Geometric ergodicity for dissipative particle dynamics

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Abstract

Dissipative particle dynamics is a model of multi phase fluid flows described by a system of stochastic differential equations. We consider the problem of N particles evolving on the one dimensional periodic domain of length L and, if the density of particles is large, prove geometric convergence to a unique invariant measure. The proof uses minorization and drift arguments, but allows elements of the drift and diffusion matrix to have compact support, in which case hypoellipticity arguments are not directly available.
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1 Introduction

Dissipative particle dynamics (DPD) was first proposed by Hoogerbrugge and Koelman [6] as a method for the mesoscopic simulation of complex fluids. DPD describes the evolution of $(q_i, p_i) \in \mathbf{R}^d \times \mathbf{R}^d$ for $i = 1, \dots, N$, the positions and velocities of a set of mesoscopic objects describing a group of atoms or fluid molecules, by a system of stochastic differential equations (SDEs). Much has been written on DPD in the physics literature [5, 4, 7, 11, 13, 1], but few papers have considered the mathematical analysis of DPD. The purpose of this paper is to study the long time behavior of DPD and prove under suitable hypothesis that the system is ergodic. One of the main features of DPD is that particles interact only at short range. This is very convenient for computer simulations, as fewer pair interactions are evaluated, but makes the study of ergodicity difficult. The diffusion is neither uniformly elliptic nor hypoelliptic for all initial data. The main work of this paper is to establish conditions that imply geometric ergodicity in one dimension ($d = 1$).

We describe the setting of our results on DPD formally. We work on a periodic spatial domain, so that particle positions q_i live in the periodic interval $\mathcal{T} = [0, L]$. Relative positions and velocities are denoted by $q_{ij} = q_i - q_j$ and $p_{ij} = p_i - p_j$. The (q_i, p_i) satisfy the SDE

$$\begin{aligned} dq_i =& p_i\, dt, \\ dp_i =& -\sum_{j=1, j\neq i}^{N} a_{ij} \frac{\partial}{\partial q_i} V(|q_{ij}|)\, dt - \gamma \sum_{j=1, j\neq i}^{N} W^D(|q_{ij}|) p_{ij}\, dt \\ &+ \sigma \sum_{j=1, j\neq i}^{N} W^R(|q_{ij}|)\, d\beta_{ij}(t), \end{aligned} \tag{1.1}$$

where initial values should be specified for q_i, p_i at $t = 0$. The $\beta_{ij}(t)$ are independent Brownian motions for $i < j$ and $\beta_{ij}(t) = -\beta_{ji}(t)$ so that momentum is conserved. The matrix a_{ij} is symmetric, with each $a_{ij} \geq 0$. The functions $V, W^D, W^R \colon [0, \infty) \to \mathbf{R}$ describe the pair potential and cut-off functions for the dissipation and noise.

We assume that (1.1) defines a strong Markov process $x(t) = (q_1, \dots, q_N, p_1, \dots, p_N)$ on S with start value $y \in S$, where

$$S = \Big\{ (q_1, \dots, q_N, p_1, \dots, p_N) \in \mathcal{T}^N \times \mathbf{R}^N \colon \frac{1}{N} \sum_{i=1}^{N} q_i = \ell, \quad \sum_{i=1}^{N} p_i = 0, \quad |p_{ij}| + |q_{ij}| > 0 \text{ if } i \neq j \Big\},$$

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some $\ell \in \mathcal{T}$. The total linear momentum $\sum_i p_i$ is conserved, and it is convenient to assume that $\sum_i p_i = 0$, which implies the average position of the particles always equals ℓ. Further, we exclude degenerate states where two particles have identical position and velocity, $p_{ij} = q_{ij} = 0$. For initial data y in S, the probability of reaching a degenerate state is zero and we may assume that $x(t)$ is S valued. Even with this assumption, the conservative term may have jump discontinuities at $q_{ij} = 0$ for $i \neq j$. Well defined solutions are available when $q_{ij} = 0$ as long as $p_{ij} \neq 0$.

We make use of the following assumptions on V, W^R, and W^D. Assumption 1.1(i) maintains temperature control and leads to the Gibbs invariant distribution, (ii) describes the regularity and support property of the functions, and (iii) selects a scaling for W^D. Denote the support of a function $W\colon [0,\infty) \to \mathbf{R}$ by $\operatorname{supp}(W) = \{r \in [0,\infty)\colon W(r) \neq 0\}$.

Assumption 1.1 *(i)* $W^D(r) = W^R(r)^2$, *and* W^R *and* V *are* C^∞ *on* $(0, r_c)$, *some* $r_c > 0$.

(ii) $\operatorname{supp}(W^R) = \operatorname{supp}(V) = [0, r_c)$ *and the limit of* $V'(r)/W^R(r)$ *as* $r \uparrow r_c$ *(approaches* r_c *from below) is finite.*

(iii) $W^D(0) = 1$.

These assumptions are sufficiently broad to include the following example, used in the early papers [5] on DPD: for a cut-off distance $r_c > 0$, $W^R(r) = W^D(r)^{1/2}$, $V(r) = W^D(r)$, and

$$W^D(r) = \begin{cases} (1 - r/r_c)^2, & 0 \le r < r_c, \\ 0, & \text{otherwise}. \end{cases} \tag{1.2}$$

We state the main result. Let $\boldsymbol{p}$ denote the vector $(p_1, \dots, p_N)$ of particle velocities and $\|\boldsymbol{p}\|_2 = (p_1^2 + \cdots + p_N^2)^{1/2}$.

Theorem 1.2 *Suppose that Assumption 1.1 holds. Suppose that* $L < N\, r_c$ *and* $\sigma, \gamma > 0$. *The solution* $x(t)$ *of* (1.1) *with start value* $y \in S$ *is geometrically ergodic: there exist a unique invariant probability measure* π *on* S *such that, for some constants* $k, K > 0$,

$$|\mathbf{E} g(x(t)) - \pi(g)| \le K(1 + \|\boldsymbol{p}\|_2^2) e^{-kt},$$

for all $y = (q_1, \dots, q_N, p_1, \dots, p_N) \in S$, *all measurable function* $g : S \to \mathbf{R}$ *with* $|g| \le (1 + \|\boldsymbol{p}\|_2^2)$, *where* $\pi(g) = \int_S g \, d\pi$.

This theory concerns only dimension $d = 1$. We are unable at this time to discuss ergodicity in the physically interesting cases of $d = 2, 3$. The key assumption is that the density of particles $N/L > 1/r_c$, so that at least two particles are interacting ($|q_{ij}| < r_c$ for some $i \neq j$). This observation applies to higher dimensions: there must be a sufficient density of particles to ensure the system mixes. For $y = (q_1, \dots, q_N, p_1, \dots, p_N)$, define

$$H(y) = \frac{1}{2} \sum_{i=1}^{N} p_i^2 + \frac{1}{2} \sum_{i,j=1, i \neq j}^{N} a_{ij} V(|q_{ij}|). \tag{1.3}$$

When the system does mix, it converges to a unique invariant distribution and, if $W^D(r) = W^R(r)^2$, Español and Warren [3] show that the Gibbs distribution with density

$$\rho(y) = \exp\Big(-\frac{1}{K_B T} H(y)\Big)$$

defines the invariant distibution, where $\sigma^2 = 2\gamma k_B T$, k_B is Boltzmann's constant, and T is the equilibrium temperature.

For $d = 2, 3$ dimensions, there are more degenerate states in the possible configurations of particles, as particles may move in parallel and not collide with one another. Also, for each pair of particles, we have one Brownian motion, which corresponds to the dimension of physical space, and this helps in the use of Hörmander's Theorem. For $d = 2, 3$, we would need to show that three or more particles are interacting to fulfill bracket conditions. Controlling the particles into such configurations will be demanding technically.

The organization of this paper is the following. In Section 2, we give some preliminary definitions and review the theory of geometric ergodicity. The key is the minorization and Lyapunov-Foster drift condition developed in Meyn-Tweedie [9]. In Sections 3–4, we prove that these conditions hold for DPD. In Section 5, we give the proof of Theorem 1.2. Finally in the Appendix, we provide technical Lemmas, which we need in Sections 3–4. We suppose that Assumption 1.1 holds throughout.

2 Preliminaries

Let $(\Omega, \mathbf{P}, \mathcal{F})$ be the underlying probability space. Let $\mathcal{F}_t$ be the σ-algebra of all events up to time t. Consider a Markov process $x(t)$ on a state space $(S, \mathcal{B}(S))$, where $\mathcal{B}(S)$ denotes the Borel σ-algebra on S. Denote $P_t(y, A)$ the transition probability:

$$P_t(y, A) = \mathbf{P}(x(t) \in A | x(0) = y), \quad \forall y \in S,\ \forall A \in \mathcal{B}(S).$$

We describe two fundamental assumptions that imply geometric ergodicity. For further details, see Meyn and Tweedie [9] or for a development of this theory for Langevin systems see Mattingly, Stuart, and Higham [8].

Assumption 2.1 (minorization condition) *For a compact set $C \subset S$, there exist $T, \eta > 0$ and a probability measure ν on S with $\nu(C) > 0$ such that*

$$P_T(y, A) \geq \eta \nu(A), \quad \forall y \in C,\ \forall A \in \mathcal{B}(S).$$

Usually, this condition is established by proving continuity of a transition density and establishing that the each set A is reachable with (strictly) positive probability from C. Because the probability is positive and continuous in the initial data, we can find a positive minimum over choice of initial data in a compact set and thereby derive the minorization condition. In this way, a continuous density is key to our arguments.

Assumption 2.2 (drift condition) *There exist $\mathcal{V} : S \to [1, \infty)$ measurable and some time $T > 0$ such that, for a set $C \subset S$ and some $\alpha, \beta > 0$,*

$$\mathbf{E}[\mathcal{V}(x(T))] - \mathcal{V}(y) \leq -\alpha \mathcal{V}(y) + \beta \mathbf{1}_C(y), \quad \forall x(0) = y \in S,$$

where $\mathbf{1}_C$ is the indicator function on the set C.

Theorem 2.3 *Assume that Assumptions 2.1 and 2.2 hold for a set C. Then $x(t)$ is $\mathcal{V}$-geometrically ergodic: there exists a unique invariant probability measure π such that, for some constants $k, K > 0$,*

$$|\mathbf{E} g(x(t)) - \pi(g)| \leq K \mathcal{V}(y) e^{-kt}, \quad \forall\, x(0) = y \in S,$$

for all measurable function $g : S \to \mathbf{R}$ with $|g| \leq \mathcal{V}$.

Proof [9, Theorem 16.0.1] or [8, Theorem 2.5]. *QED*

The proof of Theorem 1.2 is based on Theorem 2.3.

Before closing this preliminaries section, we recall a generalisation of the Hörmander Theorem that provides existence and smoothness of the density of a killed diffusion process, used to prove Assumption 2.1. For a C^∞ domain $\mathcal{D} \subset \mathbf{R}^p$, consider the process $\tilde{x}(t)$ that satisfies the following Itô SDE in $\mathcal{D}$

$$dx = X_0(x) dt + \sum_{i=1}^{m} X_i(x) dW^i(t), \qquad x(0) \in \mathcal{D} \tag{2.1}$$

and is killed on the boundary of $\mathcal{D}$, where $X_i : \mathbf{R}^p \to \mathbf{R}^p$ for $i = 0, 1, \ldots, m$. Here each $W^i(t)$ is an independent one dimensional Brownian motion. Define the Lie bracket $[X_i, X_j] = DX_j\, X_i - DX_i\, X_j$, where $DX_i : \mathbf{R}^p \to \mathbf{R}^{p\times p}$ is the Fréchet derivative of X_i.

Theorem 2.4 *Suppose that (i) the domain $\mathcal{D}$ is non-characteristic: if $\boldsymbol{n}$ is the normal to $\partial\mathcal{D}$ at $x \in \partial\mathcal{D}$ then $X_i(x) \cdot \boldsymbol{n} \neq 0$ for some $i \in \{1, \dots, m\}$ and (ii) DX_i are C^∞ smooth from $\mathbf{R}^p \to \mathbf{R}^{p\times p}$ and*

$$X_1, \cdots, X_m, [X_0, X_1], \cdots, [X_0, X_m]$$

span $\mathbf{R}^p$ for each $y \in \bar{\mathcal{D}}$. Then, the solution $\tilde{x}(t)$ of (2.1) has a jointly continuous density function.

Proof Cattiaux [2]. *QED*

Notation By K and k we denote positive constants independent of the functions and parameters concerned, but not necessarily the same at different occurrences. When necessary for clarity we distinguish constants by subscripts. For any $x = (q_1, \dots, q_N, p_1, \dots, p_N) \in \mathcal{T}^N \times \mathbf{R}^N$, we will denote

$$\|x\|_\infty = \max_{1\le i\le N} \{|q_i|, |p_i|\}$$

and denote $\|x\|_2$ the Euclidean norm of a vector $x \in \mathbf{R}^{2N}$ and $\|\Sigma\|_2$ the trace norm for matrix $\Sigma \in \mathbf{R}^{2N\times\frac{1}{2}N(N-1)}$; i.e., $|\Sigma|_2^2 = \mathrm{trace}(\Sigma^T\Sigma)$. Denote by $B_\delta(y)$ the $\|\cdot\|_\infty$ open ball of radius δ centered at y and $\bar{B}_\delta(y)$ the closure of this ball.

3 Minorization condition

We will prove the minorization condition for a variety of compact subsets. We start with $N = 3$ particles and examine configurations where every particle is interacting with another particle. In Subsection 3.1, we prove

Theorem 3.1 *Let $N = 3$. There exists a $\bar{y} \in M = S \cap \{|q_{12}| < r_c, |q_{13}| < r_c\}$ and a $\delta > 0$ such that the minorization condition holds for the process $x(t)$ on the set $C = \bar{B}_\delta(\bar{y})$ (closed ball of radius δ with centre $\bar{y}$).*

We must establish the minorization conditions for a broader class of sets to use it with the drift condition and prove geometric ergodicity.

Theorem 3.2 *Let $N = 3$. The minorization condition holds for the process $x(t)$ for any compact subset C' of $M' = S \cap \{|q_{ij}| < r_c\colon$ some $i \neq j\}$.*

To prove this (Subsection 3.2), we show how to steer a trajectory starting at an initial data $y \in M'$ (where only one pair of particles need be close together) into M. If the probability of entering M is sufficient, Theorem 3.1 can be applied to gain the minorization condition.

We develop the results for $N = 3$ in full detail to illustrate how to deal with initial conditions where particles may not be initially influenced by noise. The argument can be extended to $N > 3$ to gain the following theorem by controlling the trajectory through stages, with ever more particles being influenced by noise until we arrive in the situation where $|q_{i,i+1}| < r_c$ for $i = 1, \dots, N-1$, similar to Theorem 3.1. The proof is tedious, its main ideas are illustrated by the $N = 3$ case, and is not presented.

Theorem 3.3 *For $N \ge 2$ particles, the minorization condition holds for the process $x(t)$ for any compact subset of $S \cap \{|q_{ij}| < r_c\colon$ some $i \neq j\}$.*

To develop these proofs, it is convenient to write (1.1) as the following abstract SDE:

$$dx = f(x)dt + \Sigma(x)dW(t), \quad x(0) = y, \tag{3.1}$$

where

$$x = \begin{pmatrix} q_1 \\ \vdots \\ q_N \\ p_1 \\ \vdots \\ p_N \end{pmatrix}, \quad f(x) = \begin{pmatrix} p_1 \\ \vdots \\ p_N \\ -\sum_{j\neq 1} a_{1j} \frac{\partial}{\partial q_1} V(|q_{1j}|) - \gamma \sum_{j\neq 1} W^D(|q_{1j}|) p_{1j} \\ \vdots \\ -\sum_{j\neq N} a_{Nj} \frac{\partial}{\partial q_N} V(|q_{Nj}|) - \gamma \sum_{j\neq N} W^D(|q_{Nj}|) p_{Nj} \end{pmatrix},$$

$W = (\beta_{12}, \ldots, \beta_{1N}, \beta_{23}, \ldots, \beta_{2N}, \ldots, \beta_{N-1,N})^T \in \mathbf{R}^{\frac{1}{2}N(N-1)}$, and

$$\Sigma(x) = \begin{pmatrix} O \\ \sigma(x) \end{pmatrix} \in \mathbf{R}^{2N \times \frac{1}{2}N(N-1)},$$

where $O \in \mathbf{R}^{N \times \frac{1}{2}N(N-1)}$ is the zero matrix, and $\sigma(x) \in \mathbf{R}^{N \times \frac{1}{2}N(N-1)}$ is a matrix whose elements depend on x. One can write $\sigma(x)$ explicitly, for example, when $N = 3$,

$$\sigma(x) = \begin{pmatrix} \sigma W^R(q_{12}) & \sigma W^R(q_{13}) & 0 \\ -\sigma W^R(q_{21}) & 0 & \sigma W^R(q_{23}) \\ 0 & -\sigma W^R(q_{31}) & -\sigma W^R(q_{32}) \end{pmatrix} \in \mathbf{R}^{3\times 3}.$$

3.1 Proof of Theorem 3.1

The classical statement of Hörmander's Theorem requires smoothness of coefficients on the whole domain (for example, [10]). The drift and diffusion functions in (1.1) are not C^∞, and in particular the conservative term has a jump discontinuity. We will exploit Theorem 2.4, a version of Hörmander's Theorem for killed diffusion processes, on a domain $\mathcal{D}$ where the coefficients are smooth. The obvious candidate for $\mathcal{D}$ is

$$\tilde{\mathcal{D}} = \{(q_1, \ldots, q_N, p_1, \ldots, p_N) \in S \colon |q_{ij}| < r_c \text{ and } q_{ij} \neq 0 \text{ for } i \neq j\}.$$

This domain fails the non-characteristic condition, as the normal to the boundary of $\tilde{\mathcal{D}}$ may be orthogonal to all the p directions. To gain a non-characteristic domain, define

$$\mathcal{D} = \left\{x \in \tilde{\mathcal{D}} \colon |p_{ij}| > \frac{1}{|q_{ij}|} + \frac{1}{|r_c - q_{ij}|}, \quad i \neq j\right\},$$

in which case the boundary of the domain always varies with p and the noise pushes trajectories across the boundary.

In this subsection, $N = 3$. Consider a $\bar{y} \in \tilde{\mathcal{D}}$ and a $\delta > 0$ such that $\bar{B}_{3\delta}(\bar{y}) \subset \mathcal{D}$.

Lemma 3.4 *For each $Y \in B_\delta(\bar{y})$ and $T_1 > 0$, there exists $U \in C^1([0, T_1], \mathbf{R}^3)$ such that the solution $X(t)$ of*

$$\frac{dX}{dt} = f(X) + \Sigma(X)\, U'(t), \qquad X(0) = Y$$

satisfies $X(T_1) = \bar{y}$ and $X(t) \in B_{2\delta}(\bar{y})$ for $t \in [0, T_1]$.

Proof By Lemma A.3, we can construct continuously differentiable $X(t) = (Q(t), Q'(t))$ and $Q = (Q_1, \ldots, Q_3)$ such that $X(0) = Y$, $X(T_1) = \bar{y}$, and $X(t) \in B_{2\delta}(\bar{y})$ for $0 \le t \le T_1$. Writing the equations in detail with $Q_{ij} = Q_i - Q_j$, $P_{ij} = P_i - P_j$, and $U = (U_{12}, U_{13}, U_{23})$,

$$Q_1''(t) = -\sum_{j\neq 1} a_{1j} \frac{\partial V(|Q_{1j}|)}{\partial Q_1} - \gamma W^D(|Q_{1j}|) P_{1j} + \sigma W^R(|Q_{12}|) U_{12}'(t) + \sigma W^R(|Q_{13}|) U_{13}'(t), \tag{3.2}$$

$$Q_2''(t) = -\sum_{j\neq 2} a_{2j} \frac{\partial V(|Q_{2j}|)}{\partial Q_2} - \gamma W^D(|Q_{2j}|) P_{2j} - \sigma W^R(|Q_{21}|) U_{12}'(t) + \sigma W^R(|Q_{23}|) U_{23}'(t), \tag{3.3}$$

$$Q_3''(t) = -\sum_{j\neq 3} a_{3j} \frac{\partial V(|Q_{3j}|)}{\partial Q_3} - \gamma W^D(|Q_{3j}|) P_{3j} - \sigma W^R(|Q_{31}|) U_{13}'(t) - \sigma W^R(|Q_{32}|) U_{23}'(t). \tag{3.4}$$

As $X(t) \in \tilde{\mathcal{D}}$, all the terms are well defined (especially the term in V) and, by Assumption 1.1(ii), $W^R(|Q_{12}|) \neq 0$, $W^R(|Q_{13}|) \neq 0$. To get U_{ij}' from (3.2)–(3.4), we first define U_{ij}' by choosing arbitrary $U_{23}' \in C([0, T_1], \mathbf{R})$ and then solve U_{12}' and U_{13}' from (3.3) and (3.4). Equation (3.2) will hold because $X(t) \in S$. The control U' so constructed is continuous and therefore $U \in C^1([0, T_1], \mathbf{R}^3)$. *QED*

Lemma 3.5 *Let $\tilde{x}(t)$ be the process $x(t)$ killed on the boundary of $\mathcal{D}$. Let $\tilde{P}_t(y, A)$ be the transition probability for the killed process $\tilde{x}$ for initial $y \in \mathcal{D}$ and $A \subset \mathcal{D}$. Let $C = \bar{B}_\delta(\bar{y})$. Then, for each $t > 0$,* *(i)* $\tilde{P}_t(y, B_\delta(\bar{y})) > 0$ *for all* $y \in C$.

(ii) $\tilde{P}_t(y, A)$ *possesses a jointly continuous density* $\tilde{p}_t(y, x)$.

Proof

(i) Consider $y \in C$. By Lemma 3.4 with $Y = y$, we can construct a path $X(t)$ and control $U(t)$ connecting y to $\bar{y}$ and guarantee that the δ neighbourhood of the path remains in $B_{3\delta}(\bar{y})$. Lemma A.1 does not apply directly to our problem, as f is not Lipschitz. Consider a globally Lipschitz $\hat{f}$ that equals f on C and has Lipschitz constant K and let $\hat{x}$ solve

$$d\hat{x} = \hat{f}(\hat{x})\, dt + \Sigma(\hat{x})\, dW(t), \qquad \hat{x}(0) = y.$$

By Lemma A.1,

$$\sup_{0\le t\le T_1} \|\hat{x}(t) - X(t)\|_2 \le K\Big(\sup_{0\le s\le T_1} \|W(s) - U(s)\|_2\Big).$$

Let $\epsilon = \delta/K$. If $\sup_{0\le s\le T_1} \|W(s) - U(s)\|_2 < \epsilon$, the killed process $\tilde{x} = \hat{x}$ on $[0, T_1]$ as $\hat{x}$ does not leave $B_{3\delta}(\bar{y})$. In particular, $\tilde{x}(t)$ will reach the set $B_\delta(\bar{y})$ from y with positive probability, since the Wiener measure of any event

$$\sup_{0\le s\le T_1} \|W(s) - U(s)\|_2 < \epsilon.$$

is positive; see Stroock [12, Theorem 4.20].

(ii) We wish to apply Theorem 2.4. Because $\tilde{x}(t) \in S$ for all $t \ge 0$,

$$p_1 + p_2 + p_3 = 0, \quad \tfrac{1}{3}(q_1 + q_2 + q_3) = \ell.$$

Therefore, (1.1) is equivalent to the following

$$dz = X_0(z)dt + \sum_{i=1}^{3} X_i(z)\, dW^i(t), \tag{3.5}$$

where

$$z = \begin{pmatrix} q_2 \\ q_3 \\ p_2 \\ p_3 \end{pmatrix}, \quad X_0(z) = \begin{pmatrix} p_2 \\ p_3 \\ -\sum_{j\ne 2} a_{2j} \frac{\partial}{\partial q_2} V(|q_{2j}|) - \gamma \sum_{j\ne 2} W^D(|q_{2j}|)p_{2j} \\ -\sum_{j\ne 3} a_{3j} \frac{\partial}{\partial q_3} V(|q_{3j}|) - \gamma \sum_{j\ne 3} W^D(|q_{3j}|)p_{3j} \end{pmatrix}, \tag{3.6}$$

and

$$X_1(z) = \begin{pmatrix} 0 \\ 0 \\ \sigma W^R(|q_{21}|) \\ 0 \end{pmatrix}, \quad X_2(z) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -\sigma W^R(|q_{31}|) \end{pmatrix}, \quad X_3(z) = \begin{pmatrix} 0 \\ 0 \\ \sigma W^R(|q_{23}|) \\ -\sigma W^R(|q_{32}|) \end{pmatrix}.$$

For any start value $y \in C$, we find that $X_1, X_2, [Y, X_1], [Y, X_2]$ span $\mathbf{R}^4$. In fact,

$$[Y, X_1] = \begin{pmatrix} \sigma W^R(|q_{21}|) \\ 0 \\ * \\ * \end{pmatrix}, \quad [Y, X_2] = \begin{pmatrix} 0 \\ \sigma W^R(|q_{31}|) \\ * \\ * \end{pmatrix},$$

where $*$ denotes some different functions, which implies that $\{X_1, X_2, [Y, X_1], [Y, X_2]\}$ span $\mathbf{R}^4$, since $W^D(|q_{i1}|) > 0$ as $|q_{i1}| = |q_i - q_1| < r_c$ for $i = 2, 3$ and $y \in C$ using Assumption 1.1(ii).

We chose $\mathcal{D}$ to be non-characteristic. Theorem 2.4 provides existence of a smooth density, as required.

QED

Proof [of Theorem 3.1] By standard arguments, see [9, 8], the reachability and smoothness conditions established in Lemma 3.5 imply the minorization condition. In particular, we can find a measure ν with $\nu(C) > 0$ for the killed process $\tilde{x}$ such that for some $\eta > 0$

$$\tilde{P}_t(y, A) \geq \eta\nu(A), \qquad y \in C, A \in \mathcal{B}(S),$$

where $C = \bar{B}_\delta(\bar{y})$. For $A \subset C$ and $y \in C$, $P_t(y, A) \geq \tilde{P}_t(y, A)$, as trajectories for the killed process that reach A at time t must also be trajectories for (1.1). We conclude that

$$P_t(y, A) \geq \eta\nu(A), \qquad y \in C, A \in \mathcal{B}(S),$$

and that C obeys minorization condition for (1.1). *QED*

3.2 Proof of Theorem 3.2

We work on DPD without the conservative terms, equation (3.7), which contains only Lipschitz terms. We will use a Girsanov transformation to draw conclusions about the full system.

Lemma 3.6 *For any $\bar{y} \in \tilde{\mathcal{D}}$ and any $Y \in M'$ with $N = 3$ and any $T_1 > 0$, we can construct*

$$X(t) = (Q_1(t), \ldots, Q_N(t), P_1(t), \ldots, P_N(t))$$

with $X(0) = Y$ and $X(T_1) = \bar{y}$ and a control $U \in C^1([0, T], \mathbf{R}^3)$ such that

$$\begin{aligned} \frac{dQ_i}{dt} =& P_i, \\ \frac{dP_i}{dt} =& -\gamma \sum_{j=1, j\neq i}^{N} W^D(|Q_{ij}|)P_{ij} + \sigma \sum_{j=1, j\neq i}^{N} W^R(|Q_{ij}|)\, U'_{ij}. \end{aligned} \tag{3.7}$$

Proof Write $Y = (q_1, \ldots, q_3, p_1, \ldots, p_3)$. Let $\bar{P}_3 = p_3$ and $\bar{Q}_3 = Q_3(T_2)$, where $Q_3(t)$ is the straight line with $Q_3(0) = q_3$ with slope $Q'_3(0) = p_3$. We have

$$Q_3(t) = \bar{Q}_3 + \frac{\bar{Q}_3 - q_3}{T_2}(t - T_2). \tag{3.8}$$

For $i = 1, 2$, choose $\bar{Q}_i, \bar{P}_i$ such that

$$\begin{aligned} &\bar{Q}_1 + \bar{Q}_2 + \bar{Q}_3 = 3\ell, \\ &\bar{P}_1 + \bar{P}_2 + \bar{P}_3 = 0, \\ &|\bar{Q}_1 - \bar{Q}_2| < r_c, \quad |\bar{Q}_1 - \bar{Q}_3| < r_c, \end{aligned}$$

which is possible though not unique. Let $\bar{Y} = (\bar{Q}_1, \bar{Q}_2, \bar{Q}_3, \bar{P}_1, \bar{P}_2, \bar{P}_3)$ and note $\bar{Y} \in M$. This choice of $\bar{Y}$ depends on Y and may not equal $\bar{y}$.

We first construct X such that (3.7) holds and $X(0) = Y$ and $X(T_1) = \bar{Y}$. Set $X(t) = (Q(t), Q'(t))$ and $Q(t) = (Q_1(t), \ldots, Q_3(t))$ for $0 \leq t \leq T_2$. If $X(t)$ satisfies (3.7) then

$$Q''_1(t) + Q''_2(t) + Q''_3(t) = 0, \quad 0 \leq t \leq T_2.$$

Since $Q_3(t)$ is a straight line, we have

$$Q''_1(t) + Q''_2(t) = 0, \quad 0 \leq t \leq T_2.$$

Combining $Q_3(t)$ defined in (3.8) with $Q_i(t)$, $i = 1, 2$ constructed by Lemma A.4, we find that the following holds for $i = 1, 2, 3$ and $0 \leq t \leq T_2$

$$Q_i(0) = q_i, \quad Q'_i(0) = p_i, \tag{3.9}$$
$$Q_i(T_2) = \bar{Q}_i, \quad Q'_i(T_2) = \bar{P}_i, \tag{3.10}$$
$$|Q_{12}(t)| = |Q_1(t) - Q_2(t)| < r_c, \tag{3.11}$$
$$Q''_1(t) + Q''_2(t) = 0, \tag{3.12}$$
$$Q''_1(t) + Q''_2(t) + Q''_3(t) = 0. \tag{3.13}$$

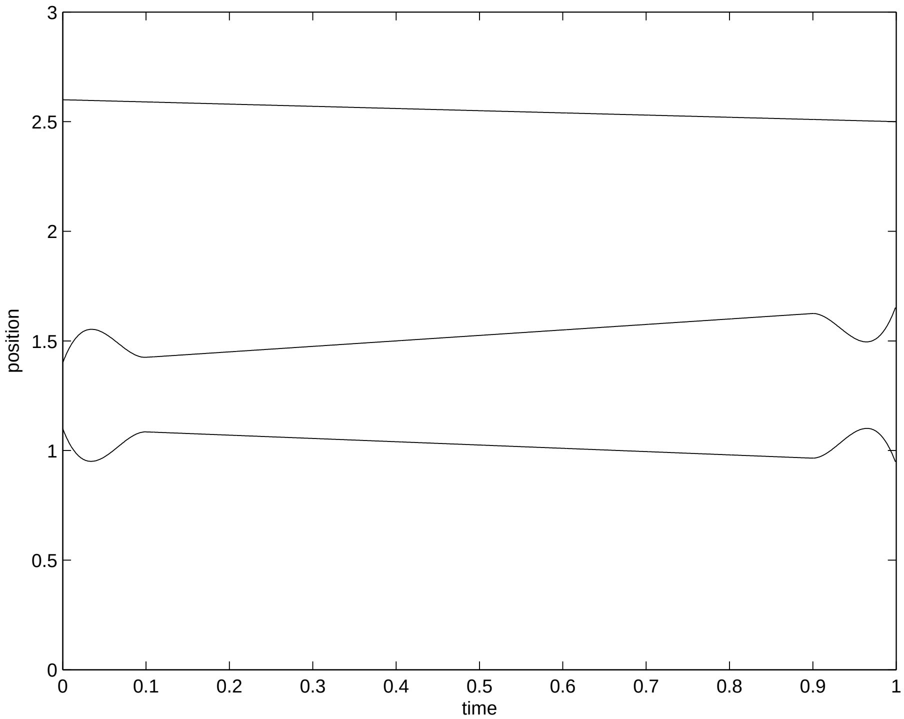

Figure 1: Paths $Q_1(t), Q_2(t), Q_3(t)$ for $Y = (1.1, 1.4, 2.6, -9.9, 10, -0.1)$ and $\bar{Y} = (0.95, 1.65, 2.5, -10, 10.1, -0.1)$,

The paths so constructed are illustrated in Figure 3.2.

Now we claim that there exist $U = (U_{12}, U_{13}, U_{23}) \in C^1([0, T_2], \mathbf{R}^3)$ such that (3.7) holds; i.e.,

$$Q_1''(t) = -\gamma \sum_{j \neq 1} W^D(|Q_{1j}|) P_{1j} + \sigma W^R(|Q_{12}|) U_{12}' + \sigma W^R(|Q_{13}|) U_{13}', \tag{3.14}$$

$$Q_2''(t) = -\gamma \sum_{j \neq 2} W^D(|Q_{2j}|) P_{2j} - \sigma W^R(|Q_{21}|) U_{12}' + \sigma W^R(|Q_{23}|) U_{23}', \tag{3.15}$$

$$Q_3''(t) = -\gamma \sum_{j \neq 3} W^D(|Q_{3j}|) P_{3j} - \sigma W^R(|Q_{31}|) U_{13}' - \sigma W^R(|Q_{32}|) U_{23}'. \tag{3.16}$$

We can choose continuous functions U_{13} and U_{23} satisfying

$$\sigma W^R(|Q_{31}|) U_{13}' = -\gamma W^D(|Q_{31}|) P_{31},$$
$$\sigma W^R(|Q_{32}|) U_{23}' = -\gamma W^D(|Q_{32}|) P_{32}.$$

The first equation defines U_{13}' if $|Q_{31}| < r_c$ and we set $U_{13}' = 0$ otherwise, so that U_{13}' is continuous by Assumption 1.1(i). Similarly, the second equation defines $U_{23}' \in C([0, T_2], \mathbf{R})$. Finally, U_{12}' can be computed from (3.14) or (3.15), since $|Q_{12}(t)| < r_c$ and therefore $W^R(|Q_{12}(t)|) \neq 0$ in $[0, T_2]$ using Assumption 1.1(ii). The two equations are consistent by (3.12). For our choice of U, each of (3.14)–(3.16) holds; the last equation by use of (3.13), and $U \in C^1([0, T_2], \mathbf{R}^3)$.

To complete the proof, we need to connect $\bar{Y}$ to $\bar{y}$. This can be done as in Lemma 3.6. The construction of a control in this case is simpler, as we can remain in M, where each particle is influenced by noise. *QED*

Lemma 3.7 *For every compact $C \subset M'$ and $T > 0$, there exists $\eta > 0$ such that $P_T(y, B_\delta(\bar{y})) \geq \eta$ for all $y \in C$.*

Proof Consider a $\tilde{W}(t) = (\tilde{\beta}_{12}, \dots, \tilde{\beta}_{23})^T$, where $\tilde{\beta}_{ij}$ are independent Brownian motions under a measure $\tilde{\mathbf{P}}$ (with expectations denoted by $\tilde{\mathbf{E}}$). Consider $x(t)$, the solution of

$$\begin{aligned} dq_i =& p_i\, dt, \\ dp_i =& -\gamma \sum_{j=1, j\neq i}^{N} W^D(|q_{ij}|) p_{ij}\, dt + \sigma \sum_{j=1, j\neq i}^{N} W^R(|q_{ij}|)\, d\tilde{\beta}_{ij}(t), \end{aligned} \tag{3.17}$$

with initial data $x(0) = y$. For $X(t)$ and $U(t)$ constructed in Lemma 3.6, Lemma A.1 yields

$$\sup_{0\le t\le T} \|x(t) - X(t)\|_2 \le K\Big(\|y - Y\|_2 + \sup_{0\le s\le T} \|\tilde{W}(s) - U(s)\|_2\Big).$$

With $\epsilon = \delta/2K$, if $\|y - Y\|_2 \le \epsilon$ and $\sup_{0\le s\le T} \|U(s) - \tilde{W}(s)\|_2 \le \epsilon$, then $\|x(T) - X(T)\|_2 \le \delta$. We now translate this into a statement for the DPD system (1.1). Define $\beta_{ij}(t)$ by

$$d\tilde{\beta}_{ij}(t) = \theta_{ij}(t)\, dt + d\beta_{ij}(t), \qquad \theta_{ij}(s) = \begin{cases} \dfrac{a_{ij}}{\sigma W^R(|q_{ij}(s)|)} \dfrac{\partial V(|q_{ij}(s)|)}{\partial q_i}, & |q_{ij}(s)| < r_c, \\ 0, & \text{otherwise.} \end{cases}$$

and $W(t) = (\beta_{12}, \dots, \beta_{23})^T$. Then $W(t)$ is a Brownian motion under the measure $\mathbf{P}$ defined by $\mathbf{P}(A) = \tilde{\mathbf{E}}(\mathbf{1}_A(W) Z_t)$, where $Z_t = \prod_{i<j} Z_{ij}(t)$ and

$$Z_{ij}(t) = \exp\Big\{ \int_0^t \theta_{ij}(s)\, d\tilde{\beta}_{ij}(s) - \frac{1}{2}\int_0^t \theta_{ij}(s)^2\, ds \Big\}.$$

Further under this measure, $x(t)$ is a (weak) solution of DPD (1.1) and to complete the proof we estimate the probability of $\sup_{0\le t\le T} \|\tilde{W}(t) - U(t)\|_2 \le \epsilon$ under $\mathbf{P}$.

Clearly, $\theta_{ij}(s)$ is bounded above Assumption 1.1(ii) and by the Itô Isometry

$$\tilde{\mathbf{E}}\Big[\Big|\int_0^t \theta_{ij}(s)\, d\tilde{\beta}_{ij}(s)\Big|^2\Big] \le \frac{a_{ij}}{\sigma^2} \sup_{0\le q<r_c} \frac{|V'(q)|^2}{|W^R(q)|^2} t.$$

Let p_* be a lower bound for $\tilde{\mathbf{P}}(\sup_{0\le t\le T} \|U(t) - \tilde{W}(t)\|_2 \le \epsilon)$ and choose Z_* suitably small that

$$\tilde{\mathbf{P}}\Big(\int_0^T \theta_{ij}(s)\, d\tilde{\beta}_{ij}(s) - \frac{1}{2}\int_0^T \theta_{ij}(s)^2\, ds > \log Z_*\Big) \ge 1 - p_*/2$$

(using Chebyshev inequality). Hence, $\tilde{\mathbf{P}}(Z_T \ge Z_*) \ge 1 - p_*/2$ and $\tilde{\mathbf{P}}(\sup_{0\le t\le T} \|U(t) - \tilde{W}(t)\|_2 \le \epsilon) \ge p_*$, which means that

$$\mathbf{P}\Big(\sup_{0\le t\le T} \|U(t) - \tilde{W}(t)\|_2 \le \epsilon\Big) = \tilde{\mathbf{E}}\Big[Z_T \mathbf{1}_{\sup_{0\le t\le T} \|U(t) - \tilde{W}(t)\|_2 \le \epsilon}\Big] \ge Z_* p_*/2.$$

Therefore, $x(T) \in B_\delta(\bar{y})$ with a positive probability, uniform over choice of initial data $y \in B_\epsilon(Y)$. By compactness of C, we can find a $\eta > 0$ such that $P_T(y, B_\delta(\bar{y})) \ge \eta$ for all $y \in C$. *QED*

Proof [of Theorem 3.2] By Theorem 3.1, there exist $T_1, \eta_1 > 0$, $C = \bar{B}_\delta(\bar{y})$, some $\delta > 0$ and $\bar{y} \in M$, and a probability measure ν on S such that

$$P_{T_1}(z, A) \ge \eta_1 \nu(A), \quad \forall\, z \in C,\ A \in \mathcal{B}(S).$$

By Lemma 3.7, we see that there exists $T_2 > 0$ such that for some $\eta_2 > 0$

$$P_{T_2}(y, C) \ge \eta_2, \quad \forall\, y \in C',$$

since C' is a compact set. Thus we have, with $T = T_1 + T_2$ and $y \in C'$,

$$\begin{aligned} P_T(y, A) &= \int_S P_{T_2}(y, dz) P_{T_1}(z, A) \\ &\ge \int_C P_{T_2}(y, dz) P_{T_1}(z, A) \\ &\ge \eta_1 \nu(A) \int_C P_{T_2}(y, dz) \\ &= \eta_1 \nu(A) P_{T_2}(y, C) \\ &\ge \eta_1 \eta_2 \nu(A) = \eta \nu(A). \end{aligned}$$

The proof is complete. *QED*

4 The drift condition

We prove the drift condition for $\mathcal{V}(y) = 1 + H(y)$, where $H(y)$ is defined by (1.3). We use $\mathcal{V}_t$ to denote $\mathcal{V}(x(t))$ and unless otherwise indicated p_i, q_i, etc. are evaluated at time t.

Theorem 4.1 *Let $x(t) = (q_1, \dots, q_N, p_1, \dots, p_N)$ denote the solution of (3.1) with initial data $x(0) = y \in S$. Then there exist $T, \alpha, \beta > 0$ such that*

$$\mathbf{E}\mathcal{V}_T - \mathcal{V}_0 \le -\alpha \mathcal{V}_0 + \beta, \quad \forall y \in S. \tag{4.1}$$

The proof will be built up from a series of Lemmas. The most important ones are included in this section; the more technical are left to the Appendix. The basic identity that we exploit is

Lemma 4.2

$$\frac{d}{dt}\mathbf{E}\mathcal{V}_t = \frac{1}{2}\sum_{i,j=1, i\neq j}^{N} \mathbf{E}W^D(|q_{ij}|)(\sigma^2 - \gamma p_{ij}^2). \tag{4.2}$$

For $\beta = \frac{1}{2}N^2\sigma^2$,

$$\mathbf{E}\mathcal{V}_t \le \mathcal{V}_0 + \beta t. \tag{4.3}$$

Proof Applying the Itô formula to $\frac{1}{2}\sum_{i=1}^N p_i^2$, we have

$$\begin{aligned} d\Big(\frac{1}{2}\sum_{i=1}^N p_i^2\Big) &= \sum_{i=1}^N p_i\Big(-\sum_{j=1,j\neq i}^N a_{ij}\frac{\partial V(|q_{ij}|)}{\partial q_i} - \gamma\sum_{j=1,j\neq i}^N W^D(|q_{ij}|)p_{ij}\Big)dt \\ &\quad + \sum_{i=1}^N p_i\Big(\sigma\sum_{j=1,j\neq i}^N W^R(|q_{ij}|)d\beta_{ij}\Big) + \frac{1}{2}\sum_{i,j=1}^N(\Sigma\Sigma^T)_{ij}\frac{\partial^2\big(\sum_{i=1}^N p_i^2\big)}{\partial p_i\partial p_j}dt \\ &= -\sum_{i,j=1,i\neq j}^N p_i a_{ij}\frac{\partial V(|q_{ij}|)}{\partial q_i}dt - \gamma\sum_{i,j=1,i\neq j}^N p_i W^D(|q_{ij}|)p_{ij}dt \\ &\quad + \sigma\sum_{i,j=1,i\neq j}^N p_i W^R(|q_{ij}|)d\beta_{ij} + \frac{1}{2}\sum_{i=1}^N(\Sigma\Sigma^T)_{ii}dt \\ &= I + II + III + IV. \end{aligned} \tag{4.4}$$

Note that, since $\dfrac{\partial V(|q_{ij}|)}{\partial q_i} = -\dfrac{\partial V(|q_{ij}|)}{\partial q_j}$ and $p_{ij} = -p_{ji}$,

$$I = -\frac{1}{2}\sum_{i,j=1,i\neq j}^N p_{ij}a_{ij}\frac{\partial V(|q_{ij}|)}{\partial q_i}dt = -\frac{1}{2}\sum_{i,j=1,i\neq j}^N a_{ij}dV(|q_{ij}|),$$

where we use

$$\begin{aligned} \frac{dV(|q_{ij}|)}{dt} &= \frac{\partial V(|q_{ij}|)}{\partial q_i}\frac{dq_i}{dt} + \frac{\partial V(|q_{ij}|)}{\partial q_j}\frac{dq_j}{dt} \\ &= (p_i - p_j)\frac{\partial V(|q_{ij}|)}{\partial q_i} = p_{ij}\frac{\partial V(|q_{ij}|)}{\partial q_i}. \end{aligned}$$

Further we have

$$II = -\gamma\sum_{i,j=1,i\neq j}^N p_i W^D(|q_{ij}|)p_{ij}dt = -\frac{1}{2}\gamma\sum_{i,j=1,i\neq j}^N p_{ij}W^D(|q_{ij}|)p_{ij}dt.$$

Taking expectations of (4.4), we get, noting that $\mathbf{E}III = 0$ and $(\Sigma\Sigma^T)_{ii} = \sigma^2 \sum_{i,j=1,i\neq j}^N W^R(|q_{ij}|)^2$,

$$\mathbf{E}d\Big(\sum_{i=1}^N \frac{1}{2}p_i^2\Big) = -\frac{1}{2}\sum_{i,j=1,i\neq j}^N a_{ij}\mathbf{E}dV(|q_{ij}|) - \frac{\gamma}{2}\mathbf{E}\sum_{i,j=1,i\neq j}^N p_{ij}W^D(|q_{ij}|)p_{ij}\,dt + \frac{\sigma^2}{2}\mathbf{E}\sum_{i,j=1,i\neq j}^N W^R(|q_{ij}|)^2 dt. \tag{4.5}$$

Moving the first term of the right hand side to the left in (4.5), we obtain (4.2). The second statement follows by integration and Assumption 1.1(i). The proof is complete. *QED*

The main work is done in the next two lemmas. The difficulty in proving the drift condition for DPD is that fast moving particles may not dissipate energy if they are separated from other particles ($|q_{ij}| > r_c$). To guarantee dissipation, we look at times at which particles collide in the following sense.

Definition 4.3 We say that two particles i and j collide at time t if $q_i(t) = q_j(t)$ and $p_i(t)\,p_j(t) < 0$.

The behaviour of the energy can be seen in Figure 2. We choose a configuration where the particles are well separated to demonstrate how $H(x(t))$ decreases in steps at times of collision.

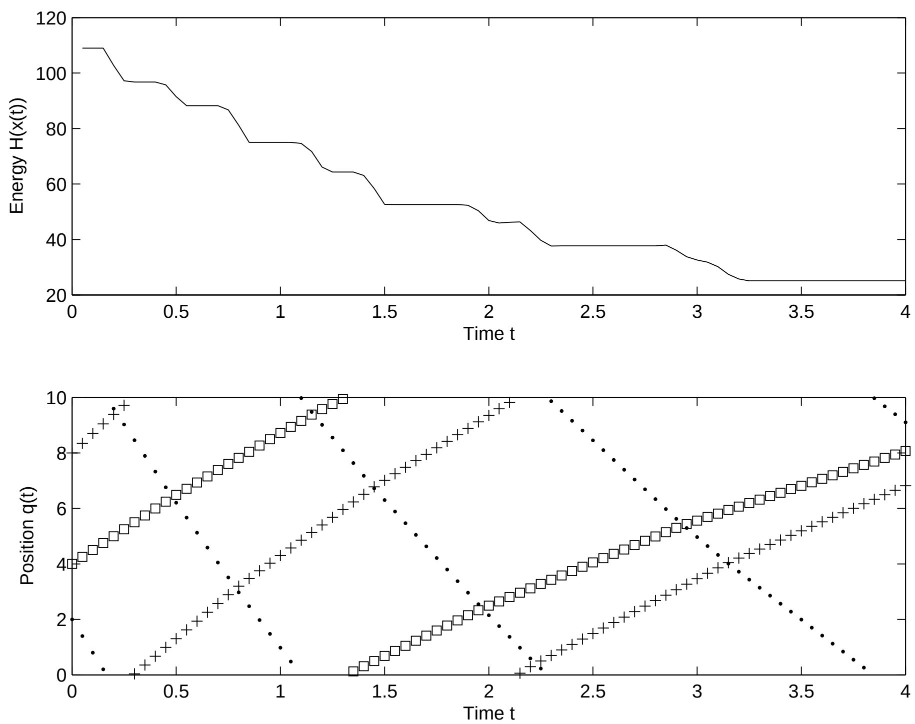

Figure 2: Plots of $H(x(t))$ and $q_i(t)$ for initial data $(2, 4, 8, -12, 5, 7)$. Parameter values $L = 10$, $\gamma = \sigma = 1$, $a_{ij} = 0$, $r_c = 1$, and W^D defined by (1.2).

If fast moving particles collide, a drift condition of the following type is available.

Lemma 4.4 *Fix $\mu > 0$. Suppose that particles 1 and 2 collide at time $t = 0$ (in the sense of Definition 4.3) and that $p_{12}^2(0) \geq \mu\mathcal{V}_0$. There exist constants $\alpha, \beta, \ell_0 > 0$ such that if $\|y\|_\infty > 1$ then*

$$\mathbf{E}\mathcal{V}_{\Delta t} \leq (1 - \alpha\Delta t)\mathcal{V}_0 + \beta\Delta t, \qquad \forall \Delta t \in (0, \ell_0/\|y\|_\infty]. \tag{4.6}$$

Proof By Lemma 4.2,

$$\frac{d}{dt}\mathbf{E}\mathcal{V}_t = \frac{1}{2}\sum_{i,j=1\, i\neq j}^N \mathbf{E}W^D(|q_{ij}|)(\sigma^2 - \gamma p_{ij}^2) \leq \beta - \frac{1}{2}\gamma\mathbf{E}W^D(|q_{12}|)p_{12}^2,$$

where $\beta = N^2\sigma^2/2$. We shall show that, with some $K_0, \gamma_0 > 0$,

$$\mathbf{E}W^D(|q_{12}|)p_{12}^2 \geq \gamma_0 \mathbf{E}\mathcal{V}_t, \quad 0 \leq t \leq K_0 \frac{\mathcal{V}_0}{\|y\|_\infty^3}. \tag{4.7}$$

Assuming this for the moment,

$$\frac{d}{dt}\mathbf{E}\mathcal{V}_t \leq \beta - \alpha \mathbf{E}\mathcal{V}_t, \tag{4.8}$$

for $\alpha = \gamma\gamma_0/2$ and $0 \leq t \leq K_0\mathcal{V}_0/\|y\|_\infty^3$. Let $\ell_0 = \inf K_0\mathcal{V}_0/\|y\|_\infty^2$ over $y \in S$ with $\|y\|_\infty \geq 1$, which is positive by definition of $\mathcal{V}_0$. Integration of (4.8) over time $\Delta t \leq \ell_0/\|y\|_\infty$ now implies (4.6). It remains to show (4.7). Using Assumption 1.1(iii)

$$W^D(|q_{12}(0)|)p_{12}(0)^2 \geq \mu\mathcal{V}_0.$$

By Lemma A.6 and using $\|y\|_\infty > 1$, for some $K > 1$,

$$\begin{aligned}\mathbf{E}W^D(|q_{12}|)p_{12}^2 &\geq W^D(|q_{12}(0)|)p_{12}(0)^2 - Kt\|y\|_\infty^3 \\ &\geq \mu\mathcal{V}_0 - \tfrac{1}{2}\mu\mathcal{V}_0\end{aligned} \tag{4.9}$$

for $0 \leq t \leq \mu\mathcal{V}_0/2K\|y\|_\infty^3$. On the other hand, by the linear growth condition (4.3),

$$\mathbf{E}\mathcal{V}_t \leq \mathcal{V}_0 + \beta t \leq \mathcal{V}_0 + \beta\mu\mathcal{V}_0/2 \tag{4.10}$$

for $0 \leq t \leq \mu\mathcal{V}_0/2$. Note that $t \leq \frac{1}{2}\mu\mathcal{V}_0/K\|y\|_\infty^3$ implies $t \leq \mu\mathcal{V}_0/2$ since $\|y\|_\infty > 1$ and $K > 1$. From (4.9) and (4.10),

$$\mathbf{E}W^D(|q_{12}(t)|)p_{12}(t)^2 \geq \tfrac{1}{2}\mu\mathcal{V}_0 \geq \frac{\frac{1}{2}\mu}{(1+\beta\mu/2)}\mathbf{E}\mathcal{V}_t,$$

and we get (4.7) with $K_0 = \mu/2K$ and $\gamma_0 = \mu/(2+\beta\mu)$. *QED*

The previous lemma only provides a drift condition under special circumstances, that two particles with large energy ($p_{12}^2(0) \geq \mu\mathcal{V}_0$) are colliding (in the sense of Definition 4.3), and this drift condition will not hold in general. We may have to wait longer for two particles to collide and dissipate energy. To describe this process, we introduce t^* to describe the maximum length of time needed for a fast moving particle to collide and Δt to describe the length of time for which the collision will dissipate energy. To make this precise for N particles, choose $\kappa \in (0,1)$ and $\mu > 0$ such that

$$\kappa\frac{1+\kappa}{1-\kappa} \leq \frac{1}{2(N-1)} \quad \text{and} \quad \mu = \frac{(1-\kappa)^2}{9(1+\kappa)^2 N}. \tag{4.11}$$

Let ℓ_0 be as in Lemma 4.4. Define

$$\Delta t = \frac{2\ell_0}{3\|y\|_\infty(1+\kappa)} \qquad \text{and} \qquad t^* = \frac{2L}{(1-\kappa)\|y\|_\infty} \tag{4.12}$$

and $t_i = i(t^* + \Delta t)$. If the particle has sufficient energy at t_i, we show there is a significant chance of a collision before $t_i + t^*$ at which Lemma 4.4 applies. Crucially though both time intervals depend on the initial data y, the ratio of Δt to t^* is fixed and we can sum to achieve the drift condition over a fixed time interval.

Lemma 4.5 *Let $T = T_0(\kappa)$, where $T_0(\kappa)$ is given by Lemma A.5. Define $N_c := \lfloor T/(t^* + \Delta t)\rfloor$, where $\lfloor t\rfloor$ denotes the largest integer less than t. There exists $\alpha, \beta, R_c > 0$ such that for $\|y\|_\infty > R_c$*

$$\mathbf{P}\Big((1-\kappa)\|y\|_\infty \leq \|x(t_i)\|_\infty \leq (1+\kappa)\|y\|_\infty, \quad i = 1, \dots, N_c\Big) \geq \frac{1}{2} \tag{4.13}$$

and for $i = 0, \dots, N_c - 1$, if $(1-\kappa)\|y\|_\infty \leq \|x(t_i)\|_\infty \leq (1+\kappa)\|y\|_\infty$, then

$$\mathbf{E}\Big[\mathcal{V}_{t_{i+1}}|\mathcal{F}_{t_i}\Big] \leq (1 - \alpha\,\Delta t)\mathcal{V}_{t_i} + \beta(t^* + \Delta t). \tag{4.14}$$

Proof By choosing $\|y\|_\infty > L$, we can assume that $\|y\|_\infty = p_1(0)$ without loss of generality. By Lemma A.5, if $\|y\|_\infty > 1$,

$$\mathbf{P}\Big(\sup_{0\le t\le T}\|x(t)-y\|_\infty \le \kappa\|y\|_\infty = \kappa p_1(0)\Big) \ge \frac{1}{2}. \tag{4.15}$$

For sample paths $x(t)$ that satisfy

$$\sup_{0\le t\le T}\|x(t)-y\|_\infty \le \kappa p_1(0) \tag{4.16}$$

we have $(1-\kappa)\|y\|_\infty \le x(t) \le (1+\kappa)\|y\|_\infty$ and hence (4.13) holds as $t_i \le T$ for $i = 1,\dots,N_c$.

To develop (4.14), we show that

$$\mathbf{E}\mathcal{V}_{t^*+\Delta t} \le (1-\alpha\Delta t)\mathcal{V}_0 + \beta(t_* + \Delta t), \tag{4.17}$$

if $(1-\kappa)\|y\|_\infty \le \|x(0)\|_\infty \le (1+\kappa)\|y\|_\infty$. In this case, we do not assume $x(0) = y$. (4.17) implies (4.14) by the Markov property if we prove (4.17) under this weaker condition on $x(0)$.

Using the hypothesis on $\|x(0)\|_\infty$ and Lemma A.5, we gain bounds on $\|x(t)\|_\infty$ on the time interval $[0,T]$: particularly, with probability at least $1/2$, using (4.11),

$$\|x(t)-x(0)\|_\infty \le \kappa\|x(0)\|_\infty \le \kappa(1+\kappa)\|y\|_\infty \le \frac{1-\kappa}{2(N-1)}\|y\|_\infty \tag{4.18}$$

for $0 \le t \le T$. Again assuming that $p_1(0) = \|x(0)\|_\infty$ and using $p_2 + \cdots + p_N = -p_1$, we gain for some particle j

$$p_j(0) \le -\frac{p_1(0)}{N-1} \le \frac{-(1-\kappa)}{N-1}\|y\|_\infty < 0.$$

Under (4.18),

$$\begin{aligned}\frac{1}{2}(1-\kappa)\|y\|_\infty &\le |p_1(0)| - |p_1(t)-p_1(0)| \le p_1(t)\\ &\le |p_1(0)| + |p_1(t)-p_1(0)| \le \frac{3}{2}(1+\kappa)\|y\|_\infty. \end{aligned}\tag{4.19}$$

Thus, particle 1 approaches particle particle j with speed at least $(1-\kappa)\|y\|_\infty/2$ and $p_1(t)p_j(t) < 0$ on $[0,T]$. As the maximum initial separation of the two particles is L and as $t^* = 2L/(1-\kappa)\|y\|_\infty < T$ for R_c large, this yields a collision at a time $\tau_c \in (0, t^*]$ with

$$\|x(\tau_c)\|_\infty \le \|x(0)\|_\infty + \|x(\tau_c)-x(0)\|_\infty \le (1+\kappa)\|y\|_\infty + \frac{1}{2}(1-\kappa)\|y\|_\infty$$

by using (4.18). In particular,

$$\|y\|_\infty^2 \ge \frac{4}{9}\frac{1}{(1+\kappa)^2}\|x(\tau_c)\|_\infty^2.$$

Choose R_c large enough that $\mathcal{V}(x) \le \|(p_1(0),\dots,p_N(0))\|_2^2$ if $\|x\|_\infty \ge R_c$ (possible by boundedness of V). Then, $\mathcal{V}_{\tau_c} \le N\|x(\tau_c)\|_\infty^2$ and

$$\frac{1}{4}(1-\kappa)^2\|y\|_\infty^2 \ge (1-\kappa)^2\frac{\|x(\tau_c)\|_\infty^2}{9(1+\kappa)^2} \ge \frac{(1-\kappa)^2}{9(1+\kappa)^2N}\mathcal{V}_{\tau_c}.$$

We have shown that $p_{1j}^2(\tau_c) \ge \mu\mathcal{V}_{\tau_c}$, with μ defined by (4.11), which is one of the conditions of Lemma 4.4.

Let $\tau \ge 0$ be the smallest time such that particles i and j (some i,j) collide at time τ with $|p_{ij}(\tau)|^2 \ge \mu V_\tau$ and

$$\|x(\tau)\|_\infty \le \frac{3}{2}(1+\kappa)\|y\|_\infty.$$

This is a stopping time. Let A denote the set where $\tau \le t^*$. Clearly $\tau \le \tau_c$ and the probability of event A is bigger than $1/2$. For samples in A, the strong Markov property and Lemma 4.4 imply

$$\mathbf{E}\Big[\mathcal{V}_{\tau+\Delta t}|\mathcal{F}_\tau\Big] \le (1-\alpha\Delta t)\mathcal{V}_\tau + \beta\Delta t \tag{4.20}$$

with $\Delta t = 2\ell_0/3(1+\kappa)\|y\|_\infty$.

Outside the event A, we may not find a suitable collision in $[0,t^*]$ and the best estimate is provided by the linear growth condition (4.3):

$$\mathbf{E}\Big[\mathcal{V}_{(\tau\wedge t^*)+\Delta t}|\mathcal{F}_{\tau\wedge t^*}\Big] \le \mathcal{V}_{\tau\wedge t^*} + \beta\Delta t. \tag{4.21}$$

Clearly,

$$\mathbf{E}\Big[\mathcal{V}_{(\tau\wedge t^*)+\Delta t}|\mathcal{F}_{\tau\wedge t_*}\Big] = \mathbf{E}\Big[1_A\mathcal{V}_{(\tau\wedge t^*)+\Delta t}|\mathcal{F}_{\tau\wedge t_*}\Big] + \mathbf{E}\Big[1_{A'}\mathcal{V}_{(\tau\wedge t^*)+\Delta t}|\mathcal{F}_{\tau\wedge t_*}\Big].$$

Using the two inequalities (4.20)–(4.21) and as $A \in \mathcal{F}_{\tau\wedge t^*}$,

$$\mathbf{E}\Big[\mathcal{V}_{(\tau\wedge t^*)+\Delta t}|\mathcal{F}_{\tau\wedge t_*}\Big] \le 1_A(1-\alpha\Delta t)\mathcal{V}_\tau + 1_{A'}\mathcal{V}_{\tau\wedge t^*} + \beta\Delta t. \tag{4.22}$$

By linear growth condition (4.3),

$$\mathbf{E}\Big[\mathcal{V}_{t^*+\Delta t}|\mathcal{F}_{(\tau\wedge t^*)+\Delta t}\Big] = \mathcal{V}_{(\tau\wedge t^*)+\Delta t} + \beta\Big[t^* - (\tau\wedge t^*)\Big]. \tag{4.23}$$

Averaging from (4.22)–(4.23),

$$\mathbf{E}\Big[\mathcal{V}_{t^*+\Delta t}|\mathcal{F}_{\tau\wedge t_*}\Big] \le 1_A(1-\alpha\Delta t)\mathcal{V}_{\tau\wedge t_*} + 1_{A'}\mathcal{V}_{\tau\wedge t_*} + \beta\Big[t^* + \Delta t - (\tau\wedge t^*)\Big]$$

and

$$\begin{aligned}\mathbf{E}\mathcal{V}_{t^*+\Delta t} &\le \mathbf{E}\Big[1_A(1-\alpha\Delta t)\mathcal{V}_{\tau\wedge t^*}\Big] + \mathbf{E}\Big[1_{A'}\mathcal{V}_{\tau\wedge t^*}\Big] + \beta\Big[(t^*+\Delta t) - \mathbf{E}(\tau\wedge t^*)\Big]\\ &\le \mathbf{E}\mathcal{V}_{\tau\wedge t^*} - \alpha\,\Delta t\,\mathbf{E}\Big[1_A\mathcal{V}_{\tau\wedge t^*}\Big] + \beta\Big[t^* + \Delta t - \mathbf{E}(\tau\wedge t^*)\Big].\end{aligned}$$

Note that $\mathbf{E}\mathcal{V}_{\tau\wedge t^*} = \mathbf{E}1_A\mathcal{V}_{\tau\wedge t^*} + \mathbf{E}1_{A'}\mathcal{V}_{\tau\wedge t^*}$, which implies, by the Hölder inequality, that

$$\mathbf{E}\Big[1_A\mathcal{V}_{\tau\wedge t^*}\Big] \ge \mathbf{E}\Big[\mathcal{V}_{\tau\wedge t^*}\Big] - P(A')^{1/2}\Big[\mathbf{E}\mathcal{V}^2_{\tau\wedge t_*}\Big]^{1/2}.$$

By Lemma A.8 and the optional stopping theorem, for some $K>0$,

$$\Big[\mathbf{E}\mathcal{V}^2_{\tau\wedge t^*}\Big]^{1/2} \le \mathcal{V}_0 e^{Kt^*}.$$

Thus,

$$\mathbf{E}1_A\mathcal{V}_{\tau\wedge t^*} \ge \mathbf{E}\mathcal{V}_{\tau\wedge t^*} - P(A')^{1/2}\mathcal{V}_0 e^{Kt^*}.$$

Further, by linear growth condition,

$$\mathbf{E}\mathcal{V}_{\tau\wedge t^*} \le \mathcal{V}_0 + \beta\mathbf{E}(\tau\wedge t^*).$$

Hence,

$$\begin{aligned}\mathbf{E}\mathcal{V}_{t^*+\Delta t} &\le \mathbf{E}\mathcal{V}_{\tau\wedge t^*} - \alpha\Delta t\Big(\mathbf{E}\mathcal{V}_{\tau\wedge t^*} - P(A')^{1/2}\mathcal{V}_0 e^{Kt^*}\Big) + \beta\Big(t^* + \Delta t - \mathbf{E}(\tau\wedge t^*)\Big)\\ &\le (1-\alpha\Delta t)\Big(\mathcal{V}_0 + \beta\mathbf{E}(\tau\wedge t^*)\Big) + P(A')^{1/2}\mathcal{V}_0 e^{Kt^*}\alpha\Delta t\\ &\quad + \beta\Big(t^* + \Delta t - \mathbf{E}(\tau\wedge t^*)\Big)\\ &= (1-\alpha\Delta t/4)\mathcal{V}_0 + \alpha\,\Delta t\,\mathcal{V}_0\Big(P(A')^{1/2}e^{Kt^*} - 3/4\Big) + \beta(t^*+\Delta t).\end{aligned}$$

As $P(A') \le \frac{1}{2}$, for sufficiently small t_*, we have $P(A')^{1/2}e^{Kt_*} - 3/4 < 0$. Hence, increasing R_c if necessary, we gain

$$\mathbf{E}\mathcal{V}_{t^*+\Delta t} \le (1-\alpha\Delta t/4)\mathcal{V}_0 + \beta(t^*+\Delta t),$$

which shows (4.17). The proof of (4.14) is complete with $\alpha \mapsto \alpha/4$. *QED*

Lemma 4.6 *With Δt defined by (4.12) and $N_c := \lfloor T/(t^* + \Delta t)\rfloor$, there exists $\lambda > 0$ such that*

$$\Big(1 - \frac{\alpha\Delta t}{4}\Big)^{N_c} \to \exp(-\alpha\lambda T) \quad \text{as } \|y\|_\infty \to \infty.$$

Proof Let $\lambda = \Delta t/(\Delta t + t^*)$. For simplicity, suppose that $N_c(t^* + \Delta t) = T$. Then $\Delta t = \lambda T/N_c$ and

$$\Big(1 - \frac{\alpha\Delta t}{4}\Big)^{N_c} = \Big(1 - \frac{\alpha\lambda T}{N_c}\Big)^{N_c} \to \exp(-\alpha\lambda T),$$

as $N_c \to \infty$, which is implied by the limit $\|y\|_\infty \to \infty$ by (4.12). *QED*

Lemma 4.7 *There exists $R_c, T > 0$ such that for $\|y\|_\infty > R_c$ and $N_c = \lfloor T/(t^* + \Delta t)\rfloor$*

$$\mathbf{E}\mathcal{V}_{t_{N_c}} \le \Big(1 - \frac{\alpha\,\Delta t}{4}\Big)^{N_c}\mathcal{V}_0 + \beta t_{N_c}. \tag{4.24}$$

Proof From (4.14),

$$\mathbf{E}\mathcal{V}_{t_1} \le (1 - \alpha\Delta t)\mathcal{V}_0 + \beta t_1.$$

We prove the following inductively:

$$\mathbf{E}\mathcal{V}_{t_k} \le (1 - \alpha\Delta t/4)^k\mathcal{V}_0 + \beta t_k.$$

It is true for $k = 1$. Let A denote the event $(1-\kappa)\|y\|_\infty \le \|x(t_k)\|_\infty \le (1+\kappa)\|y\|_\infty$. By Lemma 4.5 and the linear growth condition (4.3), with ω parameterising the sample,

$$\mathbf{E}[\mathcal{V}_{t_{k+1}}|\mathcal{F}_{t_k}] \le \begin{cases} (1-\alpha\,\Delta t)\mathcal{V}_{t_k} + \beta(t_{k+1} - t_k), & \omega \in A,\\ \mathcal{V}_{t_k} + \beta(t_{k+1} - t_k), & \omega \in A'. \end{cases}$$

Average this inequality:

$$\begin{aligned} \mathbf{E}\mathcal{V}_{t_{k+1}} &\le \mathbf{E}[1_A(1-\alpha\Delta t)\mathcal{V}_{t_k}] + \mathbf{E}[1_{A'}\mathcal{V}_{t_k}] + \beta(t_{k+1} - t_k)\\ &\le \mathbf{E}\mathcal{V}_{t_k} - \alpha\Delta t\mathbf{E}[1_A\mathcal{V}_{t_k}] + \beta(t_{k+1} - t_k). \end{aligned}$$

Note that

$$\mathbf{E}\mathcal{V}_{t_k} \le \mathbf{E}[1_A\mathcal{V}_{t_k}] + P(A')^{1/2}\mathbf{E}[\mathcal{V}_{t_k}^2]^{1/2}$$

and by Lemma A.8

$$\mathbf{E}[\mathcal{V}_{t_k}^2]^{1/2} \le \mathcal{V}_0 e^{KT}.$$

Then,

$$\begin{aligned} \mathbf{E}\mathcal{V}_{t_{k+1}} &\le \mathbf{E}\mathcal{V}_{t_k} - \alpha\Delta t\mathbf{E}\mathcal{V}_{t_k} + P(A')^{1/2}\mathcal{V}_0 e^{KT}\alpha\Delta t + \beta(t_{k+1} - t_k)\\ &\le (1-\alpha\Delta t/4)(1-\alpha\Delta t/4)^k\mathcal{V}_0 - 3\alpha\Delta t/4(1-\alpha\Delta t/4)^k\mathcal{V}_0\\ &\quad + P(A')^{1/2}\mathcal{V}_0 e^{KT}\alpha\Delta t + \beta(t_{k+1} - t_k)\\ &= (1-\alpha\Delta t/4)(1-\alpha\Delta t/4)^k\mathcal{V}_0\\ &\quad + \alpha\Delta t\mathcal{V}_0\Big[-\frac{3}{4}(1-\alpha\Delta t/4)^k + P(A')^{1/2}e^{KT}\Big] + \beta t_{k+1}. \end{aligned}$$

Because $P(A) \ge 1/2$ and Lemma 4.6 holds, for sufficiently small Δt and T, we have $-\frac{3}{4}(1-\alpha\Delta t/4)^k + P(A')^{1/2}e^{KT} < 0$. Consequently,

$$\mathbf{E}\mathcal{V}_{t_{k+1}} \le (1-\alpha\Delta t/4)^{k+1}\mathcal{V}_0 + \beta t_{k+1}.$$

Setting $k = N_c - 1$, this leads to

$$\mathbf{E}\mathcal{V}_{t_{N_c}} \le (1-\alpha\Delta t/4)^{N_c}\mathcal{V}_0 + \beta t_{N_c}.$$

The proof is complete. *QED*

Proof [of Theorem 4.1] Choose $T, R_c, N_c > 0$ as in Lemma 4.7. Then,

$$\mathbf{E}\mathcal{V}_{t_{N_c}} \le \Big(1 - \frac{\alpha\Delta t}{4}\Big)^{N_c}\mathcal{V}_0 + \beta t_{N_c}.$$

By Lemma 4.6, for R_c suitably large (and reducing λ if necessary)

$$\Big(1 - \frac{\alpha\Delta t}{4}\Big)^{N_c} \le 1 - \alpha\lambda T/2.$$

Hence, $\|y\|_\infty \ge R_c$ implies

$$\mathbf{E}\mathcal{V}_{t_{N_c}} \le (1-\alpha\lambda T/2)\mathcal{V}_0 + \beta t_{N_c}.$$

Using the linear growth condition (4.3), for $\|y\|_\infty \ge R_c$,

$$\mathbf{E}\mathcal{V}_T \le \mathbf{E}\mathcal{V}_{t_{N_c}} + \mathbf{E}\beta(T - t_{N_c}) \le (1-\alpha\lambda T/2)\mathcal{V}_0 + \beta T. \tag{4.25}$$

We still need to consider the case for $\|y\|_\infty \le R_c$. Note that $\mathcal{V}(y)$ is continuous, which implies that $\mathcal{V}(y)$ is bounded on $\|y\|_\infty \le R_c$; i.e., $|\mathcal{V}(y)| \le K_2$ for $\|y\|_\infty \le R_c$. With the linear growth condition, this implies for $\|y\|_\infty \le R_c$

$$\mathbf{E}\mathcal{V}_T \le \mathcal{V}_0 + \beta T \le (1-\alpha\lambda T/2)\mathcal{V}_0 + (K_2 + \beta T). \tag{4.26}$$

Finally, by (4.25) and (4.26), for any $y \in S$,

$$\mathbf{E}\mathcal{V}_T \le (1-\alpha\lambda T/2)V(y) + (\beta T + K_2),$$

which completes the proof of Theorem 4.1. *QED*

5 Proof of Theorem 1.2

Proof [of Theorem 1.2] By Theorem 4.1, we see that there exist $T, \alpha, \beta > 0$ such that

$$\mathbf{E}\mathcal{V}_T - \mathcal{V}_0 \le -\alpha\mathcal{V}_0 + \beta,$$

which implies that

$$\mathbf{E}\mathcal{V}_T - \mathcal{V}_0 \le -\frac{\alpha}{2}\mathcal{V}_0 - \frac{\alpha}{2}\mathcal{V}(y) + \beta \le -\frac{\alpha}{2}\mathcal{V}_0 + \beta\mathbf{1}_\Gamma(y),$$

where

$$\Gamma = \Big\{y \in S \colon \mathcal{V}(y) \le \frac{2\beta}{\alpha}\Big\}.$$

Since $L \le N r_c$, we find that for all $y \in S$ at least one pair of particles are separated by a distance less than r_c. Thus, the set $\Gamma \subset M' = \{|q_{ij}| < r_c \colon \text{ some } i \ne j\}$. By Theorem 3.3, the minorization condition holds for any compact subset of $S \cap \{|q_{12}| < r_c\}$. Therefore both the minorization condition (Assumption 2.1) and drift condition (Assumption 2.2) are fulfilled for the compact set Γ. Applying Theorem 2.3, we see the process $x(t)$ is geometrically ergodic with respect to $\mathcal{V}$. As $\mathcal{V}(y) \le K(1 + \|\boldsymbol{p}\|_2^2)$, we have proved Theorem 1.2. *QED*

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A Appendix

A.1 Lemmas for §3

Lemma A.1 *Suppose that* $U \in C^1([0,T], \mathbf{R}^{\frac{1}{2}N(N-1)})$*, that* f *and* Σ *are Lipschitz, that*

$$\frac{dX}{dt} = f(X) + \Sigma(X)U'(t), \qquad X(0) = Y$$

and that

$$dx = f(x)dt + \Sigma(x)dW(t), \qquad x(0) = y.$$

Then, for some $K > 0$,

$$\sup_{0\le t\le T} \|x(t) - X(t)\|_2 \le K\Big(\|y - Y\|_2 + \sup_{0\le s\le T} \|W(s) - U(s)\|_2\Big).$$

Proof In integral form,

$$x(t) = y + \int_0^t f(x(s))\, ds + \int_0^t \Sigma(x(s))\, dW(s),$$

$$X(t) = y + \int_0^t f(X(s))\, ds + \int_0^t \Sigma(X(s))\, dU(s).$$

Hence, we have, noting that f, Σ are Lipschitz and $U(t)$ is smooth,

$$\begin{aligned}
&\|x(t) - X(t)\|_2 \\
\leq &\|y - Y\|_2 + \int_0^t \|f(x(s)) - f(X(s))\|_2 \, ds \\
&+ \left\| \int_0^t \Sigma(x(s)) \, d(W(s) - U(s)) \right\|_2 + \left\| \int_0^t \Big(\Sigma(x(s)) - \Sigma(X(s)) \Big) \, dU(s) \right\|_2 \\
\leq &\|y - Y\|_2 + K \int_0^t \|x(s) - X(s)\|_2 \, ds + \left\| \int_0^t \Sigma(x(s)) \, d(W(s) - U(s)) \right\|_2.
\end{aligned}$$

As $\Sigma(x)$ only depends on position, which is continuous, integration by parts implies

$$\begin{aligned}
\left\| \int_0^t \Sigma(x(s)) \, d(W(s) - U(s)) \right\|_2 = &\left\| \Sigma(x(t))(W(t) - U(t)) - \int_0^t (W(s) - U(s)) \, d\Sigma(x(s)) \right\|_2 \\
\leq &K \sup_{0 \leq s \leq t} \|W(s) - U(s)\|_2.
\end{aligned}$$

Gronwall's Lemma completes the proof. *QED*

Lemma A.2 *Let $q, Q \in \mathcal{T}$ and let $p, P \in \mathbf{R}$. Let $T_0 > 0$ be arbitrary. Then, for any small $\epsilon > 0$ ($\epsilon \ll L$), there exists a twice continuously differentiable function $Q(t)$ such that*

- *(i)* $Q(0) = q$, $Q(T_0) = Q$, $Q'(0) = p$, *and* $Q'(T_0) = P$.
- *(ii)* $|Q(t) - \Phi(t)| < \epsilon$ *on* $[0, T_0]$, *where* $\Phi(t)$ *is the straight line through* $(0, q)$ *to* (T_0, Q), $\Phi(t) = q + (Q - q)t/T_0$.
- *(iii)* $\min\{p, P\} \leq Q'(t) \leq \max\{p, P\}$ *for* $0 \leq t \leq T_0$.

Proof Here we only consider the special case, $q = 0, Q = 0, p = 1, P = 1$. The proof for general case is the similar. In this case, we want to construct $Q(t)$ such that

$$Q(0) = Q(T_0) = 0, \tag{A.1}$$

$$Q'(0) = Q'(T_0) = 1, \tag{A.2}$$

$$|Q(t) - \Phi(t)| = |Q(t) - 0| = |Q(t)| < \epsilon. \tag{A.3}$$

To do this, we first construct $Q_1(t), t \in [0, \epsilon]$ such that

$$Q_1(0) = 0, \quad Q_1(\epsilon) = 0, \quad Q_1'(0) = 1, \quad Q_1'(\epsilon) = 0.$$

In fact, by standard interpolation method, we obtain $Q_1(t) = t(t - \epsilon)^3/\epsilon^3$, which has extreme value at point $t = \epsilon/4$. Thus we have

$$Q_1(t) \leq Q_1(\frac{\epsilon}{4}) < \epsilon, \quad 0 \leq t \leq \epsilon,$$

Similarly we can construct $Q_2(t),\ t \in [T_0 - \epsilon, T_0]$ such that

$$Q_2(T_0 - \epsilon) = Q_2(T_0) = 0, \quad Q_2'(T_0 - \epsilon) = 0, \quad Q_2'(T_0) = 1.$$

For example,

$$Q_2(t) = \frac{1}{\epsilon^3}(t - T_0)(t - T_0 + \epsilon)^3, \quad T_0 - \epsilon \leq t \leq T_0,$$

which has extreme value at point $t = T_0 - \epsilon/4$ so that

$$|Q_2(t)| \leq \left| Q_2(T_0 - \frac{\epsilon}{4}) \right| < \epsilon.$$

Define

$$Q(t) = \begin{cases} Q_1(t), & 0 \leq t \leq \epsilon, \\ 0, & \epsilon \leq t \leq T_0 - \epsilon, \\ Q_2(t), & T_0 - \epsilon \leq t \leq T_0. \end{cases}$$

$Q(t)$ is twice continuously differentiable and satisfies (A.1)–(A.3) *QED*

Lemma A.3 *For any $y^+, y \in M$ with $N = 3$ and any $T_1 > 0$, there exists a twice continuously differentiable function $Q(t), 0 \le t \le T_1$, which satisfies, with $X(t) = (Q(t), Q'(t))$ and $Q(t) = (Q_1(t), \dots, Q_3(t))$,*

$$X(0) = y, \quad X(T_1) = y^+, \tag{A.4}$$

$$Q_1''(t) + Q_2''(t) + Q_3''(t) = 0, \tag{A.5}$$

$$|Q_{12}(t)| = |Q_1(t) - Q_2(t)| < r_c, \quad |Q_{13}(t)| = |Q_1(t) - Q_3(t)| < r_c. \tag{A.6}$$

If $|y - y^+| < \delta$, some $\delta > 0$, then we can assure that $|X(t) - y^+| < 2\delta$ for $0 \le t \le T_1$.

Proof Write $y^+ = (Q_1^+, Q_2^+, Q_3^+, P_1^+, P_2^+, P_3^+)$ where, by the definition of M,

$$Q_1^+ + Q_2^+ + Q_3^+ = 3\ell, \quad P_1 + P_2 + P_3 = 0,$$
$$Q_i^+ \in \mathcal{T}, \quad |Q_1^+ - Q_2^+| < r_c, \quad |Q_1^+ - Q_3^+| < r_c.$$

Write $y = (q_1, q_2, q_3, p_1, p_2, p_3)$, so that

$$q_1 + q_2 + q_3 = 3\ell, \quad p_1 + p_2 + p_3 = 0,$$
$$q_i \in \mathcal{T}, \quad |q_1 - q_2| < r_c, \quad |q_1 - q_3| < r_c.$$

We shall find $Q(t) = (Q_1(t), Q_2(t), Q_3(t))$ such that (A.4)–(A.6) hold. As the first step, we construct $\tilde{Q}_i(t), i = 1, 2, 3$ which satisfy (A.4) and (A.6). Define

$$\tilde{\Phi}_i(t) = q_i + \frac{Q_i^+ - q_i}{T_1} t, \quad 0 \le t \le T_1, \quad i = 1, 2, 3. \tag{A.7}$$

For any $\epsilon > 0$, by Lemma A.2, there exist twice continuously differentiable functions $\tilde{Q}_i(t)$ such that

$$\tilde{Q}_i(0) = q_i, \quad \tilde{Q}_i'(0) = p_i,$$
$$\tilde{Q}_i(T_1) = Q_i^+, \quad \tilde{Q}_i'(T_1) = P_i^+,$$
$$|\tilde{Q}_i(t) - \tilde{\Phi}_i(t)| < \epsilon, \quad 0 \le t \le T_1, \ i = 1, 2, 3.$$

It is easy to see that $\tilde{Q}_i(t), i = 1, 2, 3$ satisfy (A.4) and (A.6). (A.4) is clear and for (A.6) we have, for sufficiently small $\epsilon > 0$,

$$\begin{aligned} |\tilde{Q}_1(t) - \tilde{Q}_2(t)| &\le |\tilde{Q}_1(t) - \tilde{\Phi}_1(t)| + |\tilde{\Phi}_1(t) - \tilde{\Phi}_2(t)| + |\tilde{\Phi}_2(t) - \tilde{Q}_2(t)| \\ &\le 2\epsilon + |\tilde{\Phi}_1(t) - \tilde{\Phi}_2(t)| < r_c, \end{aligned}$$

for $0 \le t \le T_1$, where we used the fact that $|\tilde{\Phi}_1(t) - \tilde{\Phi}_2(t)| < r_c$ for $0 \le t \le T_1$ as the endpoints of the two straight lines are separated by less than r_c. Similarly, we can show that $|\tilde{Q}_1(t) - \tilde{Q}_3(t)| < r_c$ for $0 \le t \le T_1$ and ϵ small. This provides $|y - y^+| < \delta$ implies that $|X(t) - y^+| < 2\delta$, if we take $\epsilon < \delta$.

To guarantee that (A.5) also holds, we define

$$Q_i(t) = \tilde{Q}_i(t) - \frac{\tilde{Q}_1(t) + \tilde{Q}_2(t) + \tilde{Q}_3(t)}{3} + \ell.$$

We then claim that $Q_i(t)$ satisfy (A.4)–(A.6). In fact, (A.4) follows by

$$Q_i(0) = \tilde{Q}_i(0) - \frac{\tilde{Q}_1(0) + \tilde{Q}_2(0) + \tilde{Q}_3(0)}{3} + \ell = \tilde{Q}_i(0) = q_i,$$
$$Q_i(T_1) = \tilde{Q}_i(T_1) - \frac{\tilde{Q}_1(T_1) + \tilde{Q}_2(T_1) + \tilde{Q}_3(T_1)}{3} + \ell = \tilde{Q}_i(T_1) = Q_i^+,$$
$$Q_i'(0) = \tilde{Q}_i'(0) - \frac{\tilde{Q}_1'(0) + \tilde{Q}_2'(0) + \tilde{Q}_3'(0)}{3} = \tilde{Q}_i'(0) = p_i,$$
$$Q_i'(T_1) = \tilde{Q}_i'(T_1) - \frac{\tilde{Q}_1'(T_1) + \tilde{Q}_2'(T_1) + \tilde{Q}_3'(T_1)}{3} = \tilde{Q}_i'(T_1) = P_i^+,$$

and (A.6) follows by

$$|Q_1(t) - Q_2(t)| = |\tilde{Q}_1(t) - \tilde{Q}_2(t)|, \quad |Q_1(t) - Q_3(t)| = |\tilde{Q}_1(t) - \tilde{Q}_3(t)|,$$

and (A.5) follows as $Q_1(t) + Q_2(t) + Q_3(t) = 3\ell$. *QED*

Lemma A.4 *Consider $q_i, \bar{Q}_i \in \mathcal{T}$ and $p_i, \bar{P}_i \in \mathbf{R}$ for $i = 1, 2$ such that*

$$p_1 + p_2 = \bar{P}_1 + \bar{P}_2 \qquad (\bar{Q}_1 + \bar{Q}_2) - (q_1 + q_2) = (p_1 + p_2) T_2. \tag{A.8}$$

There exist twice continuously differentiable $Q_i(t), i = 1, 2$ for $0 \le t \le T_2$ such that

$$Q_i(0) = q_i, \quad Q_i'(0) = p_i, \tag{A.9}$$
$$Q_i(T_2) = \bar{Q}_i, \quad Q_i'(T_2) = \bar{P}_i, \tag{A.10}$$
$$|Q_1(t) - Q_2(t)| < r_c, \tag{A.11}$$
$$Q_1''(t) + Q_2''(t) = 0. \tag{A.12}$$

Proof We define the straight lines $Q_i(t)$ from $(0, q_i)$ to $(T_2, \bar{Q}_i)$ for $i = 1, 2$ by

$$\Phi_i(t) = q_i + \frac{\bar{Q}_i - q_i}{T_2} t. \tag{A.13}$$

For any $\epsilon > 0$, by Lemma A.2, there exist twice continuously differentiable functions $Q_i(t)$ such that

$$\begin{aligned} &Q_i(0) = q_i, \quad Q_i'(0) = p_i, \\ &Q_i(T_2) = \bar{Q}_i, \quad Q_i'(T_2) = \bar{P}_i, \\ &|Q_i(t) - \Phi_i(t)| < \epsilon, \quad 0 \le t \le T_2, \quad i = 1, 2. \end{aligned}$$

As the end points of the two straight lines are less than r_c apart, $|\Phi_1(t) - \Phi_2(t)| < r_c$ and for ϵ small

$$|Q_1(t) - Q_2(t)| < r_c, \quad 0 \le t \le T_2.$$

To guarantee that (A.12) also holds, we introduce $\tilde{Q}_i(t) = Q_i(t) - \bar{Q}(t)$ for $i = 1, 2$, where for $L_1 = \frac{1}{2}(q_1 + q_2)$ and $L_2 = \frac{1}{2}(\bar{Q}_1 + \bar{Q}_2)$ and

$$\bar{Q}(t) = \frac{(Q_1(t) + Q_2(t))}{2} - \Big(L_1 \frac{T_2 - t}{T_2} + \frac{L_2}{T_2} t \Big).$$

Clearly, $\bar{Q}(0) = \bar{Q}(T_2) = 0$ and under (A.8) $\bar{Q}'(0) = \bar{Q}'(T_2) = 0$. Now, it is easy to check that (A.9)–(A.11) hold. Finally, (A.12) follows from

$$\tfrac{1}{2}(\tilde{Q}_1(t) + \tilde{Q}_2(t)) = \tfrac{1}{2}(Q_1(t) + Q_2(t)) - \bar{Q}(t) = \ell - L_1 \frac{T_2 - 2}{T_2} - \frac{L_2}{T_2} t,$$

for $0 \le t \le T_2$.

QED

A.2 Lemmas for §4

Lemma A.5 *Let $\|y\|_\infty > 1$. For any $\kappa > 0$, there exists $T_0 = T_0(\kappa)$ such that*

$$\mathbf{P}\Big(\sup_{0 \le t \le T_0} \|x(t) - y\|_\infty \le \kappa \|y\|_\infty \Big) \ge \frac{1}{2}.$$

Proof By Lemma A.7, noting that the maximum norm and Euclidean norm are equivalent in finite dimensional space, we have, with some $T_0 > 0$, $K > 0$,

$$\mathbf{E}\|x(t) - \mathbf{E}x(t)\|_\infty^2 \le \big(e^{Kt} - 1\big)(1 + \|y\|_\infty^2), \quad 0 \le t \le T_0.$$

Define the S-valued martingale $M(t) = x(t) - \mathbf{E}x(t)$. Doob's martingale inequality yields, for any $T_0 > 0$,

$$\mathbf{P}\Big(\sup_{0 \le t \le T_0} \|M(t)\|_\infty \ge \frac{\kappa}{2} \|y\|_\infty \Big) \le \frac{4}{\kappa^2 \|y\|_\infty^2} \mathbf{E}|M(T_0)|_\infty^2 \le \frac{4}{\kappa^2 \|y\|_\infty^2} \big(e^{KT_0} - 1\big)(1 + \|y\|_\infty^2).$$

Noting that the right hand side is convergent to 0 when $T_0 \to 0$ since $\|y\|_\infty > 1$, we can find suitable $T_0 = T_0(\kappa)$ such that

$$\mathbf{P}(\sup_{0\le t\le T_0} \|M(t)\|_\infty \ge \frac{\kappa}{2}\|y\|_\infty) \le \frac{1}{2}. \tag{A.14}$$

By Lemma A.7, we have

$$\|\mathbf{E}x(t) - y\|_\infty \le \mathbf{E}\|x(t) - y\|_\infty \le (\mathbf{E}\|x(t) - y\|_\infty^2)^{1/2} \le \left(e^{Kt} - 1\right)^{1/2}(1 + \|y\|_\infty).$$

Choosing T_0 small enough, we have, since $\|y\|_\infty \ge 1$,

$$\|\mathbf{E}x(t) - y\|_\infty \le \frac{\kappa}{4}(1 + \|y\|_\infty) \le \frac{\kappa}{2}\|y\|_\infty, \quad \text{for } 0 \le t \le T_0. \tag{A.15}$$

Since

$$x(t) - y = x(t) - \mathbf{E}x(t) + \mathbf{E}x(t) - y,$$

we have, by (A.14) and (A.15),

$$\mathbf{P}\Big(\sup_{0\le t\le T_0} \|x(t) - y\|_\infty \le \kappa\|y\|_\infty\Big) \ge \frac{1}{2},$$

which is (A.5). The proof is complete. *QED*

Lemma A.6 *For $T > 0$, there exists a constant $K > 0$ such that for $0 \le t \le T$*

$$|\mathbf{E}[W^D(|q_{12}(t)|)p_{12}^2(t) - W^D(|q_{12}(0)|)p_{12}(0)^2]| \le K\,t\,(1 + \|y\|_\infty^3).$$

Proof Let $\varphi(x(t)) = W^D(|q_{12}(t)|)p_{12}^2(t)$, where $x(t)$ is the solution of the (1.1). By Itô's formula,

$$d\varphi(x(t)) = dW^D(|q_{12}|)p_{12}^2 = I ds + II ds + III ds + IV ds,$$

where

$$I = \frac{\partial(W^D(|q_{12}|)p_{12}^2)}{\partial q_1}p_1 + \frac{\partial(W^D(|q_{12}|)p_{12}^2)}{\partial q_2}p_2 + \frac{\partial(W^D(|q_{12}|)p_{12}^2)}{\partial q_3}p_3,$$

and

$$\begin{aligned} II =& \frac{\partial(W^D(|q_{12}|)p_{12}^2)}{\partial p_1}\Big[-\sum_{j\neq 1} a_{1j}\frac{\partial V(|q_{1j}|)}{\partial q_1} - \gamma\sum_{j\neq 1} W^D(|q_{1j}|)p_{1j}\Big] \\ &+ \frac{\partial(W^D(|q_{12}|)p_{12}^2)}{\partial p_2}\Big[-\sum_{j\neq 2} a_{2j}\frac{\partial V(|q_{2j}|)}{\partial q_2} - \gamma\sum_{j\neq 2} W^D(|q_{2j}|)p_{2j}\Big] \\ &+ \frac{\partial(W^D(|q_{12}|)p_{12}^2)}{\partial p_3}\Big[-\sum_{j\neq 3} a_{3j}\frac{\partial V(|q_{3j}|)}{\partial q_3} - \gamma\sum_{j\neq 3} W^D(|q_{3j}|)p_{3j}\Big], \end{aligned}$$

and

$$III = \sum_{i=1}^{6} \frac{\partial(W^D(|q_{12}|)p_{12}^2)}{\partial x_i}\big(\Sigma(x)dW\big)_i$$

and

$$IV = \frac{1}{2}\sum_{i,j=1}^{3} \frac{\partial(W^D(|q_{12}|)p_{12}^2)}{\partial p_i \partial p_j}[\sigma(x)\sigma(x)^T]_{ij}.$$

After expectation and integration, we get

$$|\mathbf{E}W^D(|q_{12}|)p_{12}^2 - W^D(|q_{12}(0)|)p_{12}(0)^2| \le \mathbf{E}\Big|\int_0^t I\,ds\Big| + \mathbf{E}\Big|\int_0^t II\,ds\Big| + \mathbf{E}\Big|\int_0^t IV\,ds\Big|.$$

We first consider $\mathbf{E}\Big|\int_0^t I\,ds\Big|$, we have, for one typical term $\frac{\partial\left(W^D(|q_{12}|)p_{12}^2\right)}{\partial q_1}p_1$ in I,

$$
\begin{aligned}
&\mathbf{E}\Big|\int_0^t \frac{\partial\left(W^D(|q_{12}|)p_{12}^2\right)}{\partial q_1}p_1\,ds\Big| \\
&\le K\mathbf{E}\int_0^t p_{12}^2|p_1|\,ds \le K\mathbf{E}\int_0^t (p_1^2+p_2^2)|p_1|\,ds \le K\int_0^t \mathbf{E}\|x(s)\|_\infty^3\,ds.
\end{aligned}
$$

The other terms in I can be estimated similarly, thus we get

$$
\mathbf{E}\Big|\int_0^t I\,ds\Big| \le K\int_0^t \mathbf{E}\|x(s)\|_\infty^3\,ds.
$$

Next we consider $\mathbf{E}\Big|\int_0^t II\,ds\Big|$, we have, for one typical term,

$$
\begin{aligned}
&\mathbf{E}\Big|\int_0^t \frac{\partial\left(W^D(|q_{12}|)p_{12}^2\right)}{\partial p_1}W^D(|q_{13}|)p_{13}\,ds\Big| \\
&\le K\mathbf{E}\int_0^t |p_{12}||p_{13}|\,ds \le K\mathbf{E}\int_0^t |p_1-p_2||p_1-p_3|\,ds \\
&\le K\mathbf{E}\int_0^t \|x(s)\|_\infty^2\,ds = K\int_0^t \mathbf{E}\|x(s)\|_\infty^2\,ds.
\end{aligned}
$$

The other terms in II can be estimated similarly, thus we get

$$
\mathbf{E}\Big|\int_0^t II\,dt\Big| \le K\int_0^t \mathbf{E}\|x(s)\|_\infty^2\,ds.
$$

It remains to consider $\mathbf{E}\Big|\int_0^t IV\,dt\Big|$. Noting that, for one typical term in IV,

$$
\Big|\frac{\partial\left(W^D(|q_{12}|)p_{12}^2\right)}{\partial p_1\partial p_2}\Big| = \Big|W^D(|q_{12}|)\frac{\partial}{\partial p_2}\big(2(p_1-p_2)\big)\Big| = |2W^D(q_{12})| \le K.
$$

The other terms are also bounded similarly, thus we get

$$
\mathbf{E}\Big|\int_0^t IV\,ds\Big| \le K\int_0^t ds = Kt.
$$

Together these estimates we get

$$
\begin{aligned}
|\mathbf{E}W^D(|q_{12}|)p_{12}^2 - W^D(|q_{12}(0)|)p_{12}(0)^2| \le& K\Big(t+\int_0^t \mathbf{E}\|x(s)\|_\infty^2\,ds + \int_0^t \mathbf{E}\|x(s)\|_\infty^3\,ds\Big) \\
\le& K\,t\,(1+\|y\|_\infty^3), \qquad 0\le t\le T,
\end{aligned}
$$

where we have used the fact that, with $p=2,3$,

$$
\mathbf{E}\|x(t)\|_\infty^p \le K(1+\|y\|_\infty^p), \qquad 0\le t\le T.
$$

Together these estimates complete the proof. *QED*

Lemma A.7 *Assume that $x(t)$ is the solution of* (3.1). *For all $T_0>0$, there exists $K>0$ such that, for $0\le t\le T_0$,*

$$
\mathbf{E}\|x(t)-\mathbf{E}x(t)\|_2^2 \le \left(e^{Kt}-1\right)(1+\|y\|_2^2), \tag{A.16}
$$

and

$$
\mathbf{E}\|x(t)-x(0)\|_2^2 \le \left(e^{Kt}-1\right)(1+\|y\|_2^2). \tag{A.17}
$$

Proof We write the solution of (3.1) into integral form

$$x(t) = x(0) + \int_0^t f(x(s))\, ds + \int_0^t \Sigma(x(s))\, dW(s). \tag{A.18}$$

Then,

$$x(t) - \mathbf{E}x(t) = \int_0^t \big(f(x(s)) - \mathbf{E}f(x(s))\big)\, ds + \int_0^t \Sigma(x(s))\, dW(s).$$

Thus, by Cauchy-Schwartz inequality, Itô Isometry, and regularity of Y and Σ,

$$\begin{aligned}
\mathbf{E}\|x(t) - \mathbf{E}x(t)\|_2^2 &\le 2T_0\mathbf{E}\int_0^t \|f(x(s)) - \mathbf{E}f(x(s))\|_2^2\, ds + 2\mathbf{E}\int_0^t \|\Sigma(x(s))\|_2^2\, ds \\
&\le 2T_0\mathbf{E}\int_0^t \big(2|f(x(s))|_2^2 + 2|\mathbf{E}f(x(s))|_2^2\big)\, ds + 2\mathbf{E}\int_0^t \|\Sigma(x(s))\|_2^2\, ds \\
&\le 8T_0\mathbf{E}\int_0^t |f(x(s))|_2^2\, ds + 2\mathbf{E}\int_0^t \|\Sigma(x(s))\|_2^2\, ds \\
&\le K\mathbf{E}\int_0^t (1 + \|x(s)\|_2^2)\, ds.
\end{aligned}$$

Here K denotes a generic constant independent of t. To estimate the right hand side, note that by (A.18)

$$\begin{aligned}
\mathbf{E}\|x(t)\|_2^2 \le 2\mathbf{E}\|x(0)\|_2^2 &+ 2T_0K\mathbf{E}\int_0^t (1 + \|x(s)\|_2^2)\, ds + 2K\mathbf{E}\int_0^t (1 + \|x(s)\|_2^2)\, ds \\
&\le 2\|x(0)\|_2^2 + K\int_0^t \mathbf{E}(1 + \|x(s)\|_2^2)\, ds.
\end{aligned}$$

Using Gronwall's lemma, we get

$$\mathbf{E}(\|x(t)\|_2^2) \le e^{Kt}(1 + \|x(0)\|_2^2), \tag{A.19}$$

which implies that

$$\begin{aligned}
\int_0^t \mathbf{E}(1 + \|x(s)\|_2^2)\, ds &\le 2\int_0^t e^{Ks}(1 + \||x(0)\|_2^2)\, ds \\
&\le \frac{2}{K}e^{Kt}(1 + \|x(0)\|_2^2.
\end{aligned} \tag{A.20}$$

Hence,

$$\mathbf{E}\|x(t) - \mathbf{E}x(t)\|_2^2 \le \big(e^{Kt} - 1\big)(1 + \|x(0)\|_2^2),$$

which is (A.16) For (A.17), we see that, by (A.18) and (A.20),

$$\begin{aligned}
\mathbf{E}\|x(t) - x(0)\|_2^2 &\le 2T_0\mathbf{E}\int_0^t \|f(x(s))\|_2^2\, ds + 2\mathbf{E}\int_0^t \|\Sigma(x(s))\|_2^2\, ds \\
&\le K\mathbf{E}\int_0^t (1 + \|x(s)\|_2^2)\, ds \\
&\le \big(e^{Kt} - 1\big)(1 + \|x(0)\|_2^2).
\end{aligned}$$

Together these estimates complete the proof. *QED*

Lemma A.8 *Assume that $x(t)$ is the solution of (3.1). Then, there exist $K > 0$ such that*

$$\big[\mathbf{E}\mathcal{V}_t^2\big]^{1/2} \le e^{Kt}\mathcal{V}_0, \qquad 0 \le t \le T. \tag{A.21}$$

Proof For simplicity, we verify for $\mathcal{V}_t = \mathcal{V}(x(t)) = 1 + \frac{1}{2}\sum p_i^2$. It is easily extended to include the conservative terms, as they are bounded. Let $g_t = \mathcal{V}_t^2$. Applying Itô formula and taking the expectation, we get

$$\begin{aligned}\mathbf{E}g_t - \mathbf{E}g_0 = \mathbf{E}\int_0^t \sum_{i=1}^N (2\mathcal{V}_s p_i)\Big(- \sum_{j\neq i} a_{ij}\frac{\partial}{\partial q_j}V(|q_{ij}|) - W^D(|q_{ij}|)p_{ij}\Big)\, ds \\ + \frac{1}{2}\mathbf{E}\int_0^t \sum_{i,j=1}^N (\sigma^T\sigma)_{ij}\frac{\partial^2 g}{\partial p_i \partial p_j}\, ds,\end{aligned}$$

where

$$\frac{\partial^2 g_t}{\partial p_i \partial p_j} = \frac{\partial^2 \mathcal{V}_t^2}{\partial p_i \partial p_j} = \frac{\partial}{\partial p_i}(2\mathcal{V}_t p_j) = \begin{cases} p_i p_j, & j \neq i, \\ 2\mathcal{V}_t + p_i p_j, & j = i. \end{cases}$$

As $\mathcal{V}(x) \geq 1$, for $i, j = 1, 2, \cdots, N$,

$$|p_i| \leq \Big(\sum_{i=1}^N p_i^2\Big)^{1/2} \leq K\mathcal{V}_t^{1/2} \leq K\mathcal{V}_t,$$

$$|p_i p_{ij}| \leq |p_i(p_i - p_j)| \leq K\sum_{i=1}^N p_i^2 \leq K\mathcal{V}_t,$$

and

$$\Big|\frac{\partial^2 g_t}{\partial p_i \partial p_i}\Big| \leq K\mathcal{V}_t \leq K\mathcal{V}_t^2, \quad 0 \leq t \leq T.$$

Using these estimates and boundedness of W^D and $\frac{\partial V(|r|)}{\partial r}$,

$$\mathbf{E}g_t - \mathbf{E}g_0 \leq \int_0^t \mathbf{E}g_s\, ds, \quad 0 \leq t \leq T,$$

which implies (A.21) by Gronwall's lemma. *QED*