)** are satisfied for the process (1.4) on the state space $\mathcal{E} = \mathbf{O}_V \times \mathbf{R}^{dN} \times \mathbf{R}^{dN}$ given by Proposition 1.6.

3.1. On Assumptions **(C1)**, **(C2)**, **(C4)**, and **(C5)** for the generalized Langevin process with singular potentials.

Proposition 3.1. *Assume that V satisfies **[Vcoercive]**. Then, the nonkilled semigroup of the process (1.4) (see Proposition 1.6) satisfies **(C1)** and **(C2)**. Let $\mathcal{D} = \mathcal{O} \times \mathbf{R}^{dN} \times \mathbf{R}^{dN}$ where \mathcal{O} is a subdomain of \mathbf{O}_V such that $\mathbf{O}_V \setminus \mathcal{O}$ is nonempty. Then, the killed process (1.4) satisfies **(C4)** and **(C5)**.*

Before turning to the proof of Proposition 3.1, we briefly explain why, in the case $\gamma > 0$, we have not been able to adapt the arguments used in the proof of Proposition 2.3 to prove **(C1)** in the singular potential setting of Proposition 3.1. First notice that the global Girsanov formula (2.5) can be extended to the case when V is singular by adding the condition (on its r.h.s.) that $t < \sigma_{\mathbf{O}_V}^0$, where $\sigma_{\mathbf{O}_V}^0 = \inf\{t \geq 0, x_t^0 \notin \mathbf{O}_V\}$ (see (2.4)). Recall that ∇V is very large near $\partial\mathbf{O}_V$ and the problem is that, roughly speaking, there is no reason for the probability of the event $\{\text{“the process (2.4) visits the region } \partial\mathbf{O}_V\text{”}\}$ to be small. We will rather use once again the energy splitting approach introduced in Section 2.1.1 as a starting point.

Proof. We will only focus on the proof of **(C1)**. The conditions **(C2)**, **(C4)**, and **(C5)** are checked with the same tools as those used in the previous section when V satisfies **[Vpoly- x^k]**. To prove **(C1)** for any $\gamma \geq 0$, the starting point is (2.1). Equation (2.2) is then a consequence of the inequality $\mathbf{P}_z[\sigma_{\mathcal{H}_R} \leq t] \leq e^{ct} H_{\text{GL}}(z)/R$ derived in the proof of Proposition 1.6. When $\gamma = 0$, (2.3) is proved with the same arguments as those used in the proof of Theorem 2.6. To this end, we recall that one begins by introducing for $R > 0$ the process $(\bar{X}_t^R, t \geq 0)$ solution of (2.9) over \mathbf{R}^{3dN} with $\mathbf{b} = \mathbf{b}_R$ and $\gamma = 0$, where $\mathbf{b}_R : \mathbf{R}^{dN} \rightarrow \mathbf{R}^{dN}$ is a globally Lipschitz vector field such that $\mathbf{b}_R = -\nabla V$ in a neighborhood of $\{x \in \mathbf{R}^{dN}, V(x) < R\}$.

When $\gamma > 0$, (2.3) can also be proved with the same arguments as those used in the proof Theorem 2.6 extending the Gaussian upper bound [18, Theorem 1.1] to the process $(\bar{X}_t^R, t \geq 0)$ solution of (2.9) over \mathbf{R}^{3dN} with $\mathbf{b} = \mathbf{b}_R$ and $\gamma > 0$. One way to avoid such a technical extension is to actually use the arguments which will be used to prove Theorem 4.1 below for the Nosé-Hoover process and which do not rely on a Gaussian upper bound. In this case, the starting point is to introduce for $R > 0$ the process $(\hat{X}_t^R = (\hat{x}_t^R, \hat{v}_t^R, \hat{z}_t^R), t \geq 0)$ solution over \mathbf{R}^{3dN} to

$$d\hat{x}_t^R = \hat{v}_t^R dt, \quad d\hat{q}_t^R = \mathbf{F}_R(\hat{X}_t^R) dt + \Sigma d\mathbf{w}_t.$$

where $\hat{q}_t^R = (\hat{v}_t^R, \hat{z}_t^R)^T \in \mathbf{R}^{dN} \times \mathbf{R}^{dN}$ and where $\mathbf{F}_R : \mathbf{R}^{3dN} \rightarrow \mathbf{R}^{2dN}$ is a bounded and globally Lipschitz vector field such that $\mathbf{F}_R = \mathbf{F}$ in a neighborhood of \mathcal{H}_R . \square

3.2. On Assumption **(C3)** for the generalized Langevin process with singular potentials.

In all this section, we assume that **[Vsing1]** holds. We will also assume without loss of generality that $V_{\mathbf{p}} \equiv 0$ (see (1.11)), up to restricting the following computations to $\mathbf{x} = (x, v, z) \in \mathcal{E}$ with $x \in \mathbf{O}_V \cap \text{supp}(V_{\mathbf{p}})^c$.

3.2.1. *Preliminary computations.* We start by constructing two Lyapunov functions $W_\delta : \mathcal{E} \rightarrow [1, +\infty)$ satisfying Assumption **(C3)**, where $0 < \delta \leq 1$. Recall that $H_{\text{GL}}(x, v, z) = V(x) + \frac{1}{2}|v|^2 + \frac{1}{2}|z|^2$, for $x = (x, v, z) \in \mathcal{E}$ (see (1.8)). Let $\mathfrak{c} \geq 0$, and $\mathfrak{h} \geq 0$, $\mathfrak{b} \geq 0$, $\mathfrak{R} > 0$. Consider the function constructed in [24]:

$$F_0(x, v, z) = \mathfrak{h}H_{\text{GL}}(x, v, z) + \mathfrak{b}\mathfrak{R}x \cdot v + \mathfrak{c}\mathfrak{R}^2v \cdot z - \mathfrak{b}J_{\mathfrak{R}}(x, v, z)v \cdot G(x), \quad (3.1)$$

where $J_{\mathfrak{R}} : \mathcal{E} \rightarrow \mathbf{R}_+^*$ is a sufficiently smooth function which depends on \mathfrak{R} (so that $\mathcal{L}_{\text{GL}}F$ below is well defined) which will be specified later (depending on the case $\gamma > 0$ or $\gamma = 0$), and where $G : \mathbf{O}_V \rightarrow \mathbf{R}^{dN}$ was introduced in [51] and is defined by:

$$G(x) = (G^1(x), \dots, G^N(x))^T, \text{ with } G^i(x) = \sum_{j=1, j \neq i}^N \frac{x^i - x^j}{|x^i - x^j|}, i \in \{1, \dots, N\}.$$

The parameters will be chosen in particular such that

$$\inf_{\mathcal{E}} F_0 \in \mathbf{R}. \quad (3.2)$$

We then set $F_{\text{GL}} = F_0 - \inf_{\mathcal{E}} F_0 + 1$ and we define over \mathcal{E} :

$$W_\delta = \exp [F_{\text{GL}}^\delta], \text{ where } 0 < \delta \leq 1. \quad (3.3)$$

For any fixed $\mathfrak{R} > 0$, the function $J_{\mathfrak{R}}$ will satisfy $J_{\mathfrak{R}}^2 \leq CH_{\text{GL}}$ over \mathcal{E} , for some $C > 0$. Consequently, for any fixed parameters $\mathfrak{h}, \mathfrak{b}, \mathfrak{R} > 0$, there exists $c > 0$, $F_0 \leq cH_{\text{GL}}$ over \mathcal{E} , which implies that for all $\delta \in (0, 1]$ (recall that $H_{\text{GL}} \geq 1$),

$$W_\delta \leq e^{c^\delta H_{\text{GL}}^\delta} \text{ on } \mathcal{E}. \quad (3.4)$$

Anew, in the following, and for ease of notation, we simply write F for F_{GL} .

Recall that $\mathcal{L}_{\text{GL}}F = v \cdot \nabla_x F + (-\gamma v - \nabla_x V + \lambda z) \cdot \nabla_v F + \gamma \Delta_v F - (\alpha z + \lambda v) \cdot \nabla_z F + \alpha \Delta_z F$ and also that over \mathcal{E} , one has:

$$\frac{\mathcal{L}_{\text{GL}}W_\delta}{W_\delta} \leq \frac{\delta}{F^{1-\delta}} \left[\mathcal{L}_{\text{GL}}F + \delta\gamma |\nabla_v F|^2 + \delta\alpha |\nabla_z F|^2 \right]. \quad (3.5)$$

On the other hand it holds on \mathcal{E} :

$$\begin{cases} \partial_{x^i} F &= \mathfrak{h} \partial_{x^i} V + \mathfrak{b}\mathfrak{R}v^i - \mathfrak{b}J_{\mathfrak{R}} \partial_{x^i}(v \cdot G) - \mathfrak{b}v \cdot G \partial_{x^i} J_{\mathfrak{R}}, \\ \partial_{v^i} F &= \mathfrak{h}v^i + \mathfrak{b}\mathfrak{R}x^i + \mathfrak{c}\mathfrak{R}^2z^i - \mathfrak{b}J_{\mathfrak{R}}G^i - \mathfrak{b}(v \cdot G) \partial_{v^i} J_{\mathfrak{R}}, \\ \Delta_v F &= \mathfrak{h}Nd - 2\mathfrak{b}\nabla_v J_{\mathfrak{R}} \cdot G - \mathfrak{b}(v \cdot G) \Delta_v J_{\mathfrak{R}}, \\ \partial_{z^i} F &= \mathfrak{h}z^i + \mathfrak{c}\mathfrak{R}^2v^i - \mathfrak{b}(v \cdot G) \partial_{z^i} J_{\mathfrak{R}}, \\ \Delta_z F &= \mathfrak{h}Nd - \mathfrak{b}(v \cdot G) \Delta_z J_{\mathfrak{R}}, \end{cases}$$

where

$$\partial_{x^i}(v \cdot G) = \sum_{j=1; j \neq i}^N \left[\frac{v^i - v^j}{|x^i - x^j|} - \frac{(v^i - v^j) \cdot (x^i - x^j)}{|x^i - x^j|^3} (x^i - x^j) \right].$$

Thus, one has for all $(x, v, z) \in \mathcal{E}$:

$$\begin{aligned} \mathcal{L}_{\text{GL}}F &= \mathfrak{h}Nd(\gamma + \alpha) + (-\alpha\mathfrak{h} + \mathfrak{c}\mathfrak{R}^2\lambda)|z|^2 + (-\gamma\mathfrak{h} - \lambda\mathfrak{c}\mathfrak{R}^2 + \mathfrak{b}\mathfrak{R})|v|^2 - \mathfrak{b}\mathfrak{R}\nabla_x V \cdot x \\ &\quad - \gamma\mathfrak{b}\mathfrak{R}x \cdot v - \gamma\mathfrak{c}\mathfrak{R}^2v \cdot z - \alpha\mathfrak{c}\mathfrak{R}^2v \cdot z + \lambda\mathfrak{b}\mathfrak{R}x \cdot z - \mathfrak{c}\mathfrak{R}^2z \cdot \nabla_x V \\ &\quad - \mathfrak{b}(v \cdot G)v \cdot \nabla_x J_{\mathfrak{R}} + \alpha\mathfrak{b}(v \cdot G)z \cdot \nabla_z J_{\mathfrak{R}} + \lambda\mathfrak{b}(v \cdot G)v \cdot \nabla_z J_{\mathfrak{R}} \\ &\quad - 2\gamma\mathfrak{b}G \cdot \nabla_v J_{\mathfrak{R}} - \lambda\mathfrak{b}(v \cdot G)z \cdot \nabla_v J_{\mathfrak{R}} + \gamma\mathfrak{b}(v \cdot G)v \cdot \nabla_v J_{\mathfrak{R}} + \mathfrak{b}(v \cdot G)\nabla_x V \cdot \nabla_v J_{\mathfrak{R}} \\ &\quad - \gamma\mathfrak{b}(v \cdot G)\Delta_v J_{\mathfrak{R}} - \alpha\mathfrak{b}(v \cdot G)\Delta_z J_{\mathfrak{R}} \\ &\quad + \gamma\mathfrak{b}(v \cdot G)J_{\mathfrak{R}} + \mathfrak{b}\nabla_x V \cdot G J_{\mathfrak{R}} - \lambda\mathfrak{b}z \cdot G J_{\mathfrak{R}} - \mathfrak{b}J_{\mathfrak{R}}v \cdot \nabla_x(v \cdot G). \end{aligned} \quad (3.6)$$

We conclude this section with some estimates which be used later. First notice that for all $\epsilon > 0$, there exist $C_{\mathbf{I}}, c_{\mathbf{I}} > 0$, for all $y \in \mathbf{R}^d \setminus \{0\}$,

$$-c_{\mathbf{I}} + \frac{\mathbf{B}}{1+\epsilon}|y|^{-\beta} \leq \mathbf{V}_{\mathbf{I}}(y) \leq C_{\mathbf{I}} + (1+\epsilon)\mathbf{B}|y|^{-\beta}, \quad (3.7)$$

so that $V(x) \geq a_0|x|^2/2 + \frac{\mathbf{B}}{2} \sum_{i,j=1;i < j}^N |x^i - x^j|^{-\beta} - C$ for $x \in \mathbf{O}_V$. We also recall that from [51, Section 4] (see the computation of $\mathbf{p} \cdot \nabla_{\mathbf{q}} \Psi$ there), $v \cdot \nabla_x (v \cdot \mathbf{G}) \geq 0$ over \mathcal{E} . Therefore, since $\mathbf{b} \geq 0$ and $\mathbf{J}_{\mathfrak{R}} \geq 0$, the last term in (3.6) is nonpositive, i.e.

$$-\mathbf{b} \mathbf{J}_{\mathfrak{R}} v \cdot \nabla_x (v \cdot \mathbf{G}) \leq 0 \quad \text{over } \mathcal{E}. \quad (3.8)$$

3.2.2. *The case when $\gamma > 0$.* In this section, $\gamma > 0$,

$$\mathfrak{h} > \max(\mathbf{b}, \mathbf{b}/a_0), \quad \mathbf{c} = 0, \quad \mathfrak{R} = 1, \quad \text{and } \mathbf{J}_{\mathfrak{R}} \equiv 1. \quad (3.9)$$

We mention that extra conditions will be assumed on $\mathfrak{h}, \mathbf{b} > 0$ in the proof of Proposition 3.2. From (3.1), it holds in particular $F_0 = \mathfrak{h} \mathbf{H}_{\text{GL}} + \mathbf{b} \mathfrak{R} x \cdot v - \mathbf{b} v \cdot \mathbf{G}$. Let us first check (3.2). Using (3.7), it holds over \mathcal{E} ,

$$F_0 \geq \frac{a_0 \mathfrak{h} - \mathbf{b}}{2} |x|^2 + \frac{\mathbf{B} \mathfrak{h}}{2} \sum_{i,j=1;i < j}^N \frac{1}{|x^i - x^j|^\beta} + \frac{\mathfrak{h} - \mathbf{b}}{2} |v|^2 - \mathbf{b}(N-1) \sum_{i=1}^N |v^i| + \frac{\mathfrak{h}}{2} |z|^2 - C.$$

Therefore, in view (3.9), the condition (3.2) is satisfied when $[\mathbf{V}_{\text{sing1}}]$ holds.

Proposition 3.2. *Assume $\gamma > 0$, $[\mathbf{V}_{\text{sing1}}]$, and (3.9). Then, under additional conditions on the parameters $\mathfrak{h}, \mathbf{b} > 0$ (these conditions are made explicit in the proof below), Assumption **(C3)** is satisfied with the function \mathbf{W}_δ defined in (3.3) and which satisfies the upper bound (3.4).*

Proof. Assume $\gamma > 0$. The goal is to show that one can find parameters such that $\mathcal{L}_{\text{GL}} \mathbf{W}_\delta / \mathbf{W}_\delta \rightarrow -\infty$ as the energy $\mathbf{H}_{\text{GL}}(\mathbf{x}) \rightarrow +\infty$. We start by providing an upper bound on $\mathcal{L}_{\text{GL}} \mathbf{F}$ (see (3.5)), adapting essentially the same computations as in [24, Lemma 3.5] (see also [51]). By (3.6), (3.8), and (3.9), one has for all $\mathbf{x} = (x, v, z) \in \mathcal{E}$,

$$\begin{aligned} \mathcal{L}_{\text{GL}} \mathbf{F} &\leq \mathfrak{h} N d (\gamma + \alpha) - \alpha \mathfrak{h} |z|^2 - |v|^2 (\gamma \mathfrak{h} - \mathbf{b}) - \mathbf{b} \nabla_x V \cdot x \\ &\quad - \gamma \mathbf{b} x \cdot v + \lambda \mathbf{b} x \cdot z + \gamma \mathbf{b} (v \cdot \mathbf{G}) + \mathbf{b} \nabla_x V \cdot \mathbf{G} - \lambda \mathbf{b} z \cdot \mathbf{G}. \end{aligned}$$

Because $C_{\mathbf{G}}^\infty := \sup_{\mathcal{E}} |\mathbf{G}| < +\infty$, we deduce that

$$\begin{aligned} \mathcal{L}_{\text{GL}} \mathbf{F} &\leq \mathfrak{h} N d (\gamma + \alpha) - \alpha \mathfrak{h} |z|^2 - |v|^2 (\gamma \mathfrak{h} - \mathbf{b}) - \mathbf{b} \nabla_x V \cdot (x - \mathbf{G}) \\ &\quad - \gamma \mathbf{b} x \cdot v + \lambda \mathbf{b} x \cdot z + \gamma \mathbf{b} C_{\mathbf{G}}^\infty |v| + C_{\mathbf{G}}^\infty \lambda \mathbf{b} |z|. \end{aligned}$$

Let us now deal with the term $\mathbf{b} \nabla_x V \cdot (x - \mathbf{G})$. Recall that since $V_{\mathbf{I}}(x) = V_{\mathbf{I}}(-x)$ (see also (1.11)) $V(x) = \sum_{i=1}^N V_{\mathbf{c}}(x^i) + \frac{1}{2} \sum_{i,j=1;i \neq j}^N V_{\mathbf{I}}(x^i - x^j)$. Using also that for any symmetric vector field $\mathbf{v} : \mathbf{R}^d \rightarrow \mathbf{R}^d$, $\sum_{i,j=1;i \neq j}^N \mathbf{v}(x^i - x^j) \cdot x^i = \frac{1}{2} \sum_{i,j=1;i \neq j}^N \mathbf{v}(x^i - x^j) \cdot (x_i - x_j)$, we deduce that for all $x \in \mathbf{O}_V$:

$$\begin{aligned} \nabla_x V \cdot (x - \mathbf{G}(x)) &= \sum_{i=1}^N \left[a_0 x^i + \frac{1}{2} \sum_{j=1;j \neq i}^N \nabla V_{\mathbf{I}}(x^i - x^j) \right] \cdot \left[x^i - \sum_{j=1;j \neq i}^N \frac{x^i - x^j}{|x^i - x^j|} \right] \\ &= a_0 |x|^2 - \frac{a_0}{2} \sum_{i,j=1;i \neq j}^N |x^i - x^j| + \frac{1}{4} \sum_{i,j=1;i \neq j}^N \nabla V_{\mathbf{I}}(x^i - x^j) \cdot (x^i - x^j) \\ &\quad + \frac{1}{2} \sum_{i=1}^N \left[\sum_{j=1;j \neq i}^N (-\nabla V_{\mathbf{I}})(x^i - x^j) \right] \cdot \left[\sum_{k=1;k \neq i}^N \frac{x^i - x^k}{|x^i - x^k|} \right]. \end{aligned} \quad (3.10)$$

Denote by $I_{\mathbf{I}}(x)$ the last term in the previous equality. Note that $|\nabla V_{\mathbf{I}}(y) \cdot y| \leq C_{\mathbf{I}}/|y|^\beta + c_{\mathbf{I}}$ (for some $C_{\mathbf{I}}, c_{\mathbf{I}} > 0$). On the other hand, with the same computations as those made to prove [51, Lemma 4.2], for any $q > 1$,

$$\sum_{i=1}^N \left[\sum_{j=1; j \neq i}^N \frac{|x^i - x^j|^q}{|x^i - x^j|^q} \right] \cdot \left[\sum_{k=1; k \neq i}^N \frac{|x^i - x^k|^q}{|x^i - x^k|^q} \right] \geq \mathfrak{K}_{q-1}(x) := \sum_{i,j=1; i \neq j}^N \frac{1}{|x^i - x^j|^{q-1}}.$$

Therefore $I_{\mathbf{I}}(x) \geq \frac{\mathbf{B}\beta}{2} \mathfrak{K}_{\beta+1}(x) - c(\mathfrak{K}_{q^*}(x) + 1)$ (for some $c > 0$). We set

$$\mathbf{q}^* = \beta + 1, \quad \mathbf{c}^* = \frac{\mathbf{B}\beta}{2}.$$

Therefore, using all the previous estimates and the inequality $\kappa \mathbf{b} |a \cdot b| \leq \mathbf{b}^{3/2} a^2 + \kappa^2 \mathbf{b}^{1/2} b^2 / 4$, we have for all $\mathbf{x} = (x, v, z) \in \mathcal{E}$:

$$\begin{aligned} \mathcal{L}_{\text{GL}} F(\mathbf{x}) &\leq C - (a_0 \mathbf{b} - 2\mathbf{b}^{3/2}) |x|^2 - \mathbf{b} \mathbf{c}^* \mathfrak{K}_{\mathbf{q}^*}(x) - (\alpha \mathfrak{h} - \lambda^2 \mathbf{b}^{1/2} / 4) |z|^2 \\ &\quad - |v|^2 (\gamma \mathfrak{h} - \mathbf{b} - \gamma^2 \mathbf{b}^{1/2} / 4) + \mathfrak{L}(\mathbf{x}), \end{aligned}$$

where $\mathfrak{L} \in \mathcal{C}^0(\mathcal{E})$ and $\mathfrak{L}(\mathbf{x}) = o(|x|^2 + \mathfrak{K}_{\mathbf{q}^*}(x))$ when $\mathbf{x} \rightarrow \{\infty\}$ or $x \rightarrow \partial \mathbf{O}_V$, i.e. when $\mathbf{H}_{\text{GL}}(\mathbf{x}) \rightarrow +\infty$. In addition, over \mathcal{E} ,

$$\delta \gamma |\nabla_v F|^2 + \delta \alpha |\nabla_z F|^2 \leq 3\delta \gamma \mathfrak{h}^2 |v|^2 + 3\delta \gamma \mathbf{b}^2 |x|^2 + \delta \alpha \mathfrak{h}^2 |z|^2 + C.$$

This implies that $\mathcal{L}_{\text{GL}} F(\mathbf{x}) + \delta \gamma |\nabla_v F|^2 + \delta \alpha |\nabla_z F|^2 \leq C - (a_0 \mathbf{b} - 2\mathbf{b}^{3/2} - 3\delta \gamma \mathbf{b}^2) |x|^2 - \mathbf{b} \mathbf{c}^* \mathfrak{K}_{\mathbf{q}^*}(x) - (\alpha \mathfrak{h} - \delta \alpha \mathfrak{h}^2 - \lambda^2 \mathbf{b}^{1/2} / 4) |z|^2 - |v|^2 (\gamma \mathfrak{h} - \mathbf{b} - 3\delta \gamma \mathfrak{h}^2 - \gamma^2 \mathbf{b}^{1/2} / 4) + \mathfrak{L}(\mathbf{x})$. Choose $\mathfrak{h} > 0$ small enough such that $\gamma \mathfrak{h} - 3\delta \gamma \mathfrak{h}^2 > 0$ and $\alpha \mathfrak{h} - \delta \alpha \mathfrak{h}^2 > 0$. Then, in addition to $\mathfrak{h} > \max(\mathbf{b}, \mathbf{b}/a_0)$, choose $\mathbf{b} > 0$ small enough such that $a_0 \mathbf{b} - 2\mathbf{b}^{3/2} - 3\delta \gamma \mathbf{b}^2 > 0$, $\alpha \mathfrak{h} - \delta \alpha \mathfrak{h}^2 - \lambda^2 \mathbf{b}^{1/2} / 4 > 0$, and $\gamma \mathfrak{h} - \mathbf{b} - 3\delta \gamma \mathfrak{h}^2 - \gamma^2 \mathbf{b}^{1/2} / 4 > 0$. Then, $\mathcal{L}_{\text{GL}} F(\mathbf{x}) + \delta \gamma |\nabla_v F|^2 + \delta \alpha |\nabla_z F|^2 \leq C - c|x|^2 - \mathbf{b} \mathbf{c}^* \mathfrak{K}_{\mathbf{q}^*}(x) + \mathfrak{L}(\mathbf{x})$ over \mathcal{E} .

On the other hand, $F \leq C(|x|^2 + \mathfrak{K}_{\beta}(x) + 1)$ over \mathcal{E} . Since $0 \leq 1 - \delta < 1$, by (3.5), we deduce that $\mathcal{L}_{\text{GL}} W_\delta / W_\delta \rightarrow -\infty$ as $\mathbf{x} \rightarrow \{\infty\}$ or $x \rightarrow \partial \mathbf{O}_V$. This concludes the proof of the proposition. \square

3.2.3. The case when $\gamma = 0$. In this section, $\gamma = 0$,

$$\mathfrak{R} > 0, \quad \mathbf{c} = \mathbf{b}, \quad \mathbf{J}_{\mathfrak{R}}^2(\mathbf{x}) = \mathfrak{R}^6 |z|^2 + |v|^2 + 2V(x) + \mathfrak{R}^2, \quad \text{for } \mathbf{x} = (x, v, z) \in \mathcal{E}. \quad (3.11)$$

The function $\mathbf{J}_{\mathfrak{R}}$ above was introduced in [24] when $\gamma = 0$ to cancel the effect caused by the term $|z|/|x|^{\beta+1}$ which comes from the term $z \cdot \nabla V_{\mathbf{I}}$ in the computations of $\mathcal{L}_{\text{GL}}(v \cdot z)$, see at the end of the second line of (3.6) (recall that this term does not exist when $\gamma > 0$ because we chose $\mathbf{c} = 0$ in this case).

We start by checking (3.2). Using that $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ ($a, b \geq 0$), one has:

$$\begin{aligned} F_0 &\geq \left[\mathfrak{h} - \frac{\mathbf{b} C_{\mathbb{G}}^\infty}{\sqrt{2}} \right] V(x) - \frac{\mathbf{b} \mathfrak{R}}{2} |x|^2 + \left[\frac{\mathfrak{h}}{2} - \frac{\mathbf{b} \mathfrak{R}}{2} - \frac{\mathbf{b} \mathfrak{R}^2}{2} - \frac{\mathbf{b} C_{\mathbb{G}}^\infty}{2} (\mathfrak{R}^3 + \sqrt{2} + 2) \right] |v|^2 \\ &\quad - \mathbf{b} \mathfrak{R} C_{\mathbb{G}}^\infty |v| + \left[\frac{\mathfrak{h}}{2} - \frac{\mathbf{b} \mathfrak{R}^2}{2} - \frac{\mathbf{b} \mathfrak{R}^3 C_{\mathbb{G}}^\infty}{2} \right] |z|^2. \end{aligned}$$

We have $\left[\mathfrak{h} - \frac{\mathbf{b} C_{\mathbb{G}}^\infty}{\sqrt{2}} \right] V(x) - \frac{\mathbf{b} \mathfrak{R}}{2} |x|^2 = \frac{a_0}{2} \left[\mathfrak{h} - \frac{\mathbf{b} C_{\mathbb{G}}^\infty}{\sqrt{2}} \right] |x|^2 - \frac{\mathbf{b} \mathfrak{R}}{2} |x|^2 + \left[\mathfrak{h} - \frac{\mathbf{b} C_{\mathbb{G}}^\infty}{\sqrt{2}} \right] \sum_{i,j=1; i < j}^N V_{\mathbf{I}}(x^i - x^j)$. Then, (3.2) holds if $\mathfrak{h}, \mathbf{b}, \mathfrak{R} > 0$ satisfy:

$$\frac{a_0}{2} \left[\mathfrak{h} - \frac{\mathbf{b} C_{\mathbb{G}}^\infty}{\sqrt{2}} \right] - \frac{\mathbf{b} \mathfrak{R}}{2} > 0, \quad (3.12)$$

and

$$\frac{\mathfrak{h}}{2} - \frac{\mathbf{b} \mathfrak{R}^2}{2} - \frac{\mathbf{b} \mathfrak{R}^3 C_{\mathbb{G}}^\infty}{2} > 0, \quad \frac{\mathfrak{h}}{2} - \frac{\mathbf{b} \mathfrak{R}}{2} - \frac{\mathbf{b} \mathfrak{R}^2}{2} - \frac{\mathbf{b} C_{\mathbb{G}}^\infty}{2} (\mathfrak{R}^3 + \sqrt{2} + 2) > 0. \quad (3.13)$$

Proposition 3.3. *Assume $\gamma = 0$ and $[\mathbf{V}_{\text{sing}1}]$. Then, for some appropriately chosen $\mathfrak{h}, \mathbf{b}, \mathfrak{R} > 0$ (these conditions are made explicit in the proof), **(C3)** is satisfied with the function W_δ defined in (3.3).*

Proof. We start by providing an upper bound on the term \mathcal{L}_{GLF} in (3.5), for which we need to track the involved constants to get explicit conditions on the parameters $\mathfrak{h}, \mathfrak{b}, \mathfrak{R} > 0$ (the computations are at some places similar to those made in the proof of [24, Lemma 3.6]). The following identities will be needed:

$$\nabla_x \mathbf{J}_{\mathfrak{R}} = \frac{\nabla_x V}{\mathbf{J}_{\mathfrak{R}}}, \quad \nabla_v \mathbf{J}_{\mathfrak{R}} = \frac{v}{\mathbf{J}_{\mathfrak{R}}}, \quad \nabla_z \mathbf{J}_{\mathfrak{R}} = \frac{\mathfrak{R}^6 z}{\mathbf{J}_{\mathfrak{R}}}, \quad \text{and} \quad \Delta_z \mathbf{J}_{\mathfrak{R}} = \frac{\mathfrak{R}^6 dN}{\mathbf{J}_{\mathfrak{R}}} - \frac{\mathfrak{R}^{12} |z|^2}{\mathbf{J}_{\mathfrak{R}}^3}.$$

By (3.6) and (3.8), when $\gamma = 0$ and $\mathbf{c} = \mathfrak{b}$, we have for all $\mathbf{x} = (x, v, z) \in \mathcal{E}$,

$$\begin{aligned} \mathcal{L}_{\text{GLF}} &\leq \mathfrak{h}Nd\alpha + (-\alpha\mathfrak{h} + \mathfrak{b}\mathfrak{R}^2\lambda)|z|^2 + (-\lambda\mathfrak{b}\mathfrak{R}^2 + \mathfrak{b}\mathfrak{R})|v|^2 - \mathfrak{b}\mathfrak{R}\nabla_x V \cdot x \\ &\quad - \alpha\mathfrak{b}\mathfrak{R}^2 v \cdot z + \lambda\mathfrak{b}\mathfrak{R} x \cdot z - \mathfrak{R}^2 \mathfrak{b}z \cdot \nabla_x V \\ &\quad - \mathfrak{b}(v \cdot \mathbf{G})v \cdot \nabla_x \mathbf{J}_{\mathfrak{R}} + \alpha\mathfrak{b}(v \cdot \mathbf{G})z \cdot \nabla_z \mathbf{J}_{\mathfrak{R}} + \lambda\mathfrak{b}(v \cdot \mathbf{G})v \cdot \nabla_z \mathbf{J}_{\mathfrak{R}} \\ &\quad - \lambda\mathfrak{b}(v \cdot \mathbf{G})z \cdot \nabla_v \mathbf{J}_{\mathfrak{R}} + \mathfrak{b}(v \cdot \mathbf{G})\nabla_x V \cdot \nabla_v \mathbf{J}_{\mathfrak{R}} - \alpha\mathfrak{b}(v \cdot \mathbf{G})\Delta_z \mathbf{J}_{\mathfrak{R}} \\ &\quad + \mathfrak{b}\nabla_x V \cdot \mathbf{G} \mathbf{J}_{\mathfrak{R}} - \lambda\mathfrak{b}z \cdot \mathbf{G} \mathbf{J}_{\mathfrak{R}}. \end{aligned} \tag{3.14}$$

We now provide upper bounds on the terms appearing in (3.14) over \mathcal{E} as follows:

- Following the computations in (3.10), we have

$$\begin{aligned} -\mathfrak{b}\mathfrak{R}\nabla_x V \cdot x &= -a_0\mathfrak{b}\mathfrak{R}|x|^2 - \frac{\mathfrak{b}\mathfrak{R}}{4} \sum_{i,j=1;i \neq j}^N \nabla V_{\mathbf{I}}(x^i - x^j) \cdot (x^i - x^j) \\ &\leq -a_0\mathfrak{b}\mathfrak{R}|x|^2 + \mathfrak{L}(x) \end{aligned}$$

and $\nabla_x V \cdot \mathbf{G} \mathbf{J}_{\mathfrak{R}} \leq -[\mathbf{c}^* \mathfrak{R}_{\mathbf{q}^*}(x) - \mathfrak{L}(x)] \mathbf{J}_{\mathfrak{R}}$, where $\mathfrak{L} \in \mathcal{C}^0(\mathbf{O}_V)$ and $\mathfrak{L}(x) = o(|x|^2 + \mathfrak{R}_{\mathbf{q}^*}(x))$ when $x \rightarrow \{\infty\} \cup \partial \mathbf{O}_V$. In particular, it holds over \mathcal{E} :

$$\mathbf{c}^* \mathfrak{R}_{\mathbf{q}^*}(x) - \mathfrak{L}(x) \geq \frac{\mathbf{c}^*}{2} \mathfrak{R}_{\mathbf{q}^*}(x) - C.$$

In addition, since $\mathbf{J}_{\mathfrak{R}} \geq \mathfrak{R}f(z)$ (where $f(z) = \sqrt{\mathfrak{R}^4|z|^2 + 1}$), one deduces that:

$$\mathfrak{b}\nabla_x V \cdot \mathbf{G} \mathbf{J}_{\mathfrak{R}} \leq -\frac{\mathbf{c}^* \mathfrak{b}\mathfrak{R}}{2} \mathfrak{R}_{\mathbf{q}^*}(x)f(z) + C\mathfrak{b}\mathfrak{R}f(z).$$

Roughly speaking, the term $\mathfrak{b}\nabla_x V \cdot \mathbf{G} \mathbf{J}_{\mathfrak{R}}$ can absorb the bad one $-\mathfrak{R}^2 \mathfrak{b}z \cdot \nabla_x V$ when $x \rightarrow \partial \mathbf{O}_V$. Note that there exists $C > 0$ such that $|\nabla V_{\mathbf{I}}(y)| \leq A/|y|^{\mathfrak{q}^*} + C$ over $\mathbf{R}^d \setminus \{0\}$ ($A = \mathbf{B}\beta + 1$). Then, one has $|\mathfrak{R}^2 \mathfrak{b}z \cdot \nabla_x V| \leq \mathfrak{R}^2 \mathfrak{b}a_0|z||x| + A\mathfrak{R}^2 \mathfrak{b}|z|\mathfrak{R}_{\mathbf{q}^*}(x) + C\mathfrak{R}^2 \mathfrak{b}|z| \leq \mathfrak{R}^2 \mathfrak{b}a_0|z||x| + A\mathfrak{b}f(z)\mathfrak{R}_{\mathbf{q}^*}(x) + C\mathfrak{R}^2 \mathfrak{b}|z|$, so that the function $\mathfrak{b}\nabla_x V \cdot \mathbf{G} \mathbf{J}_{\mathfrak{R}} - \mathfrak{R}^2 \mathfrak{b}z \cdot \nabla_x V$ is bounded from above over \mathcal{E} by

$$-\mathfrak{b} \left[\frac{\mathbf{c}^* \mathfrak{R}}{2} - A \right] \mathfrak{R}_{\mathbf{q}^*}(x)f(z) + C\mathfrak{b}\mathfrak{R}f(z) + \mathfrak{R}^2 a_0 \frac{\mathfrak{b}^{1/2}}{2} |z|^2 + \mathfrak{R}^2 a_0 \frac{\mathfrak{b}^{3/2}}{2} |x|^2.$$

Note also that $f(z) = o(|x|^2 + \mathfrak{R}_{\mathbf{q}^*}(x))$ when $\mathbf{x} \rightarrow \{\infty\}$ or $x \rightarrow \partial \mathbf{O}_V$ (i.e. when $\mathbf{H}_{\text{GL}}(\mathbf{x}) \rightarrow +\infty$).

- For any $\epsilon_0, \epsilon_1 > 0$ to be chosen later,

$$\alpha\mathfrak{b}\mathfrak{R}^2|v \cdot z| + \lambda\mathfrak{b}\mathfrak{R}|x \cdot z| \leq \alpha\mathfrak{b}\mathfrak{R}^2 \left[\frac{|v|^2}{2\epsilon_0} + \frac{\epsilon_0}{2}|z|^2 \right] + \lambda\mathfrak{b}\mathfrak{R} \left[\frac{|x|^2}{2\epsilon_1} + \frac{\epsilon_1}{2}|z|^2 \right].$$

- Using that \mathbf{G} is bounded, we have:

$$|(v \cdot \mathbf{G})v \cdot \nabla_x \mathbf{J}_{\mathfrak{R}}| \leq C_{\mathbf{G}}^{\infty} \frac{|v|^2(a_0|x| + C)}{\sqrt{|v|^2 + 2V(x) + \mathfrak{R}^2}} + C_{\mathbf{G}}^{\infty} \frac{C|v|^2 \mathfrak{R}_{\beta+1}(x)}{\sqrt{|v|^2 + 2V(x) + \mathfrak{R}^2}},$$

where we recall that over \mathbf{O}_V , $V(x) \geq a_0|x|^2/2 + \mathbf{B}\mathfrak{R}_{\beta}(x)/2 - C$. Hence,

$$|(v \cdot \mathbf{G})v \cdot \nabla_x \mathbf{J}_{\mathfrak{R}}| = o(|x|^2 + \mathfrak{R}_{\mathbf{q}^*}(x)) \text{ as } \mathbf{H}_{\text{GL}}(\mathbf{x}) \rightarrow +\infty.$$

With similar arguments, one also has:

$$\begin{aligned} & |(v \cdot \mathbf{G})z \cdot \nabla_z \mathbf{J}_{\mathfrak{R}}| + |(v \cdot \mathbf{G})v \cdot \nabla_z \mathbf{J}_{\mathfrak{R}}| + |(v \cdot \mathbf{G})z \cdot \nabla_v \mathbf{J}_{\mathfrak{R}}| + |(v \cdot \mathbf{G}) \nabla_x V \cdot \nabla_v \mathbf{J}_{\mathfrak{R}}| \\ & + |\mathfrak{b}(v \cdot \mathbf{G})\Delta_z \mathbf{J}_{\mathfrak{R}}| = o(|x|^2 + \mathfrak{R}_{\mathfrak{q}^*}(x)) \text{ as } \mathbf{H}_{\text{GL}}(x) \rightarrow +\infty. \end{aligned}$$

- Using that $\mathbf{J}_{\mathfrak{R}} \leq \mathfrak{R}^3|z| + |v| + \sqrt{2}\sqrt{V}(x) + \mathfrak{R}$ and $V(x) \leq a_0|x|^2/2 + S_{\text{int}}(x) + C$ over \mathbf{O}_V (where $S_{\text{int}} = 2\mathfrak{R}_{\beta}$), one has:

$$\begin{aligned} \lambda \mathfrak{b} \left| z \cdot \frac{\mathbf{G}}{C_{\mathfrak{G}}^{\infty}} \mathbf{J}_{\mathfrak{R}} \right| & \leq \lambda \mathfrak{b} \mathfrak{R}^3 |z|^2 + \lambda \mathfrak{b} |z| |v| + \lambda \mathfrak{b} \sqrt{2} |z| \sqrt{V}(x) + \lambda \mathfrak{b} \mathfrak{R} |z| \\ & \leq |z|^2 \left[\lambda \mathfrak{b} \mathfrak{R}^3 + \frac{\lambda \mathfrak{b} \sqrt{a_0}}{2\epsilon_2} + \frac{\lambda \mathfrak{b}}{2\epsilon_3} + \lambda \frac{\mathfrak{b}}{\sqrt{2}} \right] + \lambda \mathfrak{b} (\mathfrak{R} + C\sqrt{2}) |z| \\ & \quad + \frac{\lambda \mathfrak{b} \epsilon_2 \sqrt{a_0}}{2} |x|^2 + \frac{\lambda \mathfrak{b} \epsilon_3}{2} |v|^2 + \frac{\lambda \mathfrak{b}}{\sqrt{2}} S_{\text{int}}(x). \end{aligned}$$

Note that $|S_{\text{int}}(x)| = o(|x|^2 + \mathfrak{R}_{\mathfrak{q}^*}(x))$ when $\mathbf{H}_{\text{GL}}(x) \rightarrow +\infty$.

Finally, setting $M_{\infty} := \sup_{x=(x,v,z) \in \mathcal{E}} |v||z|/|\mathbf{J}_{\mathfrak{R}}^2(x)| < +\infty$, one has for all $x = (x, v, z) \in \mathcal{E}$:

$$\begin{aligned} \delta \alpha |\nabla_z \mathbf{F}|^2 & \leq 3\mathfrak{h}^2 \delta \alpha |z|^2 + 3\mathfrak{b}^2 \mathfrak{R}^4 \delta \alpha |v|^2 + 3\mathfrak{b}^2 |C_{\mathfrak{G}}^{\infty}|^2 M_{\infty} \delta \alpha \mathfrak{R}^{12} |v||z| \\ & \leq 3\delta \alpha (\mathfrak{h}^2 + \mathfrak{R}^{12} \mathfrak{b}^2 |C_{\mathfrak{G}}^{\infty}|^2 M_{\infty}/2) |z|^2 + 3\delta \alpha \mathfrak{b}^2 (\mathfrak{R}^4 + \mathfrak{R}^{12} |C_{\mathfrak{G}}^{\infty}|^2 M_{\infty}/2) |v|^2. \end{aligned}$$

We now gather all the previous upper bounds, to get over \mathcal{E} ,

$$\mathcal{L}_{\text{GL}} \mathbf{F} + \delta \alpha |\nabla_z \mathbf{F}|^2 \leq c_z |z|^2 + c_v |v|^2 + c_x |x|^2 - \mathfrak{b} \left[\frac{c^* \mathfrak{R}}{2} - \mathbf{A} \right] \mathfrak{R}_{\mathfrak{q}^*}(x) f(z) + o(|x|^2 + \mathfrak{R}_{\mathfrak{q}^*}(x)),$$

where

- $c_z = -\alpha \mathfrak{h} + 3\delta \alpha \mathfrak{h}^2 + \mathfrak{b} \mathfrak{R}^2 \lambda + \alpha \mathfrak{b} \mathfrak{R}^2 \frac{\epsilon_0}{2} + \lambda \mathfrak{b} \mathfrak{R} \frac{\epsilon_1}{2} + \lambda \mathfrak{b} \mathfrak{R}^3 C_{\mathfrak{G}}^{\infty} + \mathfrak{b} C_{\mathfrak{G}}^{\infty} \frac{\lambda \sqrt{a_0}}{2\epsilon_2} + \mathfrak{b} C_{\mathfrak{G}}^{\infty} \frac{\lambda}{2\epsilon_3} + \mathfrak{R}^2 a_0 \frac{\mathfrak{b}^{1/2}}{2} + 3\delta \alpha \mathfrak{b}^2 \mathfrak{R}^{12} |C_{\mathfrak{G}}^{\infty}|^2 M_{\infty}/2 + \lambda C_{\mathfrak{G}}^{\infty} \frac{\mathfrak{b}}{\sqrt{2}}$,
- $c_v = -\mathfrak{b} \mathfrak{R} (\lambda \mathfrak{R} - 1) + \mathfrak{b} \mathfrak{R}^2 \frac{\alpha}{2\epsilon_0} + \mathfrak{b} C_{\mathfrak{G}}^{\infty} \frac{\lambda \epsilon_3}{2} + 3\delta \alpha \mathfrak{b}^2 (\mathfrak{R}^4 + |C_{\mathfrak{G}}^{\infty}|^2 \mathfrak{R}^{12} M_{\infty}/2)$,
- $c_x = -a_0 \mathfrak{b} \mathfrak{R} + \mathfrak{b} C_{\mathfrak{G}}^{\infty} \frac{\lambda \epsilon_2 \sqrt{a_0}}{2} + \mathfrak{b} \mathfrak{R} \frac{\lambda}{2\epsilon_1} + \mathfrak{R}^2 a_0 \frac{\mathfrak{b}^{3/2}}{2}$.

Let $\epsilon_0 = \mathfrak{b}^{-1/2}$, $\epsilon_1 = \mathfrak{b}^{-1/2}$, $\epsilon_2 = \mathfrak{b}^{1/2}$, and $\epsilon_3 = \mathfrak{b}^{1/2}$. Pick and fix $\mathfrak{h} > 0$ small enough such that $-\alpha \mathfrak{h} + 3\delta \alpha \mathfrak{h}^2 < 0$ and $\mathfrak{R} > 0$ large enough such that $\frac{c^* \mathfrak{R}}{2} - \mathbf{A} > 0$ and $\lambda \mathfrak{R} - 1 > 0$. Then, one has when $\mathfrak{b} \rightarrow 0^+$, $c_z = -\alpha \mathfrak{h} + 3\delta \alpha \mathfrak{h}^2 + o(1)$, $c_v = -\mathfrak{b}[\mathfrak{R}(\lambda \mathfrak{R} - 1) + o(1)]$, and $c_x = -a_0 \mathfrak{b}[\mathfrak{R} + o(1)]$. One chooses $\mathfrak{b} > 0$ small enough such that $c_x, c_v, c_z < 0$ and (3.12)-(3.13) hold. This leads to the existence of $c_1, c_2 > 0$ such that over \mathcal{E} :

$$\mathcal{L}_{\text{GL}} \mathbf{F} + \delta \alpha |\nabla_z \mathbf{F}|^2 \leq -c_1 |x|^2 - c_2 \mathfrak{R}_{\mathfrak{q}^*}(x) f(z) + o(|x|^2 + \mathfrak{R}_{\mathfrak{q}^*}(x)), \quad (3.15)$$

as $|x| \rightarrow +\infty$ or $x \rightarrow \partial \mathbf{O}_V$, or equivalently when $\mathbf{H}_{\text{GL}}(x) \rightarrow +\infty$. With the same arguments as those used to conclude the proof of Proposition 3.2, we deduce that $\mathcal{L}_{\text{GL}} \mathbf{W}_{\delta} / \mathbf{W}_{\delta} \rightarrow -\infty$ as $|x|^2 + \mathfrak{R}_{\mathfrak{q}^*}(x) \rightarrow +\infty$. This ends the proof of the proposition. \square

4. THE NOSÉ-HOOVER PROCESS: PROOF OF THEOREM 1.11

In this section, we prove Theorem 1.11. We recall that, when V satisfies $[\mathbf{V}_{\text{coercive}}]$, the Nosé-Hoover process (1.5) evolves on $\mathcal{E} = \mathbf{O}_V \times \mathbf{R}^{dN} \times \mathbf{R}$ (see (1.12) and Proposition 1.9). As it will be seen below, **(C5)** is not satisfied for this process. To this end, to prove Theorem 1.11, we will use an extension (Theorem 4.6 below) of [28, Theorem 2.2], and we will thus prove that this process satisfies **(C1)**, **(C2)**, **(C3)**, **(C4)**, and a new assumption, namely **(C5')**, which is defined at the beginning of Section 4.3 below.

4.1. On Assumptions (C1), (C2), (C4), and (C5') for the process (1.5). In this section, V satisfies $[\mathbf{V}_{\text{coercive}}]$ and we consider the solution $(X_t = (x_t, v_t, y_t), t \geq 0)$ solution to (1.5), see Proposition 1.9.

The approach we will use to prove (C1) and (C4) is the energy splitting approach introduced in Section 2.1.1 (see (2.1)). The uniform integrability of the transition probabilities was obtained in Theorem 2.6 with a Gaussian upper bound. However, Gaussian upper bound does not hold anymore for the Nosé-Hoover process. Hence, the proof of (2.3) relies on different arguments than those used in Theorem 2.6.

Theorem 4.1. *Assume that V satisfies $[\mathbf{V}_{\text{coercive}}]$. Then, the nonkilled semigroup $(P_t, t \geq 0)$ of the process (1.5) satisfies (C1).*

Proof. We want to prove that, for $f \in b\mathcal{B}(\mathcal{E})$ and $t > 0$, the following function

$$z \in \mathcal{E} \mapsto \mathbf{E}_z[f(X_t)] \text{ is continuous.} \quad (4.1)$$

Pick $R > 0$. We will start by proving (2.3), which is the purpose of Step 2 below. Then we will prove (4.1) in Step 3. Before doing that, we need a local Girsanov formula (4.3), which is the aim of Step 1.

Step 1. In this step we derive (4.3) below. We recall that (see also (1.13)),

$$\mathcal{H}_R = \{x \in \mathbf{R}^{3d}, H_{\text{NH}}(x) < R\},$$

is an open bounded domain of \mathcal{E} . Set $\Sigma = \sqrt{2\gamma}$. Recall also that $\sigma_{\mathcal{H}_R}$ is the first exit time for the process $(X_t, t \geq 0)$ from \mathcal{H}_R and a.s. $\sigma = \lim_{R \rightarrow +\infty} \sigma_{\mathcal{H}_R} = \sup_{R > 0} \sigma_{\mathcal{H}_R} = +\infty$. For $z = (x_z, v_z, y_z) \in \mathcal{E}$, set also

$$\mathbf{f}(z) = -\nabla V(x_z) - \gamma v_z - v_z y_z \in \mathbf{R}^{dN}.$$

Let us consider a globally Lipschitz and bounded \mathbf{R}^{dN} -valued vector field \mathbf{f}_R over $\mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}$ such that $\mathbf{f}_R = \mathbf{f}$ in a neighborhood of \mathcal{H}_R in \mathcal{E} . Let also $\chi_R : \mathbf{R}^{dN} \rightarrow \mathbf{R}$ be a globally Lipschitz \mathcal{C}^∞ function such that $\chi_R(v) = |v|^2$ if $|v|^2/2 \leq R + 1$. Denote by $(\hat{X}_t^R, t \geq 0)$ the strong solution³ on $\mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}$ of:

$$d\hat{x}_t^R = \hat{v}_t^R dt, \quad d\hat{v}_t^R = \mathbf{f}_R(\hat{X}_t^R) dt + \Sigma dB_t, \quad d\hat{y}_t^R = \chi_R(\hat{v}_t^R) dt - dN dt. \quad (4.2)$$

Let $\hat{\sigma}_{\mathcal{H}_R} = \inf\{t \geq 0, \hat{X}_t^R \notin \mathcal{H}_R\}$. When $z \in \mathcal{H}_R$ and $0 \leq t < \hat{\sigma}_{\mathcal{H}_R}$, it holds $\chi_R(\hat{v}_t^R(z)) = |\hat{v}_t^R(z)|^2$ and $\mathbf{f}_R(\hat{X}_t^R(z)) = \mathbf{f}(\hat{X}_t^R(z))$. Therefore, one has for all $g \in b\mathcal{B}(\mathcal{H}_R)$, $t > 0$, and $z = (x_z, v_z, y_z) \in \mathcal{H}_R$,

$$\mathbf{E}_z[g(X_t) \mathbf{1}_{t < \sigma_{\mathcal{H}_R}}] = \mathbf{E}_z[g(\hat{X}_t^R(z)) \mathbf{1}_{t < \hat{\sigma}_{\mathcal{H}_R}}],$$

since the laws of the two processes coincide up to their first exit time from \mathcal{H}_R . Let us now consider the process $(\tilde{X}_t^R = (\tilde{x}_t^R, \tilde{v}_t^R, \tilde{y}_t^R), t \geq 0)$ solution on $\mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}$ to:

$$d\tilde{x}_t^R = \tilde{v}_t^R dt, \quad d\tilde{v}_t^R = \Sigma dB_t, \quad d\tilde{y}_t^R = \chi_R(\tilde{v}_t^R) dt - dN dt.$$

Set $\tilde{\sigma}_{\mathcal{H}_R} := \inf\{t \geq 0, \tilde{X}_t^R \notin \mathcal{H}_R\}$. Since \mathbf{f}_R is bounded, $\sup_{s \in [0, t]} \mathbf{E}_z[e^{|\mathbf{f}_R(\tilde{X}_s^R)|^2}] < +\infty$ for all $t > 0$. Hence, using [25, Theorem 3.1 in Section 7] and [25, Theorem 1.1 in Section 7], one has for all $g \in b\mathcal{B}(\mathcal{H}_R)$, $t > 0$, and $z = (x_z, v_z, y_z) \in \mathcal{H}_R$,

$$\mathbf{E}_z[g(\tilde{X}_t^R) \mathbf{1}_{t < \tilde{\sigma}_{\mathcal{H}_R}}] = \mathbf{E}_z[g(\tilde{X}_t^R) \mathbf{1}_{t < \tilde{\sigma}_{\mathcal{H}_R}} \tilde{\mathfrak{M}}_t(\mathbf{f}_R)],$$

where $\tilde{\mathfrak{M}}_t(\mathbf{f}_R)$ is the exponential (true) martingale defined by $\tilde{\mathfrak{M}}_t(\mathbf{f}_R) = \exp \tilde{\mathfrak{L}}_t(\mathbf{f}_R)$ and

$$\tilde{\mathfrak{L}}_t(\mathbf{f}_R) = \int_0^t \Sigma^{-1} \mathbf{f}_R^*(X_s^R) dB_s - \frac{1}{2} \int_0^t |\Sigma^{-1} \mathbf{f}_R^*(X_s^R)|^2 ds.$$

Introduce finally the process $(X_t^0 = (x_t^0, v_t^0, y_t^0), t \geq 0)$ solution on $\mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}$ to:

$$dx_t^0 = v_t^0 dt, \quad dv_t^0 = \Sigma dB_t, \quad dy_t^0 = |v_t^0|^2 dt - dN dt.$$

³Existence and uniqueness are ensured by the fact that the coefficients are globally Lipschitz.

Anew, because the laws of $(\tilde{X}_t^R, t \geq 0)$ and $(X_t^0, t \geq 0)$ coincide up to their first exit time from \mathcal{H}_R , one finally gets that for any $\mathbf{z} \in \mathcal{H}_R$:

$$\mathbf{E}_{\mathbf{z}}[g(X_t)\mathbf{1}_{t < \sigma_{\mathcal{H}_R}}] = \mathbf{E}_{\mathbf{z}}[g(X_t^0)\mathbf{1}_{t < \sigma_{\mathcal{H}_R}^0} \mathfrak{M}_t^0(\mathbf{f}_R)], \quad (4.3)$$

where $\mathfrak{M}_t^0(\mathbf{f}_R) = \exp \mathfrak{L}_t^0(\mathbf{f}_R)$, $\mathfrak{L}_t^0(\mathbf{f}_R) = \int_0^t \Sigma^{-1} \mathbf{f}_R(X_s^0) dB_s - \frac{1}{2} \int_0^t |\Sigma^{-1} \mathbf{f}_R(X_s^0)|^2 ds$, and $\sigma_{\mathcal{H}_R}^0 := \inf\{t \geq 0, X_t^0 \notin \mathcal{H}_R\}$.

Step 2. In this step we show that for all $R > 0$, $t > 0$, and all $f \in b\mathcal{B}(\mathcal{H}_R)$, the function

$$\mathbf{z} \in \mathcal{H}_R \mapsto \mathbf{E}_{\mathbf{z}}[f(X_t)\mathbf{1}_{t < \sigma_{\mathcal{H}_R}}] \text{ is continuous.}$$

In view of (4.3), let us show that

$$\mathbf{z} \in \mathcal{H}_R \mapsto \mathbf{E}_{\mathbf{z}}[f(X_t^0)\mathbf{1}_{t < \sigma_{\mathcal{H}_R}^0} \mathfrak{M}_t^0(\mathbf{f}_R)] \text{ is continuous.} \quad (4.4)$$

We first claim that

- i. For $t > 0$ and $\mathbf{x}_n \rightarrow \mathbf{x}$, $\sup_{s \in [0, t]} |X_s^0(\mathbf{x}_n) - X_s^0(\mathbf{x})| \rightarrow 0$ a.s. as $n \rightarrow +\infty$.
- ii. For all $\psi \in b\mathcal{B}(\mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R})$ and $t > 0$, the following function

$$\mathbf{z} \in \mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R} \mapsto \wp_t(\psi)(\mathbf{z}) = \mathbf{E}_{\mathbf{z}}[e^{\mathfrak{L}_t^0(\mathbf{f}_R)} \psi(X_t^0)] \text{ is continuous.}$$

- iii. For all $\delta > 0$ and all compact subset K of $\mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}$,

$$\lim_{s \rightarrow 0^+} \sup_{\mathbf{z} \in K} \mathbf{P}_{\mathbf{z}}[\sigma_{\mathbf{B}(\mathbf{z}, \delta)}^0 \leq s] = 0,$$

where $\mathbf{B}(\mathbf{z}, \delta)$ is the open ball of $\mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}$ centered at \mathbf{z} of radius δ , and $\sigma_{\mathbf{B}(\mathbf{z}, \delta)}^0$ is the first exit time from $\mathbf{B}(\mathbf{z}, \delta)$ for the process $(X_t^0, t \geq 0)$.

The proof of Item **i** is straightforward. Let us now prove Item **ii**. Let $\mathbf{z}_n \rightarrow \mathbf{z} \in \mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}$. By Hörmander's theory, for all $t > 0$, X_t^0 admits a smooth density w.r.t. the Lebesgue measure over $\mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}$. Using also Item **i** and Proposition 1.2, we deduce that $\psi(X_t^0(\mathbf{z}_n)) \rightarrow \psi(X_t^0(\mathbf{z}))$ in \mathbf{P} -probability. In addition, using Item **i** and the regularity of \mathbf{f}_R , $\mathfrak{L}_t^0(\mathbf{f}_R)(\mathbf{z}_n) \rightarrow \mathfrak{L}_t^0(\mathbf{f}_R)(\mathbf{z})$ in \mathbf{P} -probability. By the continuous mapping theorem, $e^{\mathfrak{L}_t^0(\mathbf{f}_R)}(\mathbf{z}_n) \rightarrow e^{\mathfrak{L}_t^0(\mathbf{f}_R)}(\mathbf{z})$ in \mathbf{P} -probability. Since $\mathbf{E}_{\mathbf{z}_n}[e^{\mathfrak{L}_t^0(\mathbf{f}_R)}] = \mathbf{E}_{\mathbf{z}}[e^{\mathfrak{L}_t^0(\mathbf{f}_R)}] = 1$, one deduces using the Vitali convergence theorem, that

$$\mathbf{E}_{\mathbf{z}_n}[e^{\mathfrak{L}_t^0(\mathbf{f}_R)}] \rightarrow \mathbf{E}_{\mathbf{z}}[e^{\mathfrak{L}_t^0(\mathbf{f}_R)}] \text{ in } L^1.$$

This ends the proof of Item **ii**. Let us now prove Item **iii**. Fix $\delta > 0$ and a compact subset K of $\mathbf{R}^{dN} \times \mathbf{R}^{dN} \times \mathbf{R}$. With the same arguments as those used at the beginning of the proof of Lemma 2.4, we have

$$\mathbf{P}_{\mathbf{z}}[\sigma_{\mathbf{B}(\mathbf{z}, \delta)}^0 \leq s] \leq \mathbf{P}_{\mathbf{z}}[\sigma_{\mathbf{B}(\mathbf{z}, \delta)}^0 \leq s, |X_s^0 - X_0^0| < \delta/2] + \mathbf{P}_{\mathbf{z}}[|X_s^0 - X_0^0| \geq \delta/2]$$

and by the strong Markov property,

$$\begin{aligned} & \mathbf{P}_{\mathbf{z}}[\sigma_{\mathbf{B}(\mathbf{z}, \delta)}^0 \leq s, |X_s^0 - X_0^0| < \delta/2] \\ & \leq \mathbf{p}(s, \mathbf{z}) := \mathbf{E}_{\mathbf{z}}[\mathbf{1}_{\sigma_{\mathbf{B}(\mathbf{z}, \delta)}^0(\mathbf{z}) \leq s} \mathbf{P}_{X_{\sigma_{\mathbf{B}(\mathbf{z}, \delta)}^0(\mathbf{z})}}^0[|X_{s - \sigma_{\mathbf{B}(\mathbf{z}, \delta)}^0(\mathbf{z})}^0 - X_0^0| \geq \delta/2]]. \end{aligned}$$

Let us deal with $\mathbf{p}(s, \mathbf{z})$. For any $\mathbf{z} \in K$, $\mathbf{x} = (x, v, z) \in \partial\mathbf{B}(\mathbf{z}, \delta)$, and $u \in [0, s]$, $\mathbf{P}_{\mathbf{x}}[|X_{s-u}^0 - \mathbf{x}| \geq \delta/2] \leq \mathbf{P}_{\mathbf{x}}[|x_{s-u}^0 - x| \geq \delta/2] + \mathbf{P}_{\mathbf{x}}[|v_{s-u}^0 - v| \geq \delta/2] + \mathbf{P}_{\mathbf{x}}[|y_{s-u}^0 - y| \geq \delta/2]$. Note that $|\mathbf{x}| \leq c_{\delta, K} := \delta/2 + r_K$, where $r_K > 0$ is such that $K \subset \mathbf{B}(0, r_K)$. First, it holds $\mathbf{P}_{\mathbf{x}}[|v_{s-u}^0 - v| \geq \delta/2] \leq \mathbf{a}_s := \mathbf{P}[\sup_{t \in [0, s]} |B_t| \geq \delta/(2\Sigma)]$. On the other hand, $\mathbf{P}_{\mathbf{x}}[|x_{s-u}^0 - x| \geq \delta/2] \leq \mathbf{b}_s := \mathbf{P}[sc_{\delta, K} + \int_0^s \Sigma |B_t| dt \geq \delta/2]$. Finally, $\mathbf{P}_{\mathbf{x}}[|y_{s-u}^0 - y| \geq \delta/2] \leq \mathbf{P}_{\mathbf{x}}[\int_0^s |v_t|^2 dt + sdN \geq \delta/2] \leq \mathbf{c}_s := \mathbf{P}[2\Sigma^2 \int_0^s |B_t|^2 dt + 2sc_{\delta, K}^2 + sdN \geq \delta/2]$. Thus, one has as $s \rightarrow 0^+$:

$$\sup_{\mathbf{z} \in K} \mathbf{p}(s, \mathbf{z}) \leq \mathbf{a}_s + \mathbf{b}_s + \mathbf{c}_s \rightarrow 0.$$

Similarly, we have $\sup_{\mathbf{z} \in K} \mathbf{P}_{\mathbf{z}}[|X_s^0 - X_0^0| \geq \delta/2] \rightarrow 0$ as $s \rightarrow 0^+$. This concludes the proof of Item **iii**.

We will use the fact that Item **iii** implies that for all compact subset K of \mathcal{H}_R :

$$\lim_{s \rightarrow 0^+} \sup_{z \in K} \mathbf{P}_z[\sigma_{\mathcal{H}_R}^0 \leq s] = 0. \quad (4.5)$$

We are now in position to prove (4.4). We have by the Markov property, for $0 \leq s \leq t$ and $z \in \mathcal{H}_R$:

$$\mathbf{E}_z[f(X_t^0) \mathbf{1}_{t < \sigma_{\mathcal{H}_R}^0} \mathfrak{M}_t^0(\mathbf{f}_R)] = \mathbf{E}_z[\mathbf{1}_{s < \sigma_{\mathcal{H}_R}^0} \mathfrak{M}_s^0(\mathbf{f}_R) \mathbf{E}_{X_s^0}[f(X_{t-s}^0) \mathbf{1}_{t-s < \sigma_{\mathcal{H}_R}^0} \mathfrak{M}_{t-s}^0(\mathbf{f}_R)]]. \quad (4.6)$$

Define ψ_s by $\psi_s(z) = \mathbf{E}_z[f(X_{t-s}^0) \mathbf{1}_{t-s < \sigma_{\mathcal{H}_R}^0} \mathfrak{M}_{t-s}^0(\mathbf{f}_R)]$ for $z \in \mathcal{H}_R$ (we extend ψ_s by 0 outside \mathcal{H}_R). The function ψ_s is measurable and bounded (by $\|f\|_\infty \times \mathbf{E}_z[\mathfrak{M}_{t-s}^0(\mathbf{f}_R)] = \|f\|_\infty$). By Item **ii**, $z \mapsto \wp_s(\psi_s)(z) = \mathbf{E}_z[\mathfrak{M}_s^0(\mathbf{f}_R) \psi_s(X_s^0)]$ is continuous. In addition, from (4.6) and Doob's martingale inequality, one has for $z \in \mathcal{H}_R$ and $0 \leq s \leq t$:

$$\begin{aligned} |\mathbf{E}_z[f(X_t^0) \mathbf{1}_{t < \sigma_{\mathcal{H}_R}^0} \mathfrak{M}_t^0(\mathbf{f}_R)] - \wp_s(\psi_s)(z)| &= |\mathbf{E}_z[\mathbf{1}_{s > \sigma_{\mathcal{H}_R}^0} \mathfrak{M}_s^0(\mathbf{f}_R) \psi_s(X_s^0)]| \\ &\leq \|\psi_s\|_\infty \sqrt{\mathbf{E}_z[\sup_{s \in [0, t]} |\mathfrak{M}_s^0(\mathbf{f}_R)|^2]} \sqrt{\mathbf{P}_z[\sigma_{\mathcal{H}_R}^0 \leq s]} \\ &\leq \|\psi_s\|_\infty \sqrt{4\mathbf{E}_z[|\mathfrak{M}_t^0(\mathbf{f}_R)|^2]} \mathbf{P}_z[\sigma_{\mathcal{H}_R}^0 \leq s]. \end{aligned} \quad (4.7)$$

We claim that $\sup_z \mathbf{E}_z[|\mathfrak{M}_t^0(\mathbf{f}_R)|^2] < +\infty$. Let us prove this claim. We have

$$\begin{aligned} \mathbf{E}_z[|\mathfrak{M}_t^0(\mathbf{f}_R)|^2] &= \mathbf{E}_z[\exp(2\mathfrak{L}_t^0(\mathbf{f}_R))] \\ &= \mathbf{E}_z\left[\exp(\mathfrak{L}_t^0(2\mathbf{f}_R)) \exp\left(\int_0^t |\Sigma^{-1} \mathbf{f}_R(X_s^R)|^2 ds\right)\right] \\ &\leq \exp(\Sigma^{-2} t \|\mathbf{f}_R\|_\infty^2) \times \mathbf{E}_z[\exp(\mathfrak{L}_t^0(2\mathbf{f}_R))] = \exp(\Sigma^{-1} t \|\mathbf{f}_R\|_\infty), \end{aligned}$$

where we have used that $\mathbf{E}_z[\exp(\mathfrak{L}_t^0(2\mathbf{f}_R))] = 1$ (apply for instance [25, Theorem 1.1 in Section 7]). This proves that $\mathbf{E}_z[|\mathfrak{M}_t^0(\mathbf{f}_R)|^2] < +\infty$. Combining (4.7) and (4.5), we deduce that the continuous function $z \mapsto \wp_s(\psi_s)(z)$ converges uniformly as $s \rightarrow 0^+$ to the function $z \mapsto \mathbf{E}_z[f(X_t^0) \mathbf{1}_{t < \sigma_{\mathcal{H}_R}^0} \mathfrak{M}_t^0(\mathbf{f}_R)] = \mathbf{E}_z[f(X_t) \mathbf{1}_{t < \sigma_{\mathcal{H}_R}}]$ uniformly on the compact subsets K of \mathcal{H}_R . This ends the proof of (4.4).

Note that we actually proved that for any nonempty bounded open subset \mathcal{H} of \mathcal{E} ,

$$z \in \mathcal{H} \mapsto \mathbf{E}_z[f(X_t) \mathbf{1}_{t < \sigma_{\mathcal{H}}}] \text{ is continuous.} \quad (4.8)$$

Step 3. Let us end the proof of **(C1)**, i.e. let us prove (4.1). Fix $t > 0$ and a compact subset K of \mathcal{E} . Let $R_K > 0$ be such that $K \subset \mathcal{H}_{R_K}$ (thus $K \subset \mathcal{H}_R$ for all $R \geq R_K$). We have for all $R \geq R_K$ and $z \in K$:

$$|\mathbf{E}_z[f(X_t)] - \mathbf{E}_z[f(X_t) \mathbf{1}_{t < \sigma_{\mathcal{H}_R}}]| \leq \|f\|_\infty \sup_{z \in K} \mathbf{P}_z[\sigma_{\mathcal{H}_R} \leq t] \rightarrow 0 \text{ as } R \rightarrow +\infty,$$

since $\mathbf{P}_z[\sigma_{\mathcal{H}_R} \leq t] \leq \frac{e^{ct}}{R} \mathbf{H}_{\text{NH}}(z)$. Therefore, the continuous function $z \mapsto \mathbf{E}_z[f(X_t) \mathbf{1}_{t < \sigma_{\mathcal{H}_R}}]$ converges uniformly over K to $z \mapsto \mathbf{E}_z[f(X_t)]$ as $R \rightarrow +\infty$. This concludes the proof of Equation (4.1). \square

Proposition 4.2. *Assume that V satisfies **[Vcoercive]**. Then, the nonkilled semigroup $(P_t, t \geq 0)$ of the solution of (1.5) over $\mathcal{E} = \mathbf{O}_V \times \mathbf{R}^{dN} \times \mathbf{R}$ satisfies **(C2)**. Let $\mathcal{D} = \mathcal{O} \times \mathbf{R}^{dN} \times \mathbf{R}$ where \mathcal{O} is a subdomain of \mathbf{O}_V . Then, the killed semigroup $(P_t^\mathcal{D}, t \geq 0)$ of the process (1.5) on \mathcal{D} satisfies **(C4)**. If $\mathbf{O}_V \setminus \bar{\mathcal{O}}$ is nonempty, $(P_t^\mathcal{D}, t \geq 0)$ satisfies **(C5')** (see Section 4.3).*

Proof. Assumption **(C2)** is proved with the same arguments as those used to prove Proposition 2.2. Let us now prove **(C4)**. Let $t > 0$ and $f \in b\mathcal{B}(\mathcal{D})$. Consider $x \in \mathcal{D}$ and $r > 0$ such that $\mathbf{B}(x, r) \subset \mathcal{D}$. Set $\mathcal{D}_R = \mathcal{D} \cap \mathcal{H}_R$ which is a bounded open subset of \mathcal{E} and contains $\mathbf{B}(x, r)$ for all $R > 0$ large

enough. Since $\sigma_{\mathcal{D}_R} \leq \sigma_{\mathcal{D}}$, one has $\mathbf{1}_{t < \sigma_{\mathcal{D}}} \mathbf{1}_{t < \sigma_{\mathcal{D}_R}} = \mathbf{1}_{t < \sigma_{\mathcal{D}_R}}$. Consequently, one has for all $z \in \mathbf{B}(x, r)$,

$$\begin{aligned} |\mathbf{E}_z[f(X_t) \mathbf{1}_{t < \sigma_{\mathcal{D}}}] - \mathbf{E}_z[f(X_t) \mathbf{1}_{t < \sigma_{\mathcal{D}_R}}]| &= |\mathbf{E}_z[f(X_t) \mathbf{1}_{t < \sigma_{\mathcal{D}}} \mathbf{1}_{t \geq \sigma_{\mathcal{D}_R}}]| \\ &\leq \|f\|_{\infty} \sup_{z \in \mathbf{B}(x, r)} \mathbf{P}_z[t < \sigma_{\mathcal{D}}, t \geq \sigma_{\mathcal{D}_R}] \\ &\leq \|f\|_{\infty} \sup_{z \in \mathbf{B}(x, r)} \mathbf{P}_z[t \geq \sigma_{\mathcal{H}_R}] \rightarrow 0 \end{aligned}$$

as $R \rightarrow +\infty$. The proof of **(C4)** is complete using (4.8). Let us now check **(C5')**. Fix $t > 0$ and $\mathbf{x}_* = (x_*, v_*, y_*) \in \mathcal{D}$. With the analysis led in Section 2.2, it is not difficult to see that $\mathfrak{A}_{\mathbf{x}_*, t} := \{\mathbf{x} = (x, v, y) \in \mathcal{D}, y \geq y_* + t^{-1} \mathbf{d}_{\mathcal{O}}^2(x, x_*) - tdN\} \subset \text{supp } P_t^{\mathcal{D}}(\mathbf{x}_*, dy)$, where $\mathbf{d}_{\mathcal{O}}(x, x_*)$ is the geodesic distance between x and x_* in \mathcal{O} (actually $\mathfrak{A}_{\mathbf{x}_*, t} = \text{supp } P_t^{\mathcal{D}}(\mathbf{x}_*, dy)$ thanks to [32, Proposition 2.1 (ii)]). Then, for any open ball $\mathbf{B} = \mathbf{B}(y, r) \subset \mathcal{D}$, there exists $t(\mathbf{x}_*, \mathbf{B})$ such that for all $t \geq t(\mathbf{x}_*, \mathbf{B})$, $\mathbf{B}(y, r) \subset \mathfrak{A}_{\mathbf{x}_*, t}$. This ends the proof of **(C5')**. \square

4.2. On Assumption (C3) for the process (1.5). In this section, we consider a potential V satisfying **[Vsing2]**. Recall that the Hamiltonian of the process (1.5) is given by $\mathbf{H}_{\text{NH}}(x, v, y) = V(x) + \frac{1}{2}|v|^2 + \frac{1}{2}|y|^2$ ($(x, v, y) \in \mathcal{E}$) and its infinitesimal generator is $\mathcal{L}_{\text{NH}} = v \cdot \nabla_x - (y + \gamma)v \cdot \nabla_v - \nabla V \cdot \nabla_v + \gamma \Delta_v + (|v|^2 - dN)\partial_y$ (see (1.13) and (1.14)). Note that

$$\mathcal{L}_{\text{NH}}\mathbf{H}_{\text{NH}} = -yNd - \gamma|v|^2 + \gamma dN. \quad (4.9)$$

The purpose of [32] is to show the ergodicity of the (nonkilled) Nosé-Hoover process on \mathcal{E} . For that purpose, and based on an extension of Harris' ergodic theorem [30], the strategy consists in particular in constructing a Lyapunov function w such that at high energy \mathbf{H}_{NH} and on \mathcal{E} :

$$\mathcal{L}_{\text{NH}}w/w \leq -\alpha \text{ for some } \alpha > 0. \quad (4.10)$$

As observed there, the natural candidate $e^{\mathbf{H}_{\text{NH}}}$ does not satisfy such an estimate. In view of (4.9), though there exists $\alpha > 0$ such that on the region $\mathcal{R}_0 = \{(x, v, y), y \geq c_* \text{ or } |v|^2 \geq y_* \sqrt{|y|^2 + 1}\}$, $\mathcal{L}_{\text{NH}}\mathbf{H}_{\text{NH}} \leq -\alpha$ (choosing $c_*, y_* > 0$ large enough), one cannot obtain (4.10) in \mathcal{R}_0^c . Nevertheless, by constructing a suitable perturbation Ψ of \mathbf{H}_{NH} and by considering the Lyapunov function $w = e^{\mathbf{h}_* \mathbf{H}_{\text{NH}} + \Psi}$ ($\mathbf{h}_* > 0$), D.P. Herzog [32] managed to obtain $\mathcal{L}_{\text{NH}}w \leq -\alpha$ on the region \mathcal{R}_0^c . Nonetheless, in order to get **(C3)** (i.e. to have a Lyapunov function W such that $\mathcal{L}_{\text{NH}}W/W \rightarrow -\infty$ as $\mathbf{H}_{\text{NH}} \rightarrow +\infty$), we have to introduce another perturbation Φ of \mathbf{H}_{NH} , especially to get that $\mathcal{L}_{\text{NH}}W/W \rightarrow -\infty$ as $V(x) \rightarrow +\infty$.

Before building Φ , we start by recalling the construction of Ψ in [32]. To this end, introduce the Dawson's integral $D : \mathbf{R} \rightarrow \mathbf{R}$ defined by $D(z) = e^{-z^2} \int_0^z e^{u^2} du$ and set $D_m := \sup D$. Let us consider $k_* > 0$ and $y_* > 3\gamma + 1$. Consider the following cutoff functions in $\mathcal{C}^{\infty}(\mathbf{R}, [0, 1])$:

- $\mathbf{f}_0(z) = 1$ if $z \leq -1$, $\mathbf{f}_0(z) = 0$ if $z \geq 0$, $\mathbf{f}'_0 \leq 0$, and $|\mathbf{f}'_0| \leq 2$.
- $\mathbf{f}_1(z) = 1$ if $z \leq k_*$ and $\mathbf{f}_1(z) = 0$ if $z \geq k_* + 1$.
- $\mathbf{f}_2(z) = 1$ if $|z| \leq 1$ and $\mathbf{f}_2(z) = 0$ if $|z| \geq 2$.
- $\mathbf{f}_3(z) = 1$ if $|z| \geq 2$ and $\mathbf{f}_3(z) = 0$ if $|z| \leq 1$.
- $\mathbf{h}_1(z) = 1$ if $z \leq -y_* - 1$, $\mathbf{h}_1(z) = 0$ if $z \geq -y_*$, and $|\mathbf{h}'_1| \leq 2$.
- $\mathbf{h}_3(z) = 1$ if $|z| \leq 3$ and $\mathbf{h}_3(z) = 0$ if $|z| \geq 4$.

Pick now $p_*, u_* > 0$, and set for $\mathbf{x} = (x, v, y) \in \mathcal{E}$, $\Theta(v, y) = |v|^2 / (p_* \sqrt{|y|^2 + 1})$ and $\Upsilon(x, y) = |\nabla V(x)|^2 / [u_* (|y|^2 + 1)]$,

$$\mathbf{g}_1(\mathbf{x}) = \mathbf{f}_1(y) \mathbf{f}_2(\Theta(v, y)) \mathbf{f}_3(\Upsilon(x, y)) \text{ and } \mathbf{g}_2(\mathbf{x}) = \mathbf{h}_1(y) \mathbf{f}_2(\Theta(v, y)) \mathbf{h}_3(\Upsilon(x, y)).$$

Define for $z \in \mathbf{R}$ and $\mathbf{x} = (x, v, y) \in \mathcal{E}$:

$$\mathfrak{F}(z) = -\frac{1}{2D_{\max}^2} \int_0^z e^{-|y|^2} \int_0^y e^{u^2} du dy \text{ and } \Psi_0(\mathbf{x}) = \delta_* \mathbf{f}_0(y) \frac{|y|^2}{2},$$

where $\delta_* > 0$. For $k \in \{1, \dots, N\}$, we denote by $x^k = (x^{k,1}, \dots, x^{k,d})$ and by $v^k = (v^{k,1}, \dots, v^{k,d})$ the k^{th} -coordinate in \mathbf{R}^d of $x = (x^1, \dots, x^N) \in \mathbf{O}_V$ and of $v = (v^1, \dots, v^N) \in \mathbf{R}^{dN}$, respectively. For $\mathbf{x} = (x, v, y) \in \mathcal{E}$, one sets:

$$\Psi_1(\mathbf{x}) = \alpha_* \mathbf{1}_{\{|\nabla V(x)|^2 \geq u_*/2\}} \mathfrak{g}_1(\mathbf{x}) \sqrt{|y|^2 + 1} \frac{v \cdot \nabla V(x)}{|\nabla V(x)|^2} \text{ where } \alpha_* > 0.$$

For $k \in \{1, \dots, N\}$ and $l \in \{1, \dots, d\}$, one defines

$$\Psi_2^{k,l}(\mathbf{x}) = \mathbf{1}_{\{y \leq -3\gamma\}} \mathfrak{g}_2(\mathbf{x}) \mathfrak{F} \left(\frac{|y + \gamma|^{\frac{1}{2}}}{(2\gamma)^{\frac{1}{2}}} (v^{k,l} - \frac{\partial_{x^{k,l}} V(x)}{|y + \gamma|}) \right), \text{ and } \Psi_2(\mathbf{x}) = \sum_{k,l} \Psi_2^{k,l}(\mathbf{x}).$$

Finally, set $\Psi = \Psi_0 + \Psi_1 + \Psi_2$. We now briefly recall the result of [32] we will need. Let $\mathfrak{h}_* > 0$ be such that:

$$\mathfrak{h}_* < \frac{1}{8D_m^2}. \quad (4.11)$$

Define on the following function on \mathcal{E} : $\mathbf{L}_{\text{NH}} = \mathfrak{h}_* \mathbf{H}_{\text{NH}} + \Psi$. Then, from [32, item (i) in Theorem 4.1, Eq. (4.4), and Eq. (4.8)] (see also the last equation in the proof of [32, Lemma 4.2]), for some $\delta_0 > 0$ and any $\delta_* \in (0, \delta_0)$, there exists $\varepsilon_0 > 0$ such that for all $\varepsilon_* \in (0, \varepsilon_0)$, there exists $c_0 > 0$, for all $\alpha_* > c_0$ and $k_* > c_0$, choosing $p_*, u_*, y_* > 0$ large enough, it holds over \mathcal{E} :

$$|\Psi| \leq \varepsilon_* \mathbf{H}_{\text{NH}} \text{ and } |\nabla_v \mathbf{L}_{\text{NH}}| \leq \mathfrak{h}_* |v| + \frac{\mathfrak{g}_2 N d |y + \gamma|^{\frac{1}{2}}}{2D_m (2\gamma)^{\frac{1}{2}}} + (Nd + 1)\varepsilon_*, \quad (4.12)$$

and (see the equation after [32, Eq. (4.32)])

$$\begin{aligned} \mathcal{L}_{\text{NH}} \mathbf{L}_{\text{NH}} + \gamma |\nabla_v \mathbf{L}_{\text{NH}}|^2 &\leq -\frac{\gamma \mathfrak{h}_*}{2} (1 - \mathfrak{h}_*) |v|^2 - \mathfrak{h}_* d N (1 - \mathfrak{f}_0) |y| - \frac{\mathfrak{f}_0}{2} \delta_* |y| |v|^2 \\ &\quad - \left[\mathfrak{g}_1 \frac{\alpha_*}{2} + \mathfrak{g}_2 \frac{dN}{8D_m^2} - \mathfrak{f}_0 (\mathfrak{h}_* + \delta_* + \varepsilon_*) dN \right] |y| + \mathfrak{c}, \end{aligned} \quad (4.13)$$

where $\mathfrak{c} > 0$ is independent of $\mathbf{x} \in \mathcal{E}$, which, in the following, can change from one occurrence to another.

Let us now construct Φ . Let $R_1 > 1$ such that $|\nabla V(x)| \geq 1$ if $V(x) \geq R_1 - 1$. Consider the following two cutoff functions in $\mathcal{C}^\infty(\mathbf{R}, [0, 1])$:

- $\mathfrak{h}(z) = 1$ if $z \geq R_1$, $\mathfrak{h}(z) = 0$ if $z \leq R_1 - 1$, and $|\mathfrak{h}'| \leq 2$.
- $\mathfrak{h}_0(z) = 1$ if $z \geq 2$ and $\mathfrak{h}_0(z) = 0$ if $z \leq 1$, $\mathfrak{h}'_0 \geq 0$, $|\mathfrak{h}'_0| \leq 2$.

Let $\zeta \in (1, 2)$ be as in [Vsing2]. Define for $\mathbf{x} \in \mathcal{E}$,

$$\Phi(\mathbf{x}) = \mathfrak{h}(V(x)) \frac{v \cdot \nabla V(x)}{|\nabla V(x)|^\zeta} - \mathfrak{h}_0(y) |y|^2.$$

Remark 4.3. *The sign of the second term $-\mathfrak{h}_0(y) |y|^2$ in the definition of Φ might look strange. However we will rather consider instead of Φ , $\varepsilon_\Phi \Phi$ (with $\varepsilon_\Phi > 0$ small enough) as a perturbation of \mathbf{L}_{NH} (see indeed the definition of \mathbf{F}_{NH} below). Hence, $\mathbf{H}_{\text{NH}} + \Psi + \varepsilon_\Phi \Phi$ will stay lower bounded over \mathcal{E} (see the proof of (4.16) below).*

Let us now provide some estimates on Φ , $\nabla_v \Phi$, and $\mathcal{L}_{\text{NH}} \Phi$ which will be used later on.

On the one hand, since $\zeta \in (1, 2)$, it holds over \mathcal{E} :

$$|\Phi| \leq \mathfrak{h} |v| |\nabla V|^{1-\zeta} + |y|^2 \leq |v| + |y|^2 \leq 2\mathbf{H}_{\text{NH}} \text{ and } |\nabla_v \Phi| = \mathfrak{h} |\nabla V|^{1-\zeta} \leq 1. \quad (4.14)$$

On the other hand, using [Vsing2], there exists $M > 0$ such that

$$\mathfrak{h}(V(x)) |\text{Hess } V(x)| / |\nabla V(x)|^\zeta \leq M.$$

Set

$$\mathfrak{c}_V = 3M + 2 \sup_{\{x, V(x) \in [R_1 - 1, R_1]\}} |\nabla V|^{2-\zeta}.$$

Note that because $|\nabla V| \geq 1$ on the support of $\mathfrak{h} \circ V$ and since $\zeta - 1 > 0$, we have that $1/|\nabla V|^{\zeta-1} \leq 1$. Hence, it holds:

$$\begin{aligned}
 \mathcal{L}_{\text{NH}}\Phi &= v \cdot \left[\mathfrak{h}' \circ V \nabla V \frac{v \cdot \nabla V}{|\nabla V|^\zeta} + \mathfrak{h} \circ V \frac{\text{Hess } V v}{|\nabla V|^\zeta} - \zeta \mathfrak{h} \circ V \frac{v \cdot \nabla V \text{ Hess } V \nabla V}{|\nabla V|^{2+\zeta}} \right] \\
 &\quad - (yv + \gamma v + \nabla V) \cdot \mathfrak{h} \circ V \frac{\nabla V(x)}{|\nabla V(x)|^\zeta} - (|v|^2 - dN)(\mathfrak{h}'_0|y|^2 + 2\mathfrak{h}_0y) \\
 &\leq |v|^2 \left[|\mathfrak{h}' \circ V| |\nabla V|^{2-\zeta} + \mathfrak{h} \circ V \frac{|\text{Hess } V|}{|\nabla V|^\zeta} + 2\mathfrak{h} \circ V \frac{|\text{Hess } V|}{|\nabla V|^\zeta} \right] \\
 &\quad + (|y||v| + \gamma|v|) \frac{\mathfrak{h} \circ V}{|\nabla V|^{\zeta-1}} - \mathfrak{h} \circ V |\nabla V|^{2-\zeta} - \mathfrak{h}'_0|y|^2|v|^2 - 2\mathfrak{h}_0y|v|^2 \\
 &\quad + dN(\mathfrak{h}'_0|y|^2 + 2\mathfrak{h}_0y) \\
 &\leq \mathfrak{c}_V|v|^2 - \mathfrak{h} \circ V |\nabla V|^{2-\zeta} + (|y||v| + \gamma|v|)\mathfrak{h} \circ V - 2\mathfrak{h}_0y|v|^2 + 2\mathfrak{h}_0dNy + \mathfrak{c}.
 \end{aligned}$$

Hence, one has:

$$\mathcal{L}_{\text{NH}}\Phi \leq \mathfrak{c}_V|v|^2 - 2\mathfrak{h}_0y|v|^2 + \gamma|v| - \mathfrak{h} \circ V |\nabla V|^{2-\zeta} + |y||v|\mathfrak{h} \circ V + 2dN\mathfrak{h}_0y + \mathfrak{c}. \quad (4.15)$$

For all $\mathbf{x} \in \mathcal{E}$, $\epsilon_\Phi > 0$, set $F_0(x, v, y) = \mathcal{L}_{\text{NH}} + \epsilon_\Phi\Phi$. The parameter $\epsilon_\Phi > 0$ will be chosen such that

$$\inf_{\mathcal{E}} F_0 \in \mathbf{R}. \quad (4.16)$$

Then, we define on \mathcal{E} : $F_{\text{NH}} = F_0 - \inf_{\mathcal{E}} F_0 + 1$ and

$$W_\delta = \exp \left[F_{\text{NH}}^\delta \right], \text{ where } \delta \in (1/2, 1] \text{ is the parameter appearing in } [\mathbf{V}_{\text{sing}2}]. \quad (4.17)$$

Before going through the computations of $\mathcal{L}_{\text{NH}}W_\delta$, let us deal with (4.16). We have for all $\mathbf{x} \in \mathcal{E}$, $F_0(\mathbf{x}) \geq (\mathfrak{h}_* - \epsilon_*)\mathbf{H}_{\text{NH}}(\mathbf{x}) - \epsilon_\Phi|v| - \epsilon_\Phi|y|^2$ which is lower bounded if $\epsilon_\Phi \in (0, (\mathfrak{h}_* - \epsilon_*)/2)$. From now on $\epsilon_\Phi \in (0, (\mathfrak{h}_* - \epsilon_*)/2)$. Note that there exists $c > 0$ such that for all $\delta \in (1/2, 1]$:

$$W_\delta \leq e^{c^\delta \mathbf{H}_{\text{NH}}^\delta} \text{ on } \mathcal{E}. \quad (4.18)$$

Proposition 4.4. *Assume that V satisfies $[\mathbf{V}_{\text{sing}2}]$. Then, there are parameters such that **(C3)** is satisfied with the Lyapunov function W_δ defined in (4.17).*

Proof. We now simply write L , H , and F for \mathcal{L}_{NH} , \mathbf{H}_{NH} , and F_{NH} respectively. From the first inequalities in (4.12) and (4.14),

$$|F| \leq (\mathfrak{h}_* + \epsilon_0 + 2\epsilon_\Phi)H + |\inf_{\mathcal{E}} F_0| + 1 \leq cH, \quad (4.19)$$

for some $c > 0$. We will reduce ϵ_* , α_* , δ_* , $\epsilon_\Phi > 0$ and finally increase $p_* > 0$ such that the Lyapunov function W_δ defined in (4.17) satisfies **(C3)** on \mathcal{E} . We have over \mathcal{E} :

$$\frac{\mathcal{L}_{\text{NH}}W_\delta}{W_\delta} \leq \frac{\delta}{F^{1-\delta}} \left[\mathcal{L}_{\text{NH}}F + \gamma|\nabla_v F|^2 \right], \quad (4.20)$$

Using (4.12) and (4.14), it holds for some $\mathfrak{K} > 0$:

$$2\gamma\epsilon_\Phi|\nabla_v L||\nabla_v \Phi| \leq \epsilon_\Phi\mathfrak{K}(|v| + \mathfrak{g}_2|y| + \gamma|v|^{\frac{1}{2}} + 1).$$

Using in addition (4.13), (4.14), and (4.15), one has over \mathcal{E} :

$$\begin{aligned}
\mathcal{L}_{\text{NH}}\mathbf{F} + \gamma|\nabla_v\mathbf{F}|^2 &= \mathcal{L}_{\text{NH}}(\mathbf{L} + \epsilon_\Phi\Phi) + \gamma|\nabla_v\mathbf{L} + \epsilon_\Phi\nabla_v\Phi|^2 \\
&\leq \mathcal{L}_{\text{NH}}\mathbf{L} + \gamma|\nabla_v\mathbf{L}|^2 + \epsilon_\Phi\mathcal{L}_{\text{NH}}\Phi + \gamma\epsilon_\Phi^2|\nabla_v\Phi|^2 + 2\gamma\epsilon_\Phi|\nabla_v\mathbf{L}||\nabla_v\Phi| \\
&\leq -\frac{\gamma\mathfrak{h}_*}{2}(1 - \mathfrak{h}_*)|v|^2 - \mathfrak{h}_*dN(1 - \mathfrak{f}_0)|y| - \frac{\mathfrak{f}_0}{2}\delta_*|y||v|^2 \\
&\quad - \left[\mathfrak{g}_1\frac{\alpha_*}{2} + \mathfrak{g}_2\frac{dN}{8D_m^2} - \mathfrak{f}_0(\mathfrak{h}_* + \delta_* + \varepsilon_*)dN\right]|y| + \epsilon_\Phi\mathbf{c}_V|v|^2 \\
&\quad - 2\epsilon_\Phi\mathfrak{h}_0y|v|^2 + \epsilon_\Phi(\gamma + \mathfrak{K})|v| - \epsilon_\Phi\mathfrak{h} \circ V|\nabla V|^{2-\zeta} \\
&\quad + \epsilon_\Phi|y|(|v|^2 + 1) + 2\epsilon_\Phi dN\mathfrak{h}_0y + \epsilon_\Phi\mathfrak{K}\mathfrak{g}_2|y| + \gamma^{\frac{1}{2}} + \mathbf{c}.
\end{aligned}$$

Choose $\alpha_* > dN/(4D_m^2)$ so that $\min(\alpha_*/2, dN/(8D_m^2)) = dN/(8D_m^2)$. Note that $\epsilon_\Phi(\gamma + \mathfrak{K})|v| \leq \epsilon_\Phi|v|^2 + \mathbf{c}$. Therefore, using also that $\epsilon_\Phi|y||v|^2 \leq \epsilon_\Phi\mathbf{1}_{y \notin [-1,2]}|y||v|^2 + 2\epsilon_\Phi|v|^2$, it holds

$$\begin{aligned}
\mathcal{L}_{\text{NH}}\mathbf{F} + \gamma|\nabla_v\mathbf{F}|^2 &\leq -\frac{\gamma\mathfrak{h}_*}{2}(1 - \mathfrak{h}_*)|v|^2 + \mathbf{c}_V\epsilon_\Phi|v|^2 + 3\epsilon_\Phi|v|^2 \\
&\quad - \frac{\delta_*}{2}\mathfrak{f}_0|y||v|^2 + \epsilon_\Phi\mathbf{1}_{y \notin [-1,2]}|y||v|^2 - 2\epsilon_\Phi\mathfrak{h}_0y|v|^2 \\
&\quad - \mathfrak{h}_*dN(1 - \mathfrak{f}_0)|y| - \frac{dN}{8D_m^2}(\mathfrak{g}_1 + \mathfrak{g}_2)|y| + (\mathfrak{h}_* + \delta_* + \varepsilon_*)dN\mathfrak{f}_0|y| \\
&\quad + \epsilon_\Phi|y| + 2\epsilon_\Phi dN\mathfrak{h}_0y - \epsilon_\Phi\mathfrak{h} \circ V|\nabla V|^{2-\zeta} + \epsilon_\Phi\mathfrak{K}\mathfrak{g}_2|y| + \gamma^{\frac{1}{2}} + \mathbf{c}.
\end{aligned}$$

Note that $1 - \mathfrak{f}_0 \geq \mathbf{1}_{[1,+\infty)}$, $\mathfrak{f}_0 \geq \mathbf{1}_{(-\infty,-1]}$, $\mathfrak{f}_0 \leq \mathbf{1}_{\mathbf{R}_-}$, and $\mathfrak{h}_0 \geq \mathbf{1}_{[2,+\infty)}$. Choose $\epsilon_\Phi > 0$ small enough such that $\mathbf{m} := \frac{\gamma\mathfrak{h}_*}{2}(1 - \mathfrak{h}_*) - \epsilon_\Phi(\mathbf{c}_V + 3) > 0$. Then, one has for all $\mathbf{x} = (x, v, y) \in \mathcal{E}$:

$$\mathcal{L}_{\text{NH}}\mathbf{F}(\mathbf{x}) + \gamma|\nabla_v\mathbf{F}|^2(\mathbf{x}) \leq \mathfrak{B}(\mathbf{x}) := -\mathbf{m}|v|^2 + \mathfrak{N}(\mathbf{x}) - \epsilon_\Phi\mathfrak{h} \circ V|\nabla V|^{2-\zeta} + \mathbf{c}, \quad (4.21)$$

where

$$\begin{aligned}
\mathfrak{N}(\mathbf{x}) &= -\frac{\delta_*}{2}\mathbf{1}_{y \leq -1}|y||v|^2 + \epsilon_\Phi\mathbf{1}_{y \notin [-1,2]}|y||v|^2 - 2\epsilon_\Phi\mathbf{1}_{y \geq 2}y|v|^2 \\
&\quad - \mathfrak{h}_*dN\mathbf{1}_{y \geq 1}|y| - \frac{dN}{8D_m^2}(\mathfrak{g}_1 + \mathfrak{g}_2)|y| + (\mathfrak{h}_* + \delta_* + \varepsilon_*)dN\mathbf{1}_{y \leq 0}|y| \\
&\quad + \epsilon_\Phi\mathbf{1}_{y \leq 0}|y| + \epsilon_\Phi\mathbf{1}_{y \geq 0}|y| + 2\epsilon_\Phi dN\mathbf{1}_{y \geq 0}y + \epsilon_\Phi\mathfrak{K}\mathbf{1}_{y \leq 0}|y|.
\end{aligned}$$

We now study the function \mathfrak{N} over \mathcal{E} . There are two cases:

A. The case when $y \geq 0$. In this case, one has

$$\mathfrak{N}(\mathbf{x}) \leq \epsilon_\Phi\mathbf{1}_{y \geq 2}|y||v|^2 - 2\epsilon_\Phi\mathbf{1}_{y \geq 2}y|v|^2 - \mathfrak{h}_*dN\mathbf{1}_{y \geq 1}|y| + \epsilon_\Phi(2dN + 1)\mathbf{1}_{y \geq 0}|y|.$$

Reduce $\epsilon_\Phi > 0$ such that $\mathfrak{b} := \mathfrak{h}_*dN - \epsilon_\Phi(2dN + 1) > 0$. Then, in this case, one has:

$$\mathfrak{N}(\mathbf{x}) \leq -\epsilon_\Phi\mathbf{1}_{y \geq 2}|y||v|^2 - \mathfrak{b}\mathbf{1}_{y \geq 0}|y| + \mathbf{c}.$$

B. The case when $y \leq 0$. Then,

$$\begin{aligned}
\mathfrak{N}(\mathbf{x}) &\leq -\frac{\delta_*}{2}\mathbf{1}_{y \leq -1}|y||v|^2 + \epsilon_\Phi\mathbf{1}_{y \leq -1}|y||v|^2 - \frac{dN}{8D_m^2}(\mathfrak{g}_1 + \mathfrak{g}_2)|y| \\
&\quad + (\mathfrak{h}_* + \delta_* + \varepsilon_*)dN\mathbf{1}_{y \leq -1}|y| + \epsilon_\Phi(1 + \mathfrak{K})\mathbf{1}_{y \leq 0}|y|.
\end{aligned} \quad (4.22)$$

We then distinguish between two subcases:

- The case when $|v|^2/(p_*\sqrt{|y|^2+1}) \leq 1$. In this case one has $(\mathfrak{g}_1 + \mathfrak{g}_2) \geq \mathbf{1}_{y \leq -y_*-1}$. Then, it holds:

$$\begin{aligned} \mathfrak{N}(\mathbf{x}) &\leq -\frac{\delta_*}{2} \mathbf{1}_{y \leq -1} |y||v|^2 + \epsilon_\Phi \mathbf{1}_{y \leq -1} |y||v|^2 \\ &\quad - \left[\frac{dN}{8D_m^2} - (\mathfrak{h}_* + \delta_* + \varepsilon_*)dN - \epsilon_\Phi(1 + \mathfrak{K}) \right] \mathbf{1}_{y \leq -y_*-1} |y| + \mathfrak{c}. \end{aligned}$$

In view of (4.11), we can reduce $\delta_* > 0$ and then $\varepsilon_* > 0$ such that $\frac{dN}{8D_m^2} - (\mathfrak{h}_* + \delta_* + \varepsilon_*)dN > 0$. Then, anew, reduce $\epsilon_\Phi > 0$ such that $\epsilon_\Phi < \delta_*/4$ and such that

$$\mathfrak{n} := \frac{dN}{8D_m^2} - (\mathfrak{h}_* + \delta_* + \varepsilon_*)dN - \epsilon_\Phi(1 + \mathfrak{K}) > 0.$$

Hence, in this case, it holds: $\mathfrak{N}(\mathbf{x}) \leq -\frac{\delta_*}{4} \mathbf{1}_{y \leq -1} |y||v|^2 - \mathfrak{n} \mathbf{1}_{y \leq 0} |y| + \mathfrak{c}$.

- The case when $|v|^2/(p_*\sqrt{|y|^2+1}) \geq 1$. In this case $|v|^2 \geq p_*$ and thus, using (4.22), it holds (since $\epsilon_\Phi < \delta_*/4$):

$$\mathfrak{N}(\mathbf{x}) \leq -\frac{\delta_* p_*}{4} \mathbf{1}_{y \leq -1} |y| + \left[(\mathfrak{h}_* + \delta_* + \varepsilon_*)dN + \epsilon_\Phi(1 + \mathfrak{K}) \right] \mathbf{1}_{y \leq -1} |y| + \mathfrak{c}.$$

Choose $p_* > 0$ larger such that $\frac{\delta_* p_*}{4} > \frac{dN}{8D_m^2}$. In this case, $\frac{\delta_* p_*}{4} > (\mathfrak{h}_* + \delta_* + \varepsilon_*)dN$. Then, choose $\epsilon_\Phi > 0$ smaller such that

$$\mathfrak{j} := \frac{\delta_* p_*}{4} - (\mathfrak{h}_* + \delta_* + \varepsilon_*)dN - \epsilon_\Phi(1 + \mathfrak{K}) > 0.$$

Consequently, in this case, it holds: $\mathfrak{N}(\mathbf{x}) \leq -\mathfrak{j} \mathbf{1}_{y \leq 0} |y| + \mathfrak{c}$.

Recall $\delta \in (1/2, 1]$. Gathering the estimates obtained in Items A and B above, and using (4.21), (4.19), and (4.20), we deduce that $\mathcal{L}_{\text{NH}} \mathbf{W}_\delta / \mathbf{W}_\delta \rightarrow -\infty$ as $\mathbf{H}(\mathbf{x}) \rightarrow +\infty$ (i.e. when $V(x) + |v| + |y| \rightarrow +\infty$). This concludes the proof of the proposition. \square

4.3. Extension of [28, Theorem 2.2]. In this section, we extend [28, Theorem 2.2] when **(C5)** is replaced by the less stringent following assumption:

- (C5')** For all $\mathbf{x} \in \mathcal{D}$ and nonempty open subset \mathbf{O} of \mathcal{D} , there exists $t(\mathbf{x}, \mathbf{O}) \geq 0$, for all $t \geq t(\mathbf{x}, \mathbf{O})$, $P_t^\mathcal{D}(\mathbf{x}, \mathbf{O}) > 0$. In addition, there exists $\mathbf{x}_0 \in \mathcal{D}$ such that $\mathbf{P}_{\mathbf{x}_0}(\sigma_\mathcal{D} < +\infty) > 0$.

To this end, we first extend [28, Theorem 4.1] as follows.

Theorem 4.5. *Let \mathcal{S} be a nonempty open subset of \mathbf{R}^d , $Q = Q(\mathbf{x}, d\mathbf{y})$ be a positive bounded kernel on \mathcal{S} , and $\mathbf{W} : \mathcal{S} \rightarrow [1, +\infty)$ a continuous function. Assume that:*

- (1) *There exists $N_1 \geq 1$ such that Q^k is strong Feller for all $k \geq N_1$, i.e. $Q^k f \in \mathcal{C}^b(\mathcal{S})$ if $f \in b\mathcal{B}(\mathcal{S})$.*
- (2) *For any $\mathbf{x} \in \mathcal{S}$ and nonempty open subset \mathbf{O} of \mathcal{S} , there exists $q(\mathbf{x}, \mathbf{O}) \in \mathbf{N}$ such that for all $k \geq q(\mathbf{x}, \mathbf{O})$,*

$$Q^k(\mathbf{x}, \mathbf{O}) > 0.$$

- (3) *For some $p > 1$ and constant $C > 0$, it holds:*

$$Q\mathbf{W}^p \leq C\mathbf{W}^p.$$

Notice that this implies that Q is well defined and bounded on $b_{\mathbf{W}}\mathcal{B}(\mathcal{S})$.

- (4) *Q has a spectral gap in $b_{\mathbf{W}}\mathcal{B}(\mathcal{S})$,*

$$r_{\text{ess}}(Q|_{b_{\mathbf{W}}\mathcal{B}(\mathcal{S})}) < r_{\text{sp}}(Q|_{b_{\mathbf{W}}\mathcal{B}(\mathcal{S})}). \quad (4.23)$$

Then, all the conclusions of [28, Theorem 4.1] hold true.

Proof. We adopt the same notations as those used to prove [28, Theorem 4.1]. The proof of Theorem 4.5 is the same as the one made to prove [28, Theorem 4.1] except the end of the second step there. More precisely, we only have to prove that under our new Assumptions (1) and (2), it still holds:

- (a) $\mu(\mathbf{O}) > 0$ for all nonempty open subset \mathbf{O} of \mathcal{S} ,
- (b) $\varphi(\mathbf{x}) > 0$ for all $\mathbf{x} \in \mathcal{S}$,

where we recall that μ (resp. φ) is nonzero and nonnegative measure which is a left eigenvector (resp. a nonzero and nonnegative function which is a right eigenvector) of Q^m (where $m \in \mathbf{N}^*$ is the integer chosen at the beginning of the second step of the proof of [28, Theorem 4.1]).

Let us first prove Item (a) above. We have $\mu Q^m = \mu$ and thus $\mu Q^{mn} = \mu$ for all $n \in \mathbf{N}$. Let $n \in \mathbf{N}^*$ such that $n \geq N_1/m + 1$, so that, by Assumption (1), Q^{mn} is strong Feller. In addition, since μ is a nonzero and nonnegative measure over \mathcal{S} , its (topological) support is nonempty. Let \mathbf{z} belong to the support of μ . By definition, $\mu(\mathbf{B}(\mathbf{z}, \delta)) > 0$ for all $\delta > 0$ small enough such that $\mathbf{B}(\mathbf{z}, \delta) \subset \mathcal{S}$, where $\mathbf{B}(\mathbf{z}, \delta)$ is the open ball in \mathbf{R}^d of radius δ centered at \mathbf{z} . Assume also that $n \in \mathbf{N}^*$ is large enough such that $mn \geq q(\mathbf{z}, \mathbf{O})$ (see Assumption (2)).

It holds for any nonempty open subset \mathbf{O} of \mathcal{S} :

$$\mu(\mathbf{O}) = \int_{\mathcal{S}} Q^{mn}(\mathbf{x}, \mathbf{O}) \mu(d\mathbf{x}) \geq 0.$$

Assume that $\mu(\mathbf{O}) = 0$. Then, $Q^{mn}(\cdot, \mathbf{O}) = 0$ μ -almost surely. Consequently, there exists $\mathbf{z}_n^\delta \in \mathbf{B}(\mathbf{z}, \delta)$ such that $Q^{mn}(\mathbf{z}_n^\delta, \mathbf{O}) = 0$. Note that $\mathbf{z}_n^\delta \rightarrow \mathbf{z}$ as $\delta \rightarrow 0$, and since Q^{mn} is strong Feller, it holds $Q^{mn}(\mathbf{z}, \mathbf{O}) = 0$. This leads to a contradiction in view of Assumption (2) and because $mn \geq q(\mathbf{z}, \mathbf{O})$. The proof of Item (a) above is complete.

Let us now prove Item (b) above. We know that there exists $\mathbf{x}_0 \in \mathcal{S}$ such that $\varphi(\mathbf{x}_0) > 0$. Thus, by continuity of φ , there exists $\delta_0 > 0$ and $c_0 > 0$ such that $\mathbf{B}(\mathbf{x}_0, \delta_0) \subset \mathcal{S}$ and $\varphi \geq c_0$ on $\mathbf{B}(\mathbf{x}_0, \delta_0)$. Let $\mathbf{x} \in \mathcal{S}$. Pick $n \in \mathbf{N}^*$ such that $mn \geq q(\mathbf{x}, \mathbf{B}(\mathbf{x}_0, \delta_0))$. Since $Q^{mn}\varphi = \varphi$, one has, by Assumption (2),

$$\varphi(\mathbf{x}) = \int_{\mathcal{S}} \varphi(\mathbf{y}) Q^{mn}(\mathbf{x}, d\mathbf{y}) \geq c_0 Q^{mn}(\mathbf{x}, \mathbf{B}(\mathbf{x}_0, \delta_0)) > 0.$$

This concludes the proof of Item (b) above. □

Following exactly the same arguments as in the proof of [28, Theorem 2.2], we deduce the following extension of [28, Theorem 2.2].

Theorem 4.6. *All the conclusions of [28, Theorem 2.2] are still valid when (C5) is replaced by (C5') there.*

5. EXTENSIONS OF EXISTING RESULTS

In this section, we extend the existing results on the existence and uniqueness of the quasi-stationary distributions for the kinetic Langevin process as well as for elliptic processes.

5.1. Quasi-stationary distribution for the kinetic Langevin process. Consider the solution $((x_t, v_t), t \geq 0)$ in $\mathbf{R}^d \times \mathbf{R}^d$ to the kinetic Langevin equation

$$dx_t = v_t dt, \quad dv_t = \mathbf{b}(x_t) dt - \gamma v_t dt + \sqrt{2} dW_t. \tag{5.1}$$

Introduce the following assumption:

Assumption [V_{bounded+lip}]. *The set \mathcal{O} is a bounded subdomain of \mathbf{R}^d and $\mathbf{b} : \overline{\mathcal{O}} \rightarrow \mathbf{R}^d$ is a Lipschitz vector field.*

In [48], existence and uniqueness of the quasi-stationary distribution of the process (5.1) as well as the exponential convergence were obtained under assumption [V_{bounded+lip}] and with the two extra assumptions that $\mathbf{b} \in \mathcal{C}^\infty(\overline{\mathcal{O}})$ and $\partial\mathcal{O}$ is \mathcal{C}^2 . With the techniques used in this work, we are able to extend this result to the very weak regularity setting where only [V_{bounded+lip}] is assumed. Indeed, we have the following result.

Theorem 5.1. *Assume $[\mathbf{V}_{\text{bounded+lip}}]$ and let $\mathcal{D} = \mathcal{O} \times \mathbf{R}^d$. Assume also that $\gamma \in \mathbf{R}$. Then, there exists a unique quasi-stationary distribution $\theta_{\mathcal{D}}$ for the process (5.1) on \mathcal{D} in the whole space of probability measures $\mathcal{P}(\mathcal{D})$ over \mathcal{D} . Furthermore:*

- (1) *There exists $\kappa_{\mathcal{D}} > 0$ s.t. for all $t \geq 0$, the spectral radius of $P_t^{\mathcal{D}}$ on $b\mathcal{B}(\mathcal{D})$ is $e^{-\kappa_{\mathcal{D}}t}$, where $(P_t^{\mathcal{D}}, t \geq 0)$ is the killed semigroup of the process solution to (5.1) (see (1.7)). In addition, for all $t \geq 0$, $\theta_{\mathcal{D}}P_t^{\mathcal{D}} = e^{-\kappa_{\mathcal{D}}t}\theta_{\mathcal{D}}$ and $\theta_{\mathcal{D}}(\mathbf{O}) > 0$ for all nonempty open subsets \mathbf{O} of \mathcal{D} . There is also a unique continuous function ψ in $b\mathcal{B}(\mathcal{D})$ such that $\theta_{\mathcal{D}}(\psi) = 1$, $\psi > 0$ on \mathcal{D} , and $P_t^{\mathcal{D}}\psi = e^{-\kappa_{\mathcal{D}}t}\psi$ on \mathcal{D} , $\forall t \geq 0$.*
- (2) *There exist $L > 0$ and $c \geq 1$ such that for all $\nu \in \mathcal{P}(\mathcal{D})$,*

$$|\mathbf{P}_{\nu}[X_t \in \mathcal{A} | t < \sigma_{\mathcal{D}}] - \theta_{\mathcal{D}}(\mathcal{A})| \leq \frac{ce^{-Lt}}{\nu(\psi)}, \quad \forall \mathcal{A} \in \mathcal{B}(\mathcal{D}), t > 0.$$

- (3) *For some $t_0 > 0$, $P_t^{\mathcal{D}} : b\mathcal{B}(\mathcal{D}) \rightarrow b\mathcal{B}(\mathcal{D})$ is compact, for all $t \geq t_0$.*

Finally, $\mathbf{P}_{\mathbf{x}}(\sigma_{\mathcal{D}} < +\infty) = 1$ for all $\mathbf{x} \in \mathcal{D}$.

Proof. We extend \mathbf{b} outside $\overline{\mathcal{O}}$ as a globally Lipschitz and bounded \mathbf{R}^d -vector field over \mathbf{R}^d . Assumption **(C2)** is a consequence of the fact that for all $t \geq 0$, a.s. $X_s(\mathbf{x}_n) \rightarrow X_s(\mathbf{x})$ uniformly on $[0, t]$ when $\mathbf{x}_n \rightarrow \mathbf{x} \in \mathbf{R}^{2d}$. Assumption **(C1)** is proved using this result, together with the Gaussian upper bound (5.6) below and Proposition 1.2. On the other hand, since \mathbf{b} is globally Lipschitz, using similar arguments as those used in the proof of Lemma 2.4, one deduces that for all compact subset K of \mathbf{R}^{2d} and $\delta > 0$, it holds:

$$\lim_{s \rightarrow 0^+} \sup_{\mathbf{x}=(x,v) \in K} \mathbf{P}_{\mathbf{x}}[\sigma_{\mathcal{B}(x,\delta)} \leq s] = 0,$$

where for $\mathbf{x} = (x, v) \in \mathbf{R}^d$, $\sigma_{\mathcal{B}(x,\delta)}(\mathbf{x}) := \inf\{s \geq 0, x_s(\mathbf{x}) \notin \mathcal{B}(x, \delta)\}$ and where we recall that $\mathcal{B}(x, \delta)$ is the open ball of \mathbf{R}^d of radius $\delta > 0$ centered at $x \in \mathbf{R}^d$. Assumption **(C4)** is thus proved with the same arguments as those used to prove Proposition 2.7. Assumption **(C5)** follows from the same arguments as those used in Section 2.2.

The proof of the results stated up to Item (2) (included) in Theorem 5.1 will then be a consequence of [28, Theorem 4.1], if we prove that for some $t > 0$, the essential spectral radius of $P_t^{\mathcal{D}}$ on $b\mathcal{B}(\mathcal{D})$ is zero (see indeed the proof of [28, Theorem 2.2] made in [28, Section 5]), i.e.

$$r_{\text{ess}}(P_t^{\mathcal{D}}|_{b\mathcal{B}(\mathcal{D})}) = 0. \quad (5.2)$$

Let us recall the definition of the measure of non- w -compactness $\beta_w(Q)$ of a bounded nonnegative kernel $Q = Q(\mathbf{x}, d\mathbf{y})$ on a polish space \mathcal{S} introduced in [78]:

$$\beta_w(Q) := \inf_{K \subset \mathcal{S}} \sup_{\mathbf{x} \in \mathcal{S}} Q(\mathbf{x}, \mathcal{S} \setminus K), \quad (5.3)$$

where the infimum is on the set of compact subsets K of \mathcal{S} . Since for $t > 0$, $P_t^{\mathcal{D}}$ is strongly Feller, it satisfies the assumption **(A1)** in [78, Section 3.2]. We can thus use [78, Theorem 3.5] to deduce that (5.2) is satisfied if for $t > 0$:

$$\beta_w(P_t^{\mathcal{D}}) = 0, \quad (5.4)$$

where (see (5.3))

$$\beta_w(P_t^{\mathcal{D}}) = \inf_{K \subset \mathbf{R}^{2d}} \sup_{\mathbf{x}=(x,v) \in \mathbf{R}^{2d}} P_t^{\mathcal{D}}(\mathbf{x}, \mathbf{R}^{2d} \setminus K) = \inf_{K \subset \mathbf{R}^{2d}} \sup_{\mathbf{x}=(x,v) \in \mathcal{D}} P_t^{\mathcal{D}}(\mathbf{x}, \mathcal{D} \setminus K).$$

Choosing $K_R = \overline{\mathcal{O}} \times \{|v| \leq R\}$, one has

$$\begin{aligned} \beta_w(P_t^{\mathcal{D}}) &\leq \inf_{R>0} \sup_{\mathbf{x}=(x,v) \in \mathcal{O} \times \mathbf{R}^d} P_t^{\mathcal{D}}(\mathbf{x}, \mathcal{O} \times \{|v| > R\}) \\ &\leq \inf_{R>0} \sup_{\mathbf{x}=(x,v) \in \mathcal{O} \times \mathbf{R}^d} P_t(\mathbf{x}, \mathcal{O} \times \{|v| > R\}). \end{aligned} \quad (5.5)$$

Let us now prove (5.4). Let $t > 0$ be fixed. In what follows c_i 's are positive constants which are independent of $\mathbf{x} = (x, v), \mathbf{y} = (x', v') \in \mathbf{R}^{2d}$. By [18, Theorem 1.1], for all $\mathbf{x} \in \mathbf{R}^{2d}$, $X_t(\mathbf{x})$ admits a density $p_t(\mathbf{x}, \mathbf{y})$ (w.r.t. the Lebesgue measure $d\mathbf{y}$ over \mathbf{R}^{2d}) which satisfies the following Gaussian upper bound: for all $\mathbf{x}, \mathbf{y} \in \mathbf{R}^{3d}$,

$$p_t(\mathbf{x}, \mathbf{y}) \leq c_0 \exp(-c_1 |\boldsymbol{\psi}_t(\mathbf{x}) - \mathbf{y}|^2), \quad (5.6)$$

where $(\boldsymbol{\psi}_s(\mathbf{x}) = (\mathbf{x}_s(\mathbf{x}), \mathbf{v}_s(\mathbf{x})), s \geq 0)$ is the deterministic solution for $s \geq 0$ of:

$$\dot{\mathbf{x}}_s = \mathbf{v}_s, \dot{\mathbf{v}}_s = \mathbf{b}(\mathbf{x}_s) - \gamma \mathbf{v}_s \text{ with } \boldsymbol{\psi}_0(\mathbf{x}) = \mathbf{x}.$$

Assume that $\gamma \neq 0$ (the case when $\gamma = 0$ is treated similarly). Let us now consider the solution $(\boldsymbol{\Psi}_s(\mathbf{x}) = (\mathbf{X}_s(\mathbf{x}), \mathbf{V}_s(\mathbf{x})), s \geq 0)$ for $s \geq 0$ of the equation

$$\dot{\mathbf{X}}_s = \mathbf{V}_s, \dot{\mathbf{V}}_s = -\gamma \mathbf{V}_s \text{ with } \boldsymbol{\Psi}_0(\mathbf{x}) = \mathbf{x},$$

i.e $\mathbf{V}_s(\mathbf{x}) = v e^{-\gamma s}$ and $\mathbf{X}_s(\mathbf{x}) = x + v \gamma^{-1}(1 - e^{-\gamma s})$. Since \mathbf{b} is bounded, using Grönwall's inequality, it holds

$$\sup_{s \in [0, t]} |\boldsymbol{\psi}_s(\mathbf{x}) - \boldsymbol{\Psi}_s(\mathbf{x})| \leq c_2.$$

This previous bounds leads to, for $s \in [0, t]$, $|\boldsymbol{\psi}_s(\mathbf{x}) - \mathbf{y}|^2 \geq |\boldsymbol{\Psi}_s(\mathbf{x}) - \mathbf{y}|^2 - 2c_2 |\boldsymbol{\Psi}_s(\mathbf{x}) - \mathbf{y}|$. Since \mathcal{O} is bounded, there exists $c_5 > 0$ such that $|x - x'| \leq c_5$ for all $x, x' \in \mathcal{O}$. Setting $c_3 := \gamma^{-1}(1 - e^{-\gamma t}) > 0$ and $c_4 := e^{-\gamma t} > 0$, it thus holds for all $\epsilon > 0$ and all $\mathbf{x}, \mathbf{y} \in \mathcal{D}$:

$$\begin{aligned} |(a_t, b_t)^T(\mathbf{x}) - \mathbf{y}|^2 &\geq |x - x' + c_3 v|^2 - 2c_2 |x - x' + c_3 v| \\ &\quad + |v' - c_4 v|^2 - 2c_2 |v' - c_4 v|, \\ &\geq c_3^2 |v|^2 - 2c_3(c_2 + c_5)|v| - 2c_2 c_5 \\ &\quad + |v'|^2 + c_4^2 |v|^2 - 2c_4 v \cdot v' - 2c_2 |v'| - 2c_2 c_4 |v|, \\ &\geq c_3^2 |v|^2 - 2c_3(c_2 + c_5)|v| - 2c_2 c_5 \\ &\quad + |v'|^2 + c_4^2 |v|^2 - 2c_4 |v| |v'| - 2c_2 |v'| - 2c_2 c_4 |v|, \\ &\geq c_3^2 |v|^2 - 2c_3(c_2 + c_5)|v| - 2c_2 c_5 \\ &\quad + |v'|^2 + c_4^2 |v|^2 - c_4 \epsilon^{-1} |v|^2 - \epsilon c_4 |v'|^2 - 2c_2 |v'| - 2c_2 c_4 |v| \\ &= |v|^2 (c_3^2 + c_4^2 - \epsilon^{-1} c_4) - 2c_3(c_2 + c_5)|v| - 2c_2 c_4 |v| \\ &\quad + |v'|^2 (1 - \epsilon c_4) - 2c_2 |v'| - 2c_2 c_5. \end{aligned}$$

Choose $\epsilon \in (0, 1/c_4)$ such that $c_6 = c_3^2 + c_4^2 - \epsilon^{-1} c_4 > 0$ (this is indeed possible since $c_6 \rightarrow c_3^2 > 0$ as $\epsilon \rightarrow (1/c_4)^-$). Using the previous computations, we have since \mathcal{O} is bounded, for all $\mathbf{x} = (x, v) \in \mathcal{O} \times \mathbf{R}^d$:

$$\begin{aligned} P_t(\mathbf{x}, \mathcal{O} \times \{|v| \geq R\}) &\leq c_7 e^{-c_1 c_6 |v|^2 + c_8 |v|} \int_{|v'| \geq R} e^{-c_1(1 - \epsilon c_4) |v'|^2 + 2c_1 c_2 |v'|} dv' \\ &\leq c_9 \int_{|v'| \geq R} e^{-c_1(1 - \epsilon c_4) |v'|^2 + 2c_1 c_2 |v'|} dv' \rightarrow 0 \text{ as } R \rightarrow +\infty. \end{aligned}$$

By (5.5), this implies that $\beta_w(P_t^{\mathcal{D}}) = 0$ and then (5.2) holds. The proof of the theorem is complete. \square

We end this section by considering the case when the position domain might be unbounded and the drift is singular: we state without proof the following extension of the main results of [29].

Theorem 5.2. [29, Theorems 2.4 and 3.2] *are both still valid without any regularity assumption on the boundary of the position domain \mathcal{O} , where $\mathcal{O} \times \mathbf{R}^d$ is the subdomain where the quasi-stationary distribution is considered there.*

5.2. Elliptic processes in bounded domains. In this section, we consider the solution $(Y_t, t \geq 0)$ in \mathbf{R}^d to the equation

$$dY_t = \mathbf{b}(Y_t)dt + \sqrt{2}dW_t. \quad (5.7)$$

When \mathcal{O} is an open subset of \mathbf{R}^d , we denote by $(P_t^\mathcal{O}, t \geq 0)$ the semigroup of the killed process $(Y_t, t \geq 0)$: $P_t^\mathcal{O}f(y) = \mathbf{E}_y[f(Y_t)\mathbf{1}_{t < \sigma_\mathcal{O}}]$, for $f \in b\mathcal{B}(\mathcal{O})$, $y \in \mathcal{O}$, and where $\sigma_\mathcal{O} = \inf\{t \geq 0, Y_t \notin \mathcal{O}\}$ is the first exit time of the process $(Y_t, t \geq 0)$ from \mathcal{O} . Using the same tools as those used in this work, we are able to get the following result which holds without any regularity assumption on $\partial\mathcal{O}$:

Theorem 5.3. *Assume $[\mathbf{V}_{\text{bounded+lip}}]$. Then, there exists a unique quasi-stationary distribution $\nu_\mathcal{O}$ for the process (5.7) on \mathcal{O} in the whole space of probability measures $\mathcal{P}(\mathcal{O})$ over \mathcal{O} . Furthermore:*

- (1) *There exists $\alpha_\mathcal{O} > 0$ s.t. for all $t \geq 0$, the spectral radius of $P_t^\mathcal{O}$ on $b\mathcal{B}(\mathcal{O})$ is $e^{-\alpha_\mathcal{O}t}$, where $(P_t^\mathcal{O}, t \geq 0)$ is the killed semigroup of the process solution to (5.1) (see (1.7)). In addition, for all $t \geq 0$, $\nu_\mathcal{O}P_t^\mathcal{O} = e^{-\alpha_\mathcal{O}t}\nu_\mathcal{O}$ and $\nu_\mathcal{O}(\mathbf{O}) > 0$ for all nonempty open subsets \mathbf{O} of \mathcal{O} . There is also a unique continuous function ϕ in $b\mathcal{B}(\mathcal{O})$ such that $\nu_\mathcal{O}(\phi) = 1$, $\phi > 0$ on \mathcal{O} , and $P_t^\mathcal{O}\phi = e^{-\alpha_\mathcal{O}t}\phi$ on \mathcal{O} , $\forall t \geq 0$.*
- (2) *There exist $m_1 > 0$ and $m_2 \geq 1$ such that for all $\nu \in \mathcal{P}(\mathcal{O})$,*

$$|\mathbf{P}_\nu[Y_t \in \mathcal{A} | t < \sigma_\mathcal{O}] - \nu_\mathcal{O}(\mathcal{A})| \leq \frac{m_2 e^{-m_1 t}}{\nu(\phi)}, \quad \forall \mathcal{A} \in \mathcal{B}(\mathcal{O}), t > 0.$$

Eventually, $\mathbf{P}_y(\sigma_\mathcal{O} < +\infty) = 1$ for all $y \in \mathcal{O}$.

Proof. Theorem 5.3 is proved using the same arguments as those used to prove Theorem 5.1 above. \square

Theorem 5.3 can be extended to the case where there is a uniformly elliptic and Lipschitz diffusion coefficient in (5.7). Theorem 5.3 was already derived in [13] (see Theorem 1.1 there) with different techniques. We end this work with the following result about existence and uniqueness of quasi-stationary distributions for elliptic processes on possible unbounded domains and with singular potentials.

Theorem 5.4. [29, Proposition 4.2] *is still valid without any regularity assumption on the boundary of the subdomain \mathcal{D} on which is considered the quasi-stationary distribution there.*

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