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Quantitative propagation of chaos of
McKean-Vlasov equations via the
master equation

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Declaration

I declare that this thesis was composed by myself and that the work contained therein is my own, except where explicitly stated otherwise in the text. The work has not been submitted for any other degree or professional qualification except as specified.

(Alvin Tse)

To anyone passionate in mathematics

Lay Summary

Large systems of interacting agents occur in many different areas of science. The agents may be people, computers, flocks of animals, or particles in moving fluid. Mean-field theory aims to study particle systems by considering the asymptotic behaviour of the agents or particles, as their number goes to infinity. This thesis concerns the theoretical numerical analysis and properties of mean-field models, through various tools in PDE theory and stochastic analysis.

Abstract

McKean-Vlasov stochastic differential equations (MVSDEs) are ubiquitous in kinetic theory and in controlled games with a large number of players. They have been intensively studied since McKean, as they pave a way to probabilistic representations for many important non-linear/nonlocal PDEs. Classically, their simulation involves using standard particle systems, which replace the evolving law in MVSDEs by the evolving empirical measure of the particles. However, this type of simulation is costly in terms of computational complexity, due to the interaction between the particles.

Apart from classical techniques in stochastic analysis, the approach in this thesis relies heavily on the calculus on Wasserstein space, presented by P. Lions in his course at Collège de France. An important object in our study, is a PDE written on the product space of the space of time horizon and the Wasserstein space, which is a generalisation of the classical Feynman-Kac PDE. This PDE, namely the master equation, provides a new insight into the study of mean-field limits of particles and consequently allows us to solve many problems on MVSDEs that are very difficult/impossible to solve by classical techniques.

The layout of the thesis is as follows. We start by a recap on classical results of MVSDEs (Chapter 2), followed by a full exposition of Wasserstein calculus on the results that we need (Chapter 3). Chapters 4 and 5 propose approximating systems to MVSDEs (as alternatives to the classical particle system) via Romberg extrapolation and Antithetic Multi-level Monte-Carlo estimation respectively, which are less costly in terms of computational complexity. Finally, in Chapter 6, we explore the converse: given a standard particle system, we hope to find an alternative mean-field limit that gives a better approximation to the standard particle system.

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Convention of notations

- For any $x, y \in \mathbb{R}^d$, we denote their inner product by xy . Since different measure derivatives lie in different tensor product spaces, we use $|\cdot|$ to denote the Euclidean norm for *any* tensor product space in the form $\mathbb{R}^{d_1} \otimes \dots \otimes \mathbb{R}^{d_\ell}$.
- The law of any random variable Z is denoted by $\mathcal{L}(Z)$. For any function $f : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, its lift $\tilde{f} : L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{R}^d) \rightarrow \mathbb{R}$ is defined by $\tilde{f}(\xi) = f(\mathcal{L}(\xi))$.
- $(\hat{\Omega}, \hat{\mathcal{F}}, \hat{\mathbb{P}})$ stands for a copy of $(\Omega, \mathcal{F}, \mathbb{P})$, which is useful to represent the L-derivative of a function of w.r.t. the probability measure (to be defined in Chapter 3). Any random variable η defined on $(\Omega, \mathcal{F}, \mathbb{P})$ is represented by $\hat{\eta}$ as a pointwise copy on $(\hat{\Omega}, \hat{\mathcal{F}}, \hat{\mathbb{P}})$. Whenever necessary, we shall introduce a sequence of copies of $(\Omega, \mathcal{F}, \mathbb{P})$, denoted by $\{(\Omega^{(n)}, \mathcal{F}^{(n)}, \mathbb{P}^{(n)})\}_n$. Any random variable η defined on $(\Omega, \mathcal{F}, \mathbb{P})$ is represented by $\eta^{(n)}$ as a pointwise copy on $(\Omega^{(n)}, \mathcal{F}^{(n)}, \mathbb{P}^{(n)})$.
- $L^2 := L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{R}^d)$ denotes the set of square integrable random variables. For any sub- σ -algebra \mathcal{G} , $L^2(\mathcal{G})$ denotes the set of all random variables in $L^2(\Omega, \mathcal{G}, \mathbb{P}; \mathbb{R}^d)$.
- \mathcal{H}^2 denotes the set of square-integrable progressively measurable processes θ such that $\left(\int_0^T |\theta_s|^2 ds\right)^{\frac{1}{2}} \in L^2$.
- N represents the number of particles and h represents the discretisation step in an Euler scheme. For $a, b \in \mathbb{R}$, we write $a \lesssim b$ if $a \leq Cb$, for some constant C that does not depend on N or h . Unless otherwise specified, C denotes a constant independent of N and h , whose value varies from line to line.
- For any $t \geq 0$, \mathcal{C}_t stands for the space $C([0, t], \mathbb{R}^d)$ equipped with the supremum norm.
- $C_0^k((\mathbb{R}^d)^\ell)$ denotes the set of all functions from $(\mathbb{R}^d)^\ell$ to \mathbb{R} that are in C^k with compact support.
- $C_{b, \text{Lip}}^k((\mathbb{R}^d)^\ell)$ denotes the set of all functions from $(\mathbb{R}^d)^\ell$ to \mathbb{R} that are in C^k with bounded and Lipschitz partial derivatives up to and including order k .
- For any metric space E , $C_b(E)$ denotes the set of all bounded functions from E to \mathbb{R} .
- For any metric space E , $\mathcal{P}(E)$ denotes the set of probability measures on E .
- For any measure $\mu \in \mathcal{P}(C_t)$, μ_t denotes the marginal of μ at time t .

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Chapter 1

Introduction

Large systems of interacting individuals/agents occur in many different areas of science; the individuals/agents may be people, computers, flocks of animals, or particles in moving fluid. In theoretical physics, the microscopic interaction between fluid or gas particles can be described by a system of nonlinear PDEs. Inspired by the Hilbert's sixth problem, the first systematic study regarding this was pioneered by H. McKean. The study of systems of particles undergoing collision processes, including many-particle jump processes formulated by Kac and McKean (which also give rise to the Boltzmann equation), was further developed in the Kac's program [55]. Mean-field theory was subsequently developed to study particle systems by considering the asymptotic behaviour of the agents or particles, as their number goes to infinity. Instead of considering a system with a huge dimension, one can effectively approximate macroscopic and statistical features of the system as well as the average behaviour of particles. Despite originating from theoretical physics, applications of techniques of mean-field theory go well beyond physical particle systems into mathematical biology and economics.

The problem of interacting particles can also be viewed from a stochastic point of view, as the weak solutions for the associated PDEs are density functions of SDEs (if they exist) with interactions in the drift and diffusion terms. This approach was adopted in [61] by A. Sznitman in the context of Boltzmann equations. In a probabilistic setting, the coefficients of the type of SDEs describing this limiting behaviour typically depend on the probability distribution of the process itself. These SDEs are called McKean-Vlasov SDEs.

Example 1: Individual-Based Models in mathematical biology

We consider Individual-Based Models (IBM) in mathematical biology, which are investigated in detail in [5]. They give a particle-like description of a large set of individuals, by describing the interactions between individuals (which depend on the type of species), and the precise mechanism of the interactions through coefficients of a system of SDEs. To be concrete, let us consider a system of N individuals of some biological species, living in the space of \mathbb{R}^d . Denoting the displacement and velocity processes for each individual i respectively by $(S^{i,N})$ and $(V^{i,N})$, $1 \leq i \leq N$, the general IBM model can be described by

$$\begin{cases} dS_t^{i,N} = V_t^{i,N} dt, \\ dV_t^{i,N} = -F(S_t^{i,N}, V_t^{i,N}) dt - \frac{1}{N} \sum_{j=1}^N H(S_t^{i,N} - S_t^{j,N}, V_t^{i,N} - V_t^{j,N}) dt + dW_t^i, \end{cases}$$

where $F, H : \mathbb{R}^{2d} \rightarrow \mathbb{R}^d$ are suitable functions and (W^i) , $1 \leq i \leq N$, are N independent standard Brownian motions in \mathbb{R}^d . Some special cases of this model are of interest amongst mathematical biologists. For example, in the Cucker-Smale model, we set $F = 0$ and $H(x, v) = w(x)v$, where w is a matrix function given by

$$w_{ij}(x) = \frac{1}{(1 + |x_i - x_j|^2)^\gamma},$$

for some $\gamma \geq 0$. If we define \hat{f}_t^N as the empirical measure

$$\hat{f}_t^N = \frac{1}{N} \sum_{i=1}^N \delta_{(S_t^{i,N}, V_t^{i,N})},$$

then the general IBM model can be rewritten as

$$\begin{cases} dS_t^{i,N} = V_t^{i,N} dt, \\ dV_t^{i,N} = -F(S_t^{i,N}, V_t^{i,N}) dt - (H * \hat{f}_t^N)(S_t^{i,N}, V_t^{i,N}) dt + dW_t^i. \end{cases}$$

Since the pairwise action between any two individuals i and j is of order $\frac{1}{N}$, it is reasonable to predict that their mutual interaction diminishes as N gets large. Under a certain set of regularity assumptions imposed on F and H , each of the N interacting individuals $(S_t^{i,N}, V_t^{i,N})$ behaves like the process (\bar{S}^i, \bar{V}^i) as $N \rightarrow \infty$, with dynamics satisfying the system of SDEs

$$\begin{cases} d\bar{S}_t^i = \bar{V}_t^i dt, \\ d\bar{V}_t^i = -F(\bar{S}_t^i, \bar{V}_t^i) dt - (H * f_t)(\bar{S}_t^i, \bar{V}_t^i) dt + dW_t^i, \\ (\bar{S}_0^i, \bar{V}_0^i) = (S_0^i, V_0^i), \quad f_t = \text{Law}(\bar{S}_t^i, \bar{V}_t^i). \end{cases}$$

This is an example of McKean-Vlasov SDEs, for which the coefficients depend on the law of the process itself.

Example 2: Mean-field games

The theory of mean-field games (MFG) was proposed by J. Lasry and P. Lions ([47, 48]). It models the behaviour of multiple agents, in the situation where each individually tries to optimise one's position in space and time, but with the preference being partly determined by the choices of all the other agents. Each individual optimises according to some criterion, known as the objective function. Because equilibria of large competitive systems tend to suffer from the curse of dimensionality, MFG theory analyses infinite-population limits that are more tractable, which nonetheless provide approximations to the game.

Let $P_t^{i,N}$ be the state process of player i . Player i chooses a control process $\alpha_i = \{\alpha_t^i\}_{t \in [0, T]}$ from a set of admissible strategies, which influences the evolution of the state process according to the following dynamics:

$$\begin{cases} dP_t^{i,N} = b(P_t^{i,N}, \mu_t^N, \alpha_t^i) dt + \sigma(P_t^{i,N}, \mu_t^N, \alpha_t^i) dW_t^i, \\ \mu_t^N := \frac{1}{N} \sum_{i=1}^N \delta_{P_t^{i,N}}. \end{cases}$$

The strategy α^i is chosen to maximise the objective function

$$J^{N,i}(\alpha^i, \dots, \alpha^N) := \mathbb{E} \left[\int_0^T f(P_t^{i,N}, \mu_t^N, \alpha_t^i) dt + g(P_T^{i,N}, \mu_T^N) \right],$$

where f is called the *running cost* and g is called the *terminal cost*. The optimal strategy of player i depends through μ^N on which controls the other agents choose. Typically, the optimisation is done in the sense of Nash equilibrium, which is defined as a vector of controls $(\alpha^1, \dots, \alpha^N)$ such that

$$J^{N,i}(\alpha^i, \dots, \alpha^N) \geq J^{N,i}(\alpha^i, \dots, \alpha^{i-1}, \tilde{\alpha}, \alpha^{i+1}, \alpha^N),$$

for any alternative choice of control $\tilde{\alpha}$. There are of course other more refined concepts of Nash equilibrium, such as ϵ -Nash equilibrium (see [46]). It is well-known in the literature ([14, 21])

that the Nash equilibrium can be characterised in terms of the Hamiltonian function and the solution of an N -player PDE system (a system of Hamilton-Jacobi-Bellman (HJB) equations). Under certain conditions, the Nash equilibrium exists, although it is often not unique.

There are advantages of considering the mean-field limit for finding the Nash equilibrium. Whilst there exist existence theorems for N -player games by PDE methods [4] and BSDE methods [33, 34], the notion of mean-field equilibria in mean-field theory allows us to construct ϵ -Nash equilibria (approximate equilibria) for large-population games, for which existence of equilibria may be hard to prove directly. (See Theorem 8.3 in [46].)

Secondly, N -player PDE systems are hard to solve, especially when N is large. Closed-form solutions of N -player games are almost never available, apart from sufficiently simple linear-quadratic models. One could solve the N -dimensional system of HJB equations numerically via finite-difference schemes, but these schemes do suffer from the curse of dimensionality, as the estimates depend on the dimension. In this respect, the mean-field limit is much more tractable.

What happens as $N \rightarrow \infty$? When N is large, each player has little influence on the empirical measure flow $(\mu_t^N)_{t \in [0, T]}$. If there were a continuum of players, then each player's influence on this empirical measure would be nearly zero and the optimization problems of the players would be decoupled and identically distributed. Since each player among the continuum acts identically, the law of large numbers suggests that the statistical distribution (i.e. μ_t^N) of the player's optimally controlled state process at time t must agree with its law at time t . More precisely, the mean-field limit $\{\bar{P}_t\}_{t \in [0, T]}$ satisfies the dynamics

$$\begin{cases} d\bar{P}_t = b(\bar{P}_t, \mu_t, \alpha_t) dt + \sigma(\bar{P}_t, \mu_t, \alpha_t) dW_t, \\ \mu_t := \text{Law}(\bar{P}_t), \end{cases}$$

where strategy α is chosen to maximise the objective function

$$J^\infty(\alpha) := \mathbb{E} \left[\int_0^T f(\bar{P}_t, \mu_t, \alpha_t) dt + g(\bar{P}_T, \mu_T) \right].$$

Results regarding approximation of N -player games by their mean-field limits are abundant in the literature and can be found in [1, 46, 14, 21].

Central theme of the thesis: Interacting diffusion models

Our central object of study is the interacting particle system $(Y^{1, N}, \dots, Y^{N, N})$ defined by

$$\begin{cases} dY_t^{i, N} = b(Y_t^{i, N}, \mu_t^{Y, N}) dt + \sigma(Y_t^{i, N}, \mu_t^{Y, N}) dW_t^i, \\ \mu_t^{Y, N} := \frac{1}{N} \sum_{i=1}^N \delta_{Y_t^{i, N}}. \end{cases} \quad (1.0.1)$$

This is essentially the same model as that for N -player games, except that the controls α^i are no longer present. Indeed, this also corresponds to the case in which the optimal controls are closed-loop (i.e. $\alpha_t = \hat{\alpha}(t, X_t)$, for some Borel-measurable function $\hat{\alpha} : [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}$). The functions b and σ satisfy appropriate regularity conditions (e.g. Lipschitz continuity) so that the solution exists. We require the driving noises W^1, \dots, W^N to be independent Wiener processes and the initial positions $Y_0^{1, N}, \dots, Y_0^{N, N}$ to be i.i.d.. We also note that the particles are exchangeable, i.e. the joint distribution of $(Y^{1, N}, \dots, Y^{N, N})$ is the same as $(Y^{\pi(1), N}, \dots, Y^{\pi(N), N})$, for any permutation π of $\{1, \dots, N\}$.

A typical example of this model is when σ is constant and b is of the form

$$b(x, \mu) = \int B(x, y) \mu(dy),$$

for some function B taking two spatial variables as arguments. This model, which serves as an approximation to the Boltzmann equation in physics, was first introduced by McKean in [51] and was then further developed by Sznitman in [61] and by Mouhot *et al.* more recently in the

Kac's program [55].

As in the previous two examples, as $N \rightarrow \infty$, we expect that $Y^{i,N}$ should converge in some sense to independent copies of the solution of the McKean-Vlasov equation

$$dX_t = b(X_t, \mu_t^X) dt + \sigma(X_t, \mu_t^X) dW_t, \quad (1.0.2)$$

where $\mu_t^X := \text{Law}(X_t)$. We heuristically observe why this is indeed the case through a PDE argument in the one-dimensional case. (A thorough analysis will be done in Section 2.2.) Let $\phi : \mathbb{R} \rightarrow \mathbb{R}$ be a smooth function. By Itô's formula, we have the following Fokker-Planck PDE:

$$d\left(\int \phi d\mu_t^X\right) = \left(\int (L_{\mu_t^X} \phi) d\mu_t^X\right) dt, \quad (1.0.3)$$

where L_{μ_t} is defined by

$$(L_{\mu_t} \phi)(x) = b(x, \mu_t) \phi'(x) + \frac{1}{2} \sigma(x, \mu_t)^2 \phi''(x).$$

Equation (1.0.3) is also called the *McKean-Vlasov PDE*. Moreover, applying the Itô's formula to (1.0.1) gives

$$d\left(\int \phi d\mu_t^{Y,N}\right) = \left(\int (L_{\mu_t^{Y,N}} \phi) d\mu_t^{Y,N}\right) dt + \frac{1}{N} \sum_{i=1}^N \phi'(Y_t^{i,N}) \sigma(Y_t^{i,N}, \mu_t^{Y,N}) dW_t^i. \quad (1.0.4)$$

Since the Brownian motions W^1, \dots, W^N are independent, the stochastic integral term converges to zero in the L^2 as $N \rightarrow \infty$. Therefore, PDE (1.0.4) becomes PDE (1.0.3) as $N \rightarrow \infty$.

In fact, for fixed $k \in \mathbb{N}$, it can be shown rigorously in many settings that the sequence $(Y^{1,N}, \dots, Y^{k,N})$ converges in law. More precisely, we have

$$\text{Law}(Y^{1,N}, \dots, Y^{k,N}) \implies (\mu^X)^{\otimes k},$$

where \implies denotes weak convergence. This type of result is known as propagation of chaos, a term coined by Mark Kac. (This property will be discussed in detail in Section 2.3.)

The McKean-Vlasov limit and many of its variations (e.g., with jumps or with common noise) have been studied thoroughly in the past several decades, using a wide range of techniques. One of them is the analysis of the Fokker-Planck PDEs associated to the McKean-Vlasov limit and the particle system. This approach was adopted in various works by P-E. Jabin and Z. Wang [38, 39], as well as [55].

Another widely applicable technique is weak convergence arguments. By placing the empirical measures $(\mu_t^{Y,N})_{t \in [0, T]}$ in a good topological space, we can establish relative compactness of this sequence by generally requiring modest assumptions on the regularity of b and σ . The above heuristic argument may then be made rigorous as a means to find the limit points. This method is employed frequently to investigate the fluctuation between the particle system and its mean-field limit over the path space on $[0, T]$. (See Chapter 6.) Implementations of this strategy can be found in [21, 37, 53].

On the other hand, the results on quantitative propagation of chaos are few and far in between. One approach, called *trajectorial propagation of chaos* (which focuses on quantitative estimates of measures on the path space), tends to yield stronger convergence results but only under accordingly stronger assumptions (e.g. Lipschitz continuity). The main idea is to construct an explicit coupling between the limiting process and the particle system, by building independent copies of the unique solution of the McKean-Vlasov equation on the same probability space as the particle system and driven by the same Brownian motions. An advantage of this approach is that it permits good estimates of the rate of convergence to the limit. In the case where b and σ are linear in measure and globally Lipschitz continuous, [61] showed that $W_2(\text{Law}(Y_t^{i,N}), \text{Law}(X_t)) = O(N^{-1/2})$. We refer to Sznitman's result as strong propagation of chaos (See Theorem 2.2.6.) Nonetheless, for more general b and σ , the rate of strong convergence generally deteriorates with the dimension. Estimates regarding weak propagation of chaos (i.e. concerning the weak error between the particle system and its mean-field limit)

have been proposed very recently by two independent works [44, Ch. 9] and [56, Th. 2.1].

Why are quantitative estimates important? The simulation of standard particle systems is costly in terms of computational complexity, due to the interaction between particles. Indeed, for general first-degree interactions, one should expect the order of interactions to be $O(N^2)$ (see Definition 4.1.1). Therefore, one of the main objectives of this thesis is to propose numerical algorithms to effectively simulate McKean-Vlasov SDEs by using alternatives to the standard particle systems. To prove that these algorithms indeed reduce the complexity, one would need to use various estimates of quantitative strong and weak propagation of chaos, which are established in Chapters 4 and 5.

Framework of analysis in the thesis

In stochastic numerical analysis, one typically considers two types of error of the forms

$$\sup_{t \in [0, T]} \mathbb{E} |Y_t^{i, N} - X_t^i|$$

and

$$\sup_{t \in [0, T]} \left| \mathbb{E}[\phi(Y_t^{i, N})] - \mathbb{E}[\phi(X_t^i)] \right|,$$

where X^i is the coupling of (1.0.2) driven by Brownian motion W^i and $\phi : \mathbb{R}^d \rightarrow \mathbb{R}$ is some smooth test function. The former is called the *strong error* and the latter is called the *weak error*.

Results regarding the strong error are well-known in the literature. In particular, as mentioned above, by [61] (see Theorem 2.2.6), the order of convergence is known to be $O(1/\sqrt{N})$ if the drift and diffusion functions are Lipschitz and linear in measure. More generally, for general Lipschitz drift and diffusion functions, the order of convergence is known to be $O(1/N^{\frac{1}{d+8}})$ (see [11]). In Theorem 5.2.5 of this thesis, the order of convergence is shown to be $O(1/\sqrt{N})$ for general drift and diffusion functions that are sufficiently smooth in the space of probability measures in a certain sense (to be defined below).

Results concerning the weak error are sparse in the literature and have been recently proposed by independent works [3], [44, Ch. 9] and [56, Th. 2.1]. These results all show the rate of convergence of the weak error of $O(1/N)$ under various conditions. The methodology behind the weak error analysis is crucial in this thesis and leads us to the machinery of optimal transport and calculus in the space of probability measures.

A natural thing to do in the analysis of weak error is to proceed by the Feynman-Kac formula. We perform the calculations under the assumption of dimension one and constant diffusion $\sigma > 0$, for simplicity of notations. We fix $t \in [0, T]$ and define the flow $v(s, x) = \mathbb{E}[\phi(X_t^{s, x})]$, where $X^{s, x}$ satisfies (1.0.2) and starts at $x \in \mathbb{R}$ at time s . Suppose that $X_0, Y_0^{1, N}, \dots, Y_0^{N, N}$ are all distributed as μ . Note that

$$\mathbb{E}\phi(X_t) = \int_{\mathbb{R}} \mathbb{E}\phi(X_t^{s, x}) \mu(dx) = \int_{\mathbb{R}} v(0, x) \mu(dx) = \mathbb{E}v(0, Y_0^{i, N}).$$

Moreover, v satisfies the Feynman-Kac formula

$$\begin{cases} \frac{\partial v}{\partial s}(s, x) + \frac{1}{2}\sigma^2 \frac{\partial^2 v}{\partial x^2}(s, x) + b(x, \mu_s^X) \frac{\partial v}{\partial x}(s, x) = 0, & s \in (0, t), x \in \mathbb{R}, \\ v(t, x) = \phi(x). \end{cases} \quad (1.0.5)$$

By Itô's formula and (1.0.5), we have

$$\begin{aligned} & \mathbb{E}\phi(Y_t^{i, N}) - \mathbb{E}\phi(X_t) \\ &= \mathbb{E}v(t, Y_t^{i, N}) - \mathbb{E}v(0, Y_0^{i, N}) \\ &= \mathbb{E} \left[\int_0^t \frac{\partial v}{\partial s}(s, Y_s^{i, N}) ds + \int_0^t \frac{\partial v}{\partial x}(s, Y_s^{i, N}) b(Y_s^{i, N}, \mu_s^{Y, N}) ds + \sigma \int_0^t \frac{\partial v}{\partial x}(s, Y_s^{i, N}) dW_s \right] \end{aligned}$$

$$\begin{aligned}
& \left. + \frac{1}{2} \sigma^2 \int_0^t \frac{\partial^2 v}{\partial x^2}(s, Y_s^{i,N}) ds \right] \\
= & \mathbb{E} \left[\int_0^t \frac{\partial v}{\partial x}(s, Y_s^{i,N}) \left(b(Y_s^{i,N}, \mu_s^{Y_s^{i,N}}) - b(Y_s^{i,N}, \mu_s^X) \right) ds \right]. \tag{1.0.6}
\end{aligned}$$

In general, one would have to resort to strong error bounds to show convergence, which only yields the order of $O(1/\sqrt{N})$. For non-interacting drifts of the form $b(x, \mu) = F_1(x, \int F_2(z) \mu(dz))$, it is shown in [3] via an argument of Gronwall's inequality that the rate can be improved to $O(1/N)$.

Another approach involves the application of Feynman-Kac formula to the particle system. As before, we maintain the assumption of dimension one and constant diffusion $\sigma > 0$. Suppose that the drift takes the form $b(x, \mu) := \int B(x, y) \mu(dy)$, for some function $B : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}$ that is twice-differentiable with all its derivatives bounded up to and including the second order partial derivatives. We define a corresponding test function $F : \mathbb{R}^N \rightarrow \mathbb{R}$ by

$$F(\mathbf{x}) = \frac{1}{N} \sum_{i=1}^N \phi(x_i).$$

Fix $t \in [0, T]$. As before, let X^i be the coupling of (1.0.2) driven by Brownian motion W^i . Define $\mathbf{Y}^{\mathbf{N}} = (Y^{1,N}, \dots, Y^{N,N})$, $\mathbf{X}^{\mathbf{N}} = (X^1, \dots, X^N)$ and a function $v^N : [0, t] \times \mathbb{R}^N \rightarrow \mathbb{R}$ such that

$$v^N(s, \mathbf{x}) = \mathbb{E} \left[F \left((\mathbf{Y}_t^{\mathbf{N}})^{s, \mathbf{x}} \right) \right].$$

Clearly, $\mathbb{E} \phi(X_t^i) = \mathbb{E} F(\mathbf{X}_t^{\mathbf{N}}) = \mathbb{E} v^N(t, \mathbf{X}_t^{\mathbf{N}})$. We can also see that

$$\begin{aligned}
\mathbb{E} \phi(Y_t^{i,N}) &= \mathbb{E} F(\mathbf{Y}_t^{\mathbf{N}}) \\
&= \int_{\mathbb{R}^N} \mathbb{E} \left[F \left((\mathbf{Y}_t^{\mathbf{N}})^{0, \mathbf{x}} \right) \right] \nu^{\otimes N}(d\mathbf{x}) \\
&= \int_{\mathbb{R}^N} v^N(0, \mathbf{x}) \nu^{\otimes N}(d\mathbf{x}) \\
&= \mathbb{E} v^N(0, \mathbf{X}_0^{\mathbf{N}}),
\end{aligned}$$

where ν is the initial law of $X, Y^{1,N}, \dots, Y^{N,N}$. By the Feynman-Kac formula, v^N satisfies the PDE

$$\begin{cases} \frac{\partial v^N}{\partial s}(s, \mathbf{x}) + \frac{1}{2} \sigma^2 \sum_{p=1}^N \frac{\partial^2 v^N}{\partial x_p^2}(s, \mathbf{x}) + \sum_{p=1}^N \left[\frac{1}{N} \sum_{q=1}^N B(x_p, x_q) \right] \frac{\partial v^N}{\partial x_p}(s, \mathbf{x}) = 0, & s \in (0, t), \\ v^N(t, \mathbf{x}) = \phi(\mathbf{x}). \end{cases} \tag{1.0.7}$$

Note that it is possible to show by direct differentiation of (1.0.7) that for any distinct $i, j \in \{1, \dots, N\}$,

$$\sup_{s \in [0, t]} \sup_{\mathbf{x} \in \mathbb{R}^N} \left| \frac{\partial v^N}{\partial x_i}(s, \mathbf{x}) \right| \leq \frac{C}{N}, \quad \sup_{s \in [0, t]} \sup_{\mathbf{x} \in \mathbb{R}^N} \left| \frac{\partial^2 v^N}{\partial x_i \partial x_j}(s, \mathbf{x}) \right| \leq \frac{C}{N^2}, \tag{1.0.8}$$

where C is a constant depending on T and the functions b and ϕ , but not on the number of particles N . Therefore, by (1.0.7) and (1.0.8), we have

$$\begin{aligned}
& \mathbb{E} \phi(X_t^i) - \mathbb{E} \phi(Y_t^{i,N}) \\
= & \mathbb{E} v^N(t, \mathbf{X}_t^{\mathbf{N}}) - \mathbb{E} v^N(0, \mathbf{X}_0^{\mathbf{N}}) \\
= & \mathbb{E} \left[\int_0^t \frac{\partial v^N}{\partial s}(s, \mathbf{X}_s^{\mathbf{N}}) ds + \sum_{p=1}^N \int_0^t \frac{\partial v^N}{\partial x_p}(s, \mathbf{X}_s^{\mathbf{N}}) dX_s^p + \frac{\sigma^2}{2} \sum_{p=1}^N \int_0^t \frac{\partial^2 v^N}{\partial x_p^2}(s, \mathbf{X}_s^{\mathbf{N}}) ds \right]
\end{aligned}$$

$$\begin{aligned}
&= \mathbb{E} \left[\sum_{p=1}^N \int_0^t \frac{\partial v^N}{\partial x_p}(s, \mathbf{X}_s^N) \left[b(X_s^p, \mu_s^X) - \frac{1}{N-1} \sum_{q \neq p} B(X_s^p, X_s^q) \right] ds \right] + O\left(\frac{1}{N}\right) \\
&= \frac{1}{N-1} \sum_{p=1}^N \sum_{q \neq p} \mathbb{E} \left[\int_0^t \frac{\partial v^N}{\partial x_p}(s, \mathbf{X}_s^N) \left[b(X_s^p, \mu_s^X) - B(X_s^p, X_s^q) \right] ds \right] + O\left(\frac{1}{N}\right) \\
&= \frac{1}{N-1} \sum_{p=1}^N \sum_{q \neq p} \mathbb{E} \left[\int_0^t \left(\frac{\partial v^N(s, X_s^1, \dots, X_s^{q-1}, 0, X_s^{q+1}, \dots, X_s^N)}{\partial x_p} + \right. \right. \\
&\quad \left. \left. \int_0^{X_s^q} \frac{\partial^2 v^N(s, X_s^1, \dots, X_s^{q-1}, u, X_s^{q+1}, \dots, X_s^N)}{\partial x_q \partial x_p} du \right) \cdot \right. \\
&\quad \left. \left(b(X_s^p, \mu_s^X) - B(X_s^p, X_s^q) \right) ds \right] + O\left(\frac{1}{N}\right) \\
&= \frac{1}{N-1} \sum_{p=1}^N \sum_{q \neq p} \mathbb{E} \left[\int_0^t \left(\int_0^{X_s^q} \frac{\partial^2 v^N(s, X_s^1, \dots, X_s^{q-1}, u, X_s^{q+1}, \dots, X_s^N)}{\partial x_q \partial x_p} du \right) \cdot \right. \\
&\quad \left. \left(b(X_s^p, \mu_s^X) - B(X_s^p, X_s^q) \right) ds \right] + O\left(\frac{1}{N}\right), \tag{1.0.9}
\end{aligned}$$

where we have used the independence of the coupled processes $X^i, 1 \leq i \leq N$, in the final step, since

$$\begin{aligned}
&\mathbb{E} \left[\frac{\partial v^N(s, X_s^1, \dots, X_s^{q-1}, 0, X_s^{q+1}, \dots, X_s^N)}{\partial x_p} \left(b(X_s^p, \mu_s^X) - B(X_s^p, X_s^q) \right) \right] \\
&= \mathbb{E} \left[\mathbb{E} \left[\frac{\partial v^N(s, x_s^1, \dots, x_s^{q-1}, 0, x_s^{q+1}, \dots, x_s^N)}{\partial x_p} \cdot \left(b(X_s^p, \mu_s^X) \right. \right. \right. \\
&\quad \left. \left. \left. - B(X_s^p, X_s^q) \right) \middle| (x_s^1, \dots, x_s^{q-1}, x_s^{q+1}, \dots, x_s^N) = (X_s^1, \dots, X_s^{q-1}, X_s^{q+1}, \dots, X_s^N) \right] \right] \\
&= 0.
\end{aligned}$$

Therefore, (1.0.9) and (1.0.8) show that

$$\sup_{t \in [0, T]} \left| \mathbb{E}[\phi(Y_t^{i, N})] - \mathbb{E}[\phi(X_t^i)] \right| \leq \frac{C}{N},$$

for some constant $C > 0$.

We now analyse the pros and cons of these two approaches. Indeed, the second approach fully exploits the structure of the particle system and the mean-field coupling, which enables us to obtain the desired rate. However, suppose that we wish to obtain a higher order estimator for the limiting equation through Romberg extrapolation. Then one has to write the weak error as

$$\sup_{t \in [0, T]} \left(\mathbb{E}[\phi(Y_t^{i, N})] - \mathbb{E}[\phi(X_t^i)] \right) = \frac{C}{N} + \text{higher order terms}, \tag{1.0.10}$$

where C does not depend on N . In this respect, the second approach does not seem plausible, since it is clear from (1.0.9) that the dependence on N is intrinsic in this method, as v^N depends on the particle system in its definition.

The main idea in the thesis is to apply the first approach, but along the flow of measures $\{\frac{1}{N} \sum_{i=1}^N \delta_{Y_t^{i, N}}\}_{t \in [0, T]}$, instead of applying Itô's formula to each particle $\{Y_t^{i, N}\}_{t \in [0, T]}$. To this end, one would need a version of Feynman-Kac formula (1.0.5) and Itô's formula in the space of probability measures.

Many works in mean-field games (e.g. [9, 10, 14]) make use of an idea introduced by P. Lions

in [49]. It consists in working in a sufficiently large probability space and considering the lift

$$\tilde{U}(\theta) := U(\mathcal{L}(\theta)),$$

for any function $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, where $\mathcal{P}_2(\mathbb{R}^d)$ is the set of probability measures with finite second moments. Suppose that \tilde{U} is Fréchet differentiable with Fréchet derivative $D\tilde{U}$. Then, by the Riesz representation theorem, there exists a (\mathbb{P} -a.s.) unique random variable $L_{\theta_0} \in L^2(\mathcal{F}; \mathbb{R}^d)$ such that

$$D\tilde{U}(\theta_0)(\eta) = \mathbb{E}[L_{\theta_0}\eta], \quad \forall \eta \in L^2(\mathcal{F}; \mathbb{R}^d).$$

Moreover, it is possible to show that there exists a (deterministic) Borel-measurable function $h : \mathbb{R}^d \rightarrow \mathbb{R}^d$ such that $h(\theta) = L_\theta$, where h only depends on the law of θ . (The proof can be found in many sources in the literature, e.g. [10] and [14]. There is also an alternative compact proof in the appendix of [35] due to A. Davie.) The L-derivative $\partial_\mu U(\mu)$ of U is defined to be $\partial_\mu U(\mu) := h$. We also define the corresponding joint map $\partial_\mu U : \mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ by

$$\partial_\mu U(\mu, y) := [\partial_\mu U(\mu)](y).$$

Similarly, we can define the second-order L-derivatives by

$$\partial_\nu \partial_\mu U(\mu, y) := \partial_y [\partial_\mu U(\mu, y)] \quad \text{and} \quad \partial_\mu^2 U(\mu, y_1, y_2) := \partial_\mu [\partial_\mu U(\cdot, y_1)](\mu, y_2).$$

We remark that the concept of L-derivative is closely related to the notion introduced by Ambrosio, Gigli and Savaré in a more general setting [2].

An alternative notion of derivatives in probability measures is the *linear functional derivative*. More precisely, for any function $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, the linear functional derivative $\frac{\delta U}{\delta m} : \mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \rightarrow \mathbb{R}$ is a continuous function such that

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0^+} U(\mu + \varepsilon(\nu - \mu)) = \int_{\mathbb{R}^d} \frac{\delta U}{\delta m}(\mu, y) (\nu - \mu)(dy),$$

for any $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$. It is clear that this definition is just a straightforward extension of the notion of functional derivatives in the theory of calculus of variations. In fact, this notion can be found in many works in the literature, such as [44]. It is easy to compute that, for any $m, m' \in \mathcal{P}_2(\mathbb{R}^d)$,

$$\begin{aligned} U(m') - U(m) &= \int_0^1 \frac{d}{ds} U(m + s(m' - m)) ds \\ &= \int_0^1 \left. \frac{d}{dh} \right|_{h=0^+} U((1-s)m + sm' + h(m' - m)) ds \\ &= \int_0^1 \int_{\mathbb{R}^d} \frac{\delta U}{\delta m}((1-s)m + sm', y) (m' - m)(dy) ds. \end{aligned}$$

We shall work with either of these two notions in this thesis whenever it is convenient. Moreover, under mild conditions of regularity of $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, if one of the two derivatives exists, then the other also exists and both of them are related by the connection

$$\partial_\mu U(\mu, y) = \partial_y \frac{\delta U}{\delta m}(\mu, y).$$

For any $\Phi : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, our main PDE of interest in this thesis is

$$\begin{cases} \mathcal{A}\mathcal{V}(t, \mu) = 0, & t \in (0, T), \\ \mathcal{V}(T, \mu) = \Phi(\mu), \end{cases} \quad (1.0.11)$$

where the operator \mathcal{A} is defined by

$$\mathcal{A}\mathcal{V}(t, \mu) := \partial_t \mathcal{V}(t, \mu) + \int_{\mathbb{R}^d} [\partial_\mu \mathcal{V}(t, \mu)(y) b(y, \mu) + \frac{1}{2} \text{Tr}(\partial_v \partial_\mu \mathcal{V}(t, \mu)(y) a(y, \mu))] \mu(dy)$$

and $a := \sigma \sigma^T$. This type of PDE has been well-studied in the literature and is called the *master equation* in the context of mean-field games ([11, 21]). Despite not working in a framework of stochastic controls, we shall abuse the terminology slightly and call (1.0.11) the *master equation*. It is well-known that (1.0.11) admits a classical solution when the coefficients are sufficiently smooth ([15]). Moreover, by [9], its solution has a stochastic representation of

$$\mathcal{V}(t, \mu) = \Phi(\mathcal{L}(X_T^{t, \mu})), \quad t \in [0, T].$$

Let us recall the first approach of weak error analysis. As before, we perform the following two steps:

- (i) Application of Feynman-Kac formula to the flow of $\{\mathcal{L}(X_T^{t, \mu})\}_{t \in [0, T]}$;
- (ii) Application of standard Itô's formula to the particle system $\{(Y_t^{1, N}, \dots, Y_t^{N, N})\}_{t \in [0, T]}$.

For simplicity, suppose that $X, Y^{1, N}, \dots, Y^{N, N}$ all start at a deterministic point $c \in \mathbb{R}^d$. Let $\Phi(\mu) := \int_{\mathbb{R}^d} \phi(x) \mu(dx)$. Then we have

$$\mathbb{E}[\mathcal{V}(T, \mu_T^{Y, N})] = \mathbb{E}[\Phi(\mu_T^{Y, N})] = \mathbb{E}[\phi(Y_T^{i, N})]$$

and

$$\mathcal{V}(0, \mu_0^{Y, N}) = \Phi(\mathcal{L}(X_T)) = \mathbb{E}[\phi(X_T)].$$

Define a function $u^N : [0, T] \times (\mathbb{R}^d)^N \rightarrow \mathbb{R}$ by

$$u^N(t, x_1, \dots, x_N) = \mathcal{V}\left(t, \frac{1}{N} \sum_{j=1}^N \delta_{x_j}\right).$$

By Theorem 3.2.5 (also found in Proposition 3.1 of [16]),

$$\partial_{x_i} u^N(t, x_1, \dots, x_N) = \frac{1}{N} \partial_\mu \mathcal{V}\left(t, \frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}\right)(x_i)$$

and

$$\partial_{x_j x_i}^2 u^N(t, x_1, \dots, x_N) = \frac{1}{N} \partial_v \left[\partial_\mu \mathcal{V}\left(t, \frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}\right) \right](x_i) \delta_{i, j} + \frac{1}{N^2} \partial_\mu^2 \mathcal{V}\left(t, \frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}\right)(x_i, x_j).$$

Therefore, by Itô's formula, we obtain that

$$\begin{aligned} & \mathbb{E}[\phi(Y_T^{i, N})] - \mathbb{E}[\phi(X_T)] \\ &= \mathbb{E}[u^N(T, Y_T^{1, N}, \dots, Y_T^{N, N}) - u^N(0, Y_0^{1, N}, \dots, Y_0^{N, N})] \\ &= \mathbb{E}\left[\int_0^T \frac{\partial u^N}{\partial s}(s, Y_s^{1, N}, \dots, Y_s^{N, N}) + \sum_{i=1}^N \frac{\partial u^N}{\partial x_i}(s, Y_s^{1, N}, \dots, Y_s^{N, N}) b\left(Y_s^{i, N}, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j, N}}\right) \right. \\ & \quad \left. + \frac{1}{2} \text{Tr}\left(a\left(Y_s^{i, N}, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j, N}}\right) \sum_{i=1}^N \frac{\partial^2 u^N}{\partial x_i^2}(s, Y_s^{1, N}, \dots, Y_s^{N, N})\right) ds \right] \\ &= \mathbb{E}\left[\int_0^T \partial_s \mathcal{V}\left(s, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j, N}}\right) + \sum_{i=1}^N \left[\frac{1}{N} \partial_\mu \mathcal{V}\left(s, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j, N}}\right)(Y_s^{i, N}) b\left(Y_s^{i, N}, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j, N}}\right) \right. \right. \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \text{Tr} \left(a \left(Y_s^{i,N}, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j,N}} \right) \left(\frac{1}{N} \partial_v \left[\partial_\mu \mathcal{V} \left(s, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j,N}} \right) \right] \left(Y_s^{i,N} \right) \right. \right. \\
& \left. \left. + \frac{1}{N^2} \partial_\mu^2 \mathcal{V} \left(s, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j,N}} \right) \left(Y_s^{i,N}, Y_s^{i,N} \right) \right) \right) ds.
\end{aligned}$$

Therefore, by (1.0.11), the first three terms are cancelled and we are left with

$$\begin{aligned}
& \mathbb{E}[\phi(Y_T^{i,N})] - \mathbb{E}[\phi(X_T)] \\
& = \frac{1}{2N^2} \sum_{i=1}^N \int_0^T \mathbb{E} \left[\text{Tr} \left(a \left(Y_s^{i,N}, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j,N}} \right) \partial_\mu^2 \mathcal{V} \left(s, \frac{1}{N} \sum_{j=1}^N \delta_{Y_s^{j,N}} \right) \left(Y_s^{i,N}, Y_s^{i,N} \right) \right) \right] ds.
\end{aligned} \tag{1.0.12}$$

Equation (1.0.12) is one of the most important formulae in this thesis. It allows us to capture the weak error between a particle system and its mean-field limit by a single term, as opposed to (1.0.6) and (1.0.9), with multiple terms. Note that this compact representation of the weak error is due to the fact that \mathcal{V} already encodes all the information of the dynamics of the mean-field limit. Most of the theory of this thesis is based on this formula.

If we can show that $\partial_\mu^2 \mathcal{V}$ is uniformly bounded (or of a polynomial growth), then (1.0.12) shows that the weak error converges with the order of $O(1/N)$. Nonetheless, as we shall see in Section 3.5, it is in general highly nontrivial to establish regularity properties of the L-derivatives of \mathcal{V} . As the matter of fact, in most cases (other than a few trivial examples), there are no explicit formulae for the L-derivatives of \mathcal{V} . Therefore, (1.0.12) does not really give us much information, apart from its theoretical value in numerical analysis.

Layout of the thesis

We start by a recap on classical results of MVSDEs (Chapter 2), followed by a full exposition of Wasserstein calculus on the results that we need (Chapter 3). Chapters 4 and 5 propose approximating systems to MVSDEs (as alternatives to the classical particle system) via Romberg extrapolation and Antithetic Multi-level Monte-Carlo estimation respectively, which are less costly in terms of computational complexity. Finally, in Chapter 6, we explore the converse: given a standard particle system $\{Y^{i,N}\}$, we hope to find an alternative mean-field limit that gives a better approximation to the standard particle system.

Chapter 2

Preliminaries: An overview of the theory of McKean-Vlasov SDEs

2.1 Set-up of the mean-field model

We continue the discussion on the mean-field model through a probabilistic approach. The particles interact with one another through smooth drift and diffusion functions (also called *interacting kernels*) of the empirical measure of the particles, both in drift and diffusion components.

For the rest of the thesis, unless otherwise specified, we always work with a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ endowed with a d -dimensional Brownian motion W .

To define the framework for McKean-Vlasov SDEs, we need the notion of Wasserstein metric. It is a very important notion in the theory of optimal transport. (See [65] for further details.) Let (M, ρ) be a separable metric space. For $p \geq 1$, let $\mathcal{P}_p(M)$ denote the collection of all probability measures μ on M with finite p^{th} moment, i.e. for some $x_0 \in M$,

$$\int_M \rho(x, x_0)^p \mu(dx) < +\infty.$$

Then the p^{th} Wasserstein distance between two probability measures μ and ν in $\mathcal{P}_p(M)$ is defined as

$$W_{M,p}(\mu, \nu) := \left(\inf_{\gamma \in \Gamma(\mu, \nu)} \int_{M \times M} \rho(x, y)^p d\gamma(x, y) \right)^{\frac{1}{p}},$$

where $\Gamma(\mu, \nu)$ denotes the collection of all measures on $M \times M$ with marginals μ and ν on the first and second factors respectively. (The set $\Gamma(\mu, \nu)$ is also called the set of all *couplings* of μ and ν .) Whenever there is no ambiguity from context, we shall denote $W_{M,p}$ by W_p . Note that if M is a Polish space (i.e. a complete and separable metric space), then the space $(\mathcal{P}_p(M), W_p)$ is also Polish. Furthermore, it is immediate from the definition of the Wasserstein metric that for random variables R_1 and R_2 taking values in M and for probability measures μ and ν on M , we have

$$W_p(\mu, \nu)^p = \inf \left\{ \mathbb{E} \rho(R_1, R_2)^p \mid \begin{array}{l} (R_1, R_2) \text{ has a joint law with marginals } \mu \\ \text{and } \nu \text{ respectively} \end{array} \right\}.$$

Proposition 2.1.1 (Kantorovich-Rubinstein duality theorem). *Let (M, ρ) be a Polish space and let $\mu, \nu \in \mathcal{P}_1(M)$. Then*

$$W_1(\mu, \nu) = \sup_{\phi \in Lip_1(M)} \left[\int_M \phi d\mu - \int_M \phi d\nu \right],$$

where $Lip_1(M)$ denotes the set of all functions $f : M \rightarrow \mathbb{R}$ such that

$$\sup \left\{ \frac{|f(x) - f(y)|}{\rho(x, y)} \mid x, y \in M, x \neq y \right\} \leq 1.$$

Moreover, if $\mu, \nu \in \mathcal{P}_2(M)$, then

$$W_2(\mu, \nu)^2 = \sup_{\substack{\phi_1, \phi_2 \text{ Lipschitz} \\ \phi_1(x) + \phi_2(y) \leq \rho(x, y)^2}} \left[\int_M \phi_1 d\mu + \int_M \phi_2 d\nu \right].$$

The first statement on W_1 can be found in Remark 6.5 in [65], whereas the second statement on W_2 can be found in (8.3.5) in [66].

Let $b : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}^d$ and $\sigma : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d$ be interacting kernels. As usual, let $\{\mathcal{F}_t\}_{t \in [0, T]}$ be the filtration generated by the Brownian motion W . We are interested in the McKean-Vlasov process $\{X_t^{s, \xi}\}_{t \in [s, T]}$ with interacting kernels b and σ , starting from a random variable $\xi \in L^2(\mathcal{F}_s)$, defined by the SDE¹

$$\begin{cases} X_t^{s, \xi} = \xi + \int_s^t b(X_r^{s, \xi}, \mathcal{L}(X_r^{s, \xi})) dr + \int_s^t \sigma(X_r^{s, \xi}, \mathcal{L}(X_r^{s, \xi})) dW_r, & t \in [s, T], \\ \mathcal{L}(X_r^{s, \xi}) := \text{Law}(X_r^{s, \xi}). \end{cases} \quad (2.1.1)$$

Existence and uniqueness to (2.1.1) are known under various assumptions on b and σ . In particular, throughout this work, we assume the condition

Assumption 2.1.2.

b and σ are Lipschitz continuous with respect to the Euclidean norm and the W_2 norm, (Lip)

which guarantees existence and uniqueness by [61]. (See Theorem 2.1.5 below.) On the other hand, weak existence is guaranteed by [57] under the assumption of continuous interacting kernels with linear growth, along with a non-degeneracy assumption on the diffusion. Sufficient conditions for weak existence and pathwise uniqueness in terms of Lyapunov functions of measures are proposed in [35].

The first property to be proven is the uniqueness in law of (2.1.1), which is stated in Lemma 3.1 of [9].

Proposition 2.1.3. *Assume (Lip). Then for any random variables η, η' such that $\mathcal{L}(\eta) = \mathcal{L}(\eta') = \mu$, we have $\mathcal{L}(X_t^{s, \eta}) = \mathcal{L}(X_t^{s, \eta'})$.*

Proof. The main idea of the proof relies on the decoupled process of (2.1.1), defined by

$$X_t^{s, x, \xi} = x + \int_s^t b(X_r^{s, x, \xi}, \mathcal{L}(X_r^{s, \xi})) dr + \int_s^t \sigma(X_r^{s, x, \xi}, \mathcal{L}(X_r^{s, \xi})) dW_r, \quad t \in [s, T], \quad x \in \mathbb{R}^d.$$

By uniqueness of the solution of (2.1.1) (see Theorem 2.1.5), we have

$$X_t^{s, \xi} = X_t^{s, x, \xi} \Big|_{x=\xi}. \quad (2.1.2)$$

Denoting $W^s := \{W_u - W_s\}_{s \leq u \leq T}$, by Yamada-Watanabe theorem, for each $\xi \in L^2(\mathcal{F}_s)$, there exists a $(\mathcal{B}(\mathbb{R}^d) \otimes \mathcal{B}(C([s, T], \mathbb{R}^d))) / \mathcal{B}(C([s, T], \mathbb{R}^d))$ -measurable function $h_\xi : \mathbb{R}^d \times C([s, T], \mathbb{R}^d) \rightarrow C([s, T], \mathbb{R}^d)$ such that

$$X^{s, x, \xi} = h_\xi(x, W^s) \quad \text{almost surely.} \quad (2.1.3)$$

¹We assume without loss of generality that the dimensions of X and W are the same because we will not make any non-degeneracy assumption on the diffusion coefficient σ in our work. In particular, one dimension of X could be time itself.

Let (ξ'_1, ξ'_2) have the same joint law as (ξ_1, ξ_2) , where $\xi_1, \xi_2 \in L^2(\mathcal{F}_s)$. Then, by (2.1.2) and (2.1.3), for every $t' \in [s, T]$,

$$\begin{aligned}
& \sup_{t \in [s, t']} \left[W_2 \left(\mathcal{L}(X_t^{s, \xi_1}), \mathcal{L}(X_t^{s, \xi_2}) \right) \right] \\
& \leq \sup_{t \in [s, t']} \mathbb{E} \left| X_t^{s, \xi_1} - X_t^{s, \xi_2} \right|^2 \\
& = \sup_{t \in [s, t']} \mathbb{E} \left[\left| h_{\xi_1}(\xi_1, W^s) - h_{\xi_2}(\xi_2, W^s) \right|^2 \right] \\
& = \sup_{t \in [s, t']} \mathbb{E} \left[\mathbb{E} \left[\left| h_{\xi_1}(x_1, W^s) - h_{\xi_2}(x_2, W^s) \right|^2 \right] \Big|_{(x_1, x_2) = (\xi_1, \xi_2)} \right] \\
& = \sup_{t \in [s, t']} \mathbb{E} \left[\mathbb{E} \left[\left| X_t^{s, x_1, \xi_1} - X_t^{s, x_2, \xi_2} \right|^2 \right] \Big|_{(x_1, x_2) = (\xi'_1, \xi'_2)} \right] \\
& \leq C \mathbb{E} \left[|\xi'_1 - \xi'_2|^2 + \int_s^{t'} W_2 \left(\mathcal{L}(X_t^{s, \xi_1}), \mathcal{L}(X_t^{s, \xi_2}) \right) dt \right],
\end{aligned} \tag{2.1.4}$$

for some constant $C > 0$ depending only on the Lipschitz constants of b and σ . Gronwall's inequality gives

$$\sup_{t \in [s, T]} \left[W_2 \left(\mathcal{L}(X_t^{s, \xi_1}), \mathcal{L}(X_t^{s, \xi_2}) \right) \right] \leq C \mathbb{E} |\xi'_1 - \xi'_2|^2,$$

which concludes the proof by the definition of the W_2 metric. \square

Remark 2.1.4. Since we work exclusively under assumption (Lip), for any η with $\mathcal{L}(\eta) = \mu$, we adopt the notation $X_t^{s, \mu} := X_t^{s, \eta}$ if only the law of the process is concerned. Similarly, we adopt the notation $X_t^{s, x, \mu} := X_t^{s, x, \eta}$, since any two processes X_t^{s, x, η_1} and X_t^{s, x, η_2} are indistinguishable, provided that η_1 and η_2 have the same law.

Since the initial condition of the process (2.1.1) is fixed to be $\xi \sim \nu \in \mathcal{P}_2(\mathbb{R}^d)$, we denote X to be the process $\{X_t^{0, \xi}\}_{t \in [0, T]}$ with marginal laws $\mu_t^X := \mathcal{L}(X_t^{0, \xi})$:

$$X_t = \xi + \int_0^t b(X_r, \mu_r^X) dr + \int_0^t \sigma(X_r, \mu_r^X) dW_r, \quad t \in [0, T]. \tag{2.1.5}$$

Theorem 2.1.5 (Existence and uniqueness of solutions to McKean-Vlasov SDEs, [61]). *Assume (Lip). Then (2.1.5) admits a strong solution $X \in \mathcal{H}^2$ which satisfies the property of pathwise uniqueness.*

Proof. For every $t \in [0, T]$, let $C([0, t], \mathbb{R}^d)$ be the set of continuous functions from $[0, t]$ to \mathbb{R}^d . We define the metric $d_t(f, g) = \sup_{u \in [0, t]} |f(u) - g(u)|$. Then $\mathcal{C}_t := (C([0, t], \mathbb{R}^d), d_t)$ is a Polish space, for each $t \in [0, T]$.

We consider a mapping $\Phi : \mathcal{P}_2(\mathcal{C}_T) \rightarrow \mathcal{P}_2(\mathcal{C}_T)$, which maps any measure $\mu \in \mathcal{P}_2(\mathcal{C}_T)$ to the law of X^μ defined by

$$dX_t^\mu = b(X_t^\mu, \mu_t) dt + \sigma(X_t^\mu, \mu_t) dW_t, \quad X_0^\mu = \xi, \quad t \in [0, T], \tag{2.1.6}$$

with μ_t being the t -marginal of μ . We first show that Φ is well-defined. By (Lip), it is clear that the functions

$$\underline{b}(t, x) := b(x, \mu_t); \quad \underline{\sigma}(t, x) := \sigma(x, \mu_t)$$

are Lipschitz continuous and have linear growth, uniform in time. Hence, it follows from standard results of SDE theory (e.g. Theorem 3.1 in [50]) that (2.1.6) has a strong solution in \mathcal{H}^2 which also satisfies the property of pathwise uniqueness, for each probability measure $\mu \in \mathcal{P}_2(\mathcal{C}_T)$. By the Yamada-Watanabe theorem, the solution also satisfies uniqueness in law.

Finally, since $X^\mu \in \mathcal{H}^2$,

$$\int_{\mathcal{C}_T} \sup_{0 \leq t \leq T} |y(t)|^2 \mathcal{L}(X^\mu)(dy) = \mathbb{E} \left[\sup_{0 \leq t \leq T} |X_t^\mu|^2 \right] < +\infty,$$

which shows that $\mathcal{L}(X^\mu) \in \mathcal{P}_2(\mathcal{C}_T)$.

We now observe that the process X^μ is a strong solution to (2.1.6) if and only if μ is a fixed point of Φ .

For $\mu_1, \mu_2 \in \mathcal{P}_2(\mathcal{C}_T)$, we denote $\delta X_s = X_s^{\mu_1} - X_s^{\mu_2}$, $\delta b_s = b(X_s^{\mu_1}, (\mu_1)_s) - b(X_s^{\mu_2}, (\mu_2)_s)$ and $\delta \sigma_s = \sigma(X_s^{\mu_1}, (\mu_1)_s) - \sigma(X_s^{\mu_2}, (\mu_2)_s)$. By the Cauchy-Schwarz inequality,

$$|\delta X_s|^2 \leq 2 \left(\left| \int_0^s \delta b_u du \right|^2 + \left| \int_0^s \delta \sigma_u dW_u \right|^2 \right) \leq 2 \left(s \int_0^s |\delta b_u|^2 du + \left| \int_0^s \delta \sigma_u dW_u \right|^2 \right).$$

By the Burkholder-Davis-Gundy inequality, for each $t \in [0, T]$,

$$\begin{aligned} \mathbb{E} \left[\sup_{s \in [0, t]} |\delta X_s|^2 \right] &\lesssim \int_0^t \mathbb{E} [|\delta b_u|^2] du + \int_0^t \mathbb{E} [|\delta \sigma_u|^2] du \\ &\lesssim \int_0^t \mathbb{E} [|\delta X_u|^2] du + \int_0^t W_{\mathbb{R}^d, 2}^2((\mu_1)_u, (\mu_2)_u) du \\ &\lesssim \int_0^t \mathbb{E} \left[\sup_{r \in [0, u]} |\delta X_r|^2 \right] du + \int_0^t W_{\mathbb{R}^d, 2}^2((\mu_1)_u, (\mu_2)_u) du. \end{aligned}$$

Gronwall's lemma implies that for each $t \in [0, T]$,

$$\mathbb{E} \left[\sup_{s \in [0, t]} |\delta X_s|^2 \right] \leq C \int_0^t W_{\mathbb{R}^d, 2}^2((\mu_1)_u, (\mu_2)_u) du. \quad (2.1.7)$$

For any $\mu \in \mathcal{P}_2(\mathcal{C}_T)$, we define the restriction $\mu|_{[0, t]} \in \mathcal{P}_2(\mathcal{C}_t)$ by

$$\mu|_{[0, t]}(A) := \mu \left\{ \gamma \in \mathcal{C}_T \mid \gamma|_{[0, t]} \in A \right\}, \quad A \in \mathcal{B}(\mathcal{C}_t).$$

Next, we notice that $W_{\mathcal{C}_t, 2}^2(\Phi(\mu_1)|_{[0, t]}, \Phi(\mu_2)|_{[0, t]}) \leq \mathbb{E} \left[\sup_{s \in [0, t]} |\delta X_s|^2 \right]$ and that $W_{\mathbb{R}^d, 2}^2((\mu_1)_u, (\mu_2)_u) \leq W_{\mathcal{C}_u, 2}^2(\mu_1|_{[0, u]}, \mu_2|_{[0, u]})$. Inequality (2.1.7) then gives

$$W_{\mathcal{C}_t, 2}^2(\Phi(\mu_1)|_{[0, t]}, \Phi(\mu_2)|_{[0, t]}) \leq C \int_0^t W_{\mathcal{C}_u, 2}^2(\mu_1|_{[0, u]}, \mu_2|_{[0, u]}) du.$$

By iterating this inequality, we obtain that for any $N \in \mathbb{N}$,

$$\begin{aligned} W_{\mathcal{C}_T, 2}^2(\Phi^N(\mu_1), \Phi^N(\mu_2)) &\leq C \int_0^T W_{\mathcal{C}_u, 2}^2(\Phi^{N-1}(\mu_1)|_{[0, u]}, \Phi^{N-1}(\mu_2)|_{[0, u]}) du \\ &\leq C^2 \int_0^T (T-u) W_{\mathcal{C}_u, 2}^2(\Phi^{N-2}(\mu_1)|_{[0, u]}, \Phi^{N-2}(\mu_2)|_{[0, u]}) du \\ &\vdots \\ &\leq C^N \int_0^T \frac{(T-u)^{N-1}}{(N-1)!} W_{\mathcal{C}_u, 2}^2(\mu_1|_{[0, u]}, \mu_2|_{[0, u]}) du \\ &\leq C^N \frac{T^N}{N!} W_{\mathcal{C}_T, 2}^2(\mu_1, \mu_2). \end{aligned}$$

For sufficiently large N , Φ^N is a contraction, so Φ admits a fixed point.

It remains to show strong uniqueness. Suppose that X^1 and X^2 are both strong solutions

of (2.1.5), with laws μ_1 and μ_2 respectively. Then, by inequality (2.1.7),

$$\begin{aligned} \mathbb{E} \left[\sup_{s \in [0, t]} |X_s^1 - X_s^2|^2 \right] &= \mathbb{E} \left[\sup_{s \in [0, t]} |X_s^{\mu_1} - X_s^{\mu_2}|^2 \right] \\ &\leq C \int_0^t W_{\mathbb{R}^d, 2}^2((\mu_1)_u, (\mu_2)_u) du \\ &\leq C \int_0^t \mathbb{E} |X_u^1 - X_u^2|^2 du \\ &\leq C \int_0^t \mathbb{E} \left[\sup_{s \in [0, u]} |X_s^1 - X_s^2|^2 \right] du. \end{aligned}$$

Gronwall's lemma concludes that X^1 and X^2 are indistinguishable processes. \square

2.2 Fokker-Planck PDE and the standard interacting particle system

With the issue of existence of solutions to the McKean-Vlasov SDE out of the way, we can be able to perform formal computations and obtain its corresponding Fokker-Planck PDE.

Suppose, for convenience, that the McKean-Vlasov SDE admits a probability density function $p(t, x)$. Assume that b and σ satisfy (Lip). Let $a : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d$ be a function defined as

$$a(x, \mu) = \sigma(x, \mu) \sigma^T(x, \mu). \quad (2.2.1)$$

By Itô's formula, for $f \in C_b^\infty(\mathbb{R}^d)$,

$$\begin{aligned} f(X_t) &= f(X_0) + \int_0^t \sum_{i=1}^d \sum_{l=1}^d \frac{\partial f}{\partial x_i}(X_s) \sigma_{il}(X_s, \mu_s^X) dW_s^l + \int_0^t \left(\sum_{i,j=1}^d \frac{1}{2} a_{ij}(X_s, \mu_s^X) \frac{\partial^2 f}{\partial x_i \partial x_j}(X_s) \right. \\ &\quad \left. + \sum_{i=1}^d b_i(X_s, \mu_s^X) \frac{\partial f}{\partial x_i}(X_s) \right) ds. \end{aligned}$$

By (Lip), it is clear that the expectation of the stochastic integral vanishes. Taking the expectation and differentiating both sides with respect to t , we have

$$\frac{\partial}{\partial t} \int_{\mathbb{R}^d} f(x) p(t, x) dx = \int_{\mathbb{R}^d} \left(\frac{1}{2} \sum_{i,j=1}^d a_{ij}(x, \mu_t^X) \frac{\partial^2 f}{\partial x_i \partial x_j}(x) + \sum_{i=1}^d b_i(x, \mu_t^X) \frac{\partial f}{\partial x_i}(x) \right) p(t, x) dx. \quad (2.2.2)$$

Integrating by parts yields the weak form

$$\frac{\partial p}{\partial t}(t, x) = \frac{1}{2} \sum_{i,j=1}^d \frac{\partial^2}{\partial x_i \partial x_j} \left(a_{ij}(x, \mu_t^X) p(t, x) \right) - \sum_{i=1}^d \frac{\partial}{\partial x_i} \left(b_i(x, \mu_t^X) p(t, x) \right),$$

keeping in mind that it is to be interpreted as in (2.2.2).

To fully understand the relationship with PDEs, we consider the following one-dimensional McKean-Vlasov SDE:

$$dX_t = A' \left(\int_{\mathbb{R}} H(X_t - y) \mu_t^X(dy) \right) dt + \sigma dW_t, \quad 0 \leq t \leq T, \quad (2.2.3)$$

where $A : \mathbb{R} \rightarrow \mathbb{R}$ is a C^3 function and $\sigma > 0$ and $H(x) = \mathbf{1}_{\{x \geq 0\}}$ is the Heaviside function. By the Girsanov's theorem, it is easy to show that the process $\{X_t\}_{t \in [0, T]}$ has a probability density function $p(t, x)$. (See Proposition 1.1 in [54].) The corresponding weak formulation is

thus given by

$$\frac{\partial p}{\partial t}(t, x) = -\frac{\partial}{\partial x} \left\{ A' \left(\int_{\mathbb{R}} H(X_t - y) \mu_t^X(dy) \right) p(t, x) \right\} + \frac{\sigma^2}{2} \frac{\partial^2}{\partial x^2} p(t, x).$$

Let $V(t, x)$ be the cumulative distribution of $\{X_t\}_{t \in [0, T]}$. Noting that $\int_{\mathbb{R}} H(x - y) \mu_t^X(dy) = V(t, x)$ and that $p(t, x) = \frac{\partial V}{\partial x}(t, x)$, we obtain the following equivalent form.

Example 2.2.1 (1D viscous scalar conservation law).

$$\begin{cases} \frac{\partial V}{\partial t}(t, x) = \frac{\sigma^2}{2} \frac{\partial^2 V}{\partial x^2}(t, x) - \frac{\partial}{\partial x} A(V(t, x)), & \forall (t, x) \in (0, T] \times \mathbb{R}, \\ V(0, x) = V_0(x), & \forall x \in \mathbb{R}. \end{cases}$$

In the special case when $A(v) = \frac{v^2}{2}$, the conversation law is the viscous Burgers equation.

Example 2.2.2 (Burgers equation).

$$\begin{cases} \frac{\partial V}{\partial t}(t, x) = \frac{\sigma^2}{2} \frac{\partial^2 V}{\partial x^2}(t, x) - V(t, x) \frac{\partial V}{\partial x}(t, x), & \forall (t, x) \in (0, T] \times \mathbb{R}, \\ V(0, x) = V_0(x), & \forall x \in \mathbb{R}. \end{cases}$$

This approach is one of the probabilistic interpretations of PDEs. We interpret the solution of a PDE as the cumulative distribution function (or probability density function) of a stochastic nonlinear process. This approach from a probabilistic point of view has been studied by several authors. (See the works of Sznitman [61] and Bossy, Jourdain [6], for example.) Theorem 2.1.5 merely gives us an existence result via a fixed-point argument. It does not tell us about the nature of the solution. Thanks to the propagation of chaos result for systems of interacting particles, many numerical algorithms can be formulated. Note that (2.2.3) involves the Heaviside function, which is not a smooth function. Therefore, its properties and approximation are not covered in this work.

The stochastic simulation of the McKean-Vlasov SDE is very natural. It consists of replacing the law μ_t^X , which appears explicitly in the drift and diffusion coefficients, by its approximation given by the empirical distribution of the particle system $(Y^{1, N}, \dots, Y^{N, N})$, which is defined by the $(\mathbb{R}^d)^N$ -dimensional classical SDE

$$\begin{cases} Y_t^{i, N} = \xi_i + \int_0^t b(Y_s^{i, N}, \mu_s^{Y, N}) ds + \int_0^t \sigma(Y_s^{i, N}, \mu_s^{Y, N}) dW_s^i, & 1 \leq i \leq N, \quad t \in [0, T], \\ \mu_s^{Y, N} := \frac{1}{N} \sum_{i=1}^N \delta_{Y_s^{i, N}}, \end{cases} \quad (2.2.4)$$

where $(W^i)_{i \in \mathbb{N}}$ are independent \mathbb{R}^d -valued Brownian motions and $(\xi_i)_{i \in \mathbb{N}}$ are i.i.d. random variables with the same law as $\xi \sim \nu$, independent of $(W^i)_{i \in \mathbb{N}}$. Equation (2.2.4) exhibits the essence of interaction between particles. For any particle i , the knowledge of $Y_t^{i, N}$ is not sufficient to approximate $Y_{t+\Delta t}^{i, N}$: the knowledge of the positions of the other particles $Y^{j, N}$, $j \neq i$, is also required. We also observe that, by standard results of SDE theory (e.g. Theorem 3.1 in [50]), (2.2.4) has a unique strong solution if (Lip) holds.

To compare this particle system with the original McKean-Vlasov SDE, we can introduce a *coupling* between the system $(Y^{i, N})$ and a system (X^i) of independent processes with the same law as X and being defined on the same probability space as $(Y^{i, N})$:

$$X_t^i = \xi_i + \int_0^t b(X_s^i, \mu_s^X) ds + \int_0^t \sigma(X_s^i, \mu_s^X) dW_s^i, \quad 1 \leq i \leq N, \quad t \in [0, T]. \quad (2.2.5)$$

The next theorem is stated for b and σ having first-order interaction.

Assumption 2.2.3.

$$b(x, \mu) := \int_{\mathbb{R}^d} B(x, y) \mu(dy) \quad \text{and} \quad \sigma(x, \mu) := \int_{\mathbb{R}^d} \Sigma(x, y) \mu(dy). \quad (\text{First order})$$

Assumption 2.2.4.

$B : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $\Sigma : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d$ are Lipschitz continuous. (B and Σ -Lip)

Note that (First order) and (B and Σ -Lip) imply (Lip), since

$$\begin{aligned} & |b(x, \mu_1) - b(y, \mu_2)| \\ &= \left| \int_{\mathbb{R}^d} B(x, z) \mu_1(dz) - \int_{\mathbb{R}^d} B(y, z) \mu_2(dz) \right| \\ &\leq \left| \int_{\mathbb{R}^d} B(x, z) \mu_1(dz) - \int_{\mathbb{R}^d} B(x, z) \mu_2(dz) \right| + \left| \int_{\mathbb{R}^d} B(x, z) \mu_2(dz) - \int_{\mathbb{R}^d} B(y, z) \mu_2(dz) \right| \\ &\leq \|B\|_{\text{Lip}} \left(W_1(\mu_1, \mu_2) + |x - y| \right) \leq \|B\|_{\text{Lip}} \left(W_2(\mu_1, \mu_2) + |x - y| \right), \end{aligned}$$

where the second inequality comes from Proposition 2.1.1 and the final inequality comes from Jensen's inequality. The argument for σ is identical.

Note that if the initial law ν satisfies

Assumption 2.2.5.

$$\int_{\mathbb{R}^d} |x|^{2p} \nu(dx) < +\infty, \quad (p\text{-Int})$$

for some $p > 1$, then it follows by a standard Gronwall-type argument that

$$\sup_{u \in [0, T]} \mathbb{E}[|X_u|^{2p}] < +\infty, \quad \sup_{N \in \mathbb{N}} \sup_{u \in [0, T]} \mathbb{E}[|Y_u^{1, N}|^{2p}] < +\infty, \quad \sup_{N \in \mathbb{N}} \mathbb{E}[\|Y_t^{1, N} - Y_s^{1, N}\|^{2p}] \leq C|t-s|^p, \quad (2.2.6)$$

for each $0 \leq s, t \leq T$, for some $C > 0$. The following theorem ([61]) gives a bound on the strong error of the particle approximation.

Theorem 2.2.6. Assume (First order), (B and Σ -Lip) and (p -Int), for $p = 2$. Then

$$\sup_{t \in [0, T]} \mathbb{E} \left[|Y_t^{i, N} - X_t^i|^2 \right] \leq \frac{C}{N},$$

where C is a constant independent of N .

Proof. By Itô's formula,

$$\begin{aligned} \mathbb{E}[(Y_t^{i, N} - X_t^i)^2] &= 2\mathbb{E} \left[\int_0^t (Y_s^{i, N} - X_s^i) \left(\frac{1}{N} \sum_{j=1}^N \Sigma(Y_s^{i, N}, Y_s^{j, N}) - \int_{\mathbb{R}^d} \Sigma(X_s^i, y) \mu_s^X(dy) \right) dW_s^i \right] \\ &\quad + \int_0^t \mathbb{E} \left[\left(\frac{1}{N} \sum_{j=1}^N \Sigma(Y_s^{i, N}, Y_s^{j, N}) - \int_{\mathbb{R}^d} \Sigma(X_s^i, y) \mu_s^X(dy) \right)^2 \right] ds \\ &\quad + 2 \int_0^t \mathbb{E} \left[(Y_s^{i, N} - X_s^i) \left(\frac{1}{N} \sum_{j=1}^N B(Y_s^{i, N}, Y_s^{j, N}) - \int_{\mathbb{R}^d} B(X_s^i, y) \mu_s^X(dy) \right) \right] ds. \end{aligned}$$

By the Cauchy-Schwarz inequality and (2.2.6), the first term vanishes. Using the simple inequality that $(a + b + c)^2 \leq 3(a^2 + b^2 + c^2)$, we decompose the second term as

$$\begin{aligned} \left(\frac{1}{N} \sum_{j=1}^N \Sigma(Y_s^{i, N}, Y_s^{j, N}) - \int_{\mathbb{R}^d} \Sigma(X_s^i, y) \mu_s^X(dy) \right)^2 &\leq 3 \left(\frac{1}{N} \sum_{j=1}^N (\Sigma(Y_s^{i, N}, Y_s^{j, N}) - \Sigma(Y_s^{i, N}, X_s^j)) \right)^2 \\ &\quad + 3 \left(\frac{1}{N} \sum_{j=1}^N (\Sigma(Y_s^{i, N}, X_s^j) - \Sigma(X_s^i, X_s^j)) \right)^2 \\ &\quad + 3A_s(\Sigma), \end{aligned}$$

where $A_s(h) = \left(\frac{1}{N} \sum_{j=1}^N h(X_s^i, X_s^j) - \int_{\mathbb{R}^d} h(X_s^i, y) \mu_s^X(dy) \right)^2$, for $h \in \{B, \Sigma\}$. By the Cauchy-Schwarz inequality and the Lipschitz property of Σ , we obtain that

$$\mathbb{E} \left[\left(\frac{1}{N} \sum_{j=1}^N \Sigma(Y_s^{i,N}, Y_s^{j,N}) - \int_{\mathbb{R}^d} \Sigma(X_s^i, y) \mu_s^X(dy) \right)^2 \right] \leq 6 \|\Sigma\|_{\text{Lip}}^2 \mathbb{E} \left[|Y_s^{i,N} - X_s^i|^2 \right] + 3 \mathbb{E} [A_s(\Sigma)].$$

Similarly,

$$\mathbb{E} \left[\left(\frac{1}{N} \sum_{j=1}^N B(Y_s^{i,N}, Y_s^{j,N}) - \int_{\mathbb{R}^d} B(X_s^i, y) \mu_s^X(dy) \right)^2 \right] \leq 6 \|B\|_{\text{Lip}}^2 \mathbb{E} \left[|Y_s^{i,N} - X_s^i|^2 \right] + 3 \mathbb{E} [A_s(B)].$$

For the third term, we have

$$\begin{aligned} & \mathbb{E} \left[2(Y_s^{i,N} - X_s^i) \left(\frac{1}{N} \sum_{j=1}^N B(Y_s^{i,N}, Y_s^{j,N}) - \int_{\mathbb{R}^d} B(X_s^i, y) \mu_s^X(dy) \right) \right] \\ & \leq (6 \|B\|_{\text{Lip}}^2 + 1) \mathbb{E} \left[|Y_s^{i,N} - X_s^i|^2 \right] + 3 \mathbb{E} [A_s(B)]. \end{aligned}$$

We therefore get the inequality

$$\mathbb{E} [(Y_t^{i,N} - X_t^i)^2] \leq (6 \|\Sigma\|_{\text{Lip}}^2 + 6 \|B\|_{\text{Lip}}^2 + 1) \int_0^t \mathbb{E} [(Y_s^{i,N} - X_s^i)^2] ds + 3 \int_0^t \mathbb{E} [A_s(\Sigma) + A_s(B)] ds.$$

Gronwall's lemma implies that

$$\mathbb{E} [(Y_t^{i,N} - X_t^i)^2] \leq 3 \exp \left\{ (6 \|\Sigma\|_{\text{Lip}}^2 + 6 \|B\|_{\text{Lip}}^2 + 1)t \right\} \int_0^t \mathbb{E} [A_s(\Sigma) + A_s(B)] ds.$$

Fix $h \in \{B, \Sigma\}$. Then

$$\begin{aligned} \mathbb{E} [A_s(h)] &= \mathbb{E} \left[\left(\frac{1}{N} \sum_{j=1}^N h(X_s^i, X_s^j) - \int_{\mathbb{R}^d} h(X_s^i, y) \mu_s^X(dy) \right)^2 \right] \\ &\leq 3 \left(\mathbb{E} \left[\frac{1}{N^2} h(X_s^i, X_s^i)^2 \right] + \mathbb{E} \left[\left(\frac{1}{N} \sum_{j \neq i} h(X_s^i, X_s^j) - \frac{1}{N-1} \sum_{j \neq i} h(X_s^i, X_s^j) \right)^2 \right] \right. \\ &\quad \left. + \mathbb{E} \left[\left(\frac{1}{N-1} \sum_{j \neq i} h(X_s^i, X_s^j) - \int_{\mathbb{R}^d} h(X_s^i, y) \mu_s^X(dy) \right)^2 \right] \right) \\ &\lesssim \frac{1}{N^2} + \mathbb{E} \left[\text{Var} \left[\frac{1}{N-1} \sum_{j \neq i} \left(h(x, X_s^j) - \int_{\mathbb{R}^d} h(x, y) \mu_s^X(dy) \right) \right] \Big|_{x=X_s^i} \right] \\ &= \frac{1}{N^2} + \mathbb{E} \left[\left[\frac{1}{(N-1)^2} \sum_{j \neq i} \text{Var} \left(h(x, X_s^j) - \int_{\mathbb{R}^d} h(x, y) \mu_s^X(dy) \right) \right] \Big|_{x=X_s^i} \right] \\ &\lesssim \frac{1}{N}, \end{aligned} \tag{2.2.7}$$

where the final estimate uses the fact that B and Σ are Lipschitz and therefore have linear growth as well. This completes the proof. \square

2.3 Propagation of Chaos

In this section, we explore the phenomenon in which interacting particles become asymptotically independent as their number goes to infinity, known as *propagation of chaos*. The goal of this section is to establish the result that the interacting particle system (2.2.4) indeed satisfies this property, by following closely the works of [61] and [53].

Definition 2.3.1. In a Polish space E , let $(Q^n)_n$ be a sequence of symmetric probability measures on E^n . Moreover, let Q be a probability measure on E . We say that $(Q^n)_n$ is *Q-chaotic* if for all $k \geq 1$, $\phi_1, \dots, \phi_k \in C_b(E)$,

$$\int_{E^n} \phi_1(x_1) \dots \phi_k(x_k) Q^n(d(x_1, \dots, x_n)) \xrightarrow{n \rightarrow \infty} \left(\int_E \phi_1 dQ \right) \dots \left(\int_E \phi_k dQ \right).$$

We start by giving equivalent conditions to chaotic sequences of measures.

Let us first recall the notion of a convergence determining class. Suppose that $\{X_n\}$ is a sequence of random variables taking values in (E, d) . To show that X_n converges to X in distribution, we need to prove that

$$\mathbb{E}[f(X_n)] \rightarrow \mathbb{E}[f(X)],$$

for all bounded continuous $f : E \rightarrow \mathbb{R}$. However, this is usually not practical because the class of bounded continuous functions is too large. Instead, we typically find a special class U of functions which are easier to evaluate, such that $\mathbb{E}[f(X_n)] \rightarrow \mathbb{E}[f(X)]$, for all $f \in U$ still implies $X_n \Rightarrow X$. Such a class U is called a convergence determining class. The following result gives a sufficient condition for convergence determining classes in a Polish space. (See, for example, Chapter 3 in [24], for details of the proof.)

Lemma 2.3.2. *Let (E, d) be a Polish space. Let $M \subseteq C_b(E)$ be an algebra (i.e. a vector space closed under pointwise multiplication). If M strongly separates points, i.e. for every $x \in E$ and $\delta > 0$, there exists a finite set $\{h_1, \dots, h_k\} \subseteq M$ such that*

$$\inf_{y: d(y, x) \geq \delta} \max_{1 \leq i \leq k} |h_i(y) - h_i(x)| > 0,$$

then M is convergence determining.

Theorem 2.3.3. *Let E be a Polish space. Let $(Q^n)_n$ be a sequence of symmetric probability measures on E^n and Q be a probability measure on E . Moreover, let $X^{1,n}, \dots, X^{n,n}$ be E -valued random variables such that $\mathcal{L}((X^{1,n}, \dots, X^{n,n})) = Q^n$. We define their empirical measure as $\mu^n = \frac{1}{n} \sum_{i=1}^n \delta_{X^{i,n}}$. Then, the following statements are equivalent.*

- (i) $(Q^n)_n$ is *Q-chaotic*,
- (ii) $\mathbb{E}[|\int_E f d\mu^n - \int_E f dQ|] \xrightarrow{n \rightarrow \infty} 0$, $\forall f \in C_b(E)$,
- (iii) μ^n converges weakly to Q (as $\mathcal{P}(E)$ -valued random variables).

Proof. (i) \implies (ii). By definition, for each n , $(X^{1,n}, \dots, X^{n,n})$ is exchangeable. Hence, for each $f \in C_b(E)$,

$$\begin{aligned} \mathbb{E} \left[\left(\int_E f d\mu^n - \int_E f dQ \right)^2 \right] &= \mathbb{E} \left[\left(\frac{1}{n} \sum_{i=1}^n f(X^{i,n}) - \int_E f dQ \right)^2 \right] \\ &= \mathbb{E} \left[\frac{1}{n^2} \sum_{i,j=1}^n f(X^{i,n}) f(X^{j,n}) - \frac{2}{n} \int_E f dQ \sum_{i=1}^n f(X^{i,n}) \right. \\ &\quad \left. + \left(\int_E f dQ \right)^2 \right] \\ &= \frac{1}{n} \mathbb{E} \left[(f(X^{1,n}))^2 \right] + \frac{n-1}{n} \mathbb{E} \left[f(X^{1,n}) f(X^{2,n}) \right] \\ &\quad - 2 \left(\int_E f dQ \right) \mathbb{E} \left[f(X^{1,n}) \right] + \left(\int_E f dQ \right)^2 \\ &\xrightarrow{n \rightarrow \infty} \left(\int_E f dQ \right)^2 - 2 \left(\int_E f dQ \right)^2 + \left(\int_E f dQ \right)^2 = 0. \end{aligned}$$

This establishes L^1 convergence.

(ii) \implies (i). Let $k \geq 1$ and $f_1, \dots, f_k \in C_b(E)$. Then, by assumption, $\int_E f_j d\mu^n \rightarrow \int_E f_j dQ$ in L^1 , for $j \in \{1, \dots, k\}$. Therefore, $\int_E f_j d\mu^n \rightarrow \int_E f_j dQ$ in probability, for $j \in \{1, \dots, k\}$. By a standard result concerning convergence in probability, we deduce that

$$\int_E f_1 d\mu^n \dots \int_E f_k d\mu^n \rightarrow \int_E f_1 dQ \dots \int_E f_k dQ \quad \text{in probability.}$$

Since the sequence of random variables $\{\int_E f_1 d\mu^n \dots \int_E f_k d\mu^n\}$ is uniformly bounded by $\|f_1\|_\infty \dots \|f_k\|_\infty$, we also have

$$\int_E f_1 d\mu^n \dots \int_E f_k d\mu^n \rightarrow \int_E f_1 dQ \dots \int_E f_k dQ \quad \text{in } L^1.$$

By the triangle inequality,

$$\begin{aligned} & \left| \mathbb{E}[f_1(X^{1,n}) \dots f_k(X^{k,n})] - \int_E f_1 dQ \dots \int_E f_k dQ \right| \\ &= \left| \mathbb{E}[f_1(X^{1,n}) \dots f_k(X^{k,n})] - \mathbb{E}\left[\int_E f_1 d\mu^n \dots \int_E f_k d\mu^n\right] \right| \\ & \quad + \left| \mathbb{E}\left[\int_E f_1 d\mu^n \dots \int_E f_k d\mu^n\right] - \int_E f_1 dQ \dots \int_E f_k dQ \right|. \end{aligned}$$

By above, the second term on the right converges to zero. The first term can be rewritten as

$$\begin{aligned} & \left| \mathbb{E}[f_1(X^{1,n}) \dots f_k(X^{k,n})] - \frac{1}{n^k} \sum_{i_1, \dots, i_k=1}^n \mathbb{E}[f_1(X^{i_1,n}) \dots f_k(X^{i_k,n})] \right| \\ & \leq \left| \mathbb{E}[f_1(X^{1,n}) \dots f_k(X^{k,n})] - \frac{1}{n^k} \sum_{\substack{i_1, \dots, i_k=1 \\ i_1, \dots, i_k \text{ all different}}}^n \mathbb{E}[f_1(X^{i_1,n}) \dots f_k(X^{i_k,n})] \right| \\ & \quad + \frac{1}{n^k} \sum_{\substack{i_1, \dots, i_k=1 \\ \text{some of } i_1, \dots, i_k \text{ are the same}}}^n \left| \mathbb{E}[f_1(X^{i_1,n}) \dots f_k(X^{i_k,n})] \right| \\ & \leq \mathbb{E}[f_1(X^{1,n}) \dots f_k(X^{k,n})] \left[1 - \frac{1}{n^k} \frac{n!}{(n-k)!} \right] + \frac{1}{n^k} \left[\sum_{j=1}^k \|f_j\|_\infty \right]^k \left[n^k - \frac{n!}{(n-k)!} \right] \\ & = \left(1 - \frac{1}{n^k} \frac{n!}{(n-k)!} \right) \left[\mathbb{E}[f_1(X^{1,n}) \dots f_k(X^{k,n})] + \left(\sum_{j=1}^k \|f_j\|_\infty \right)^k \right] \\ & \leq 2 \left(\sum_{j=1}^k \|f_j\|_\infty \right)^k \left(1 - \frac{1}{n^k} \frac{n!}{(n-k)!} \right) \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

(iii) \implies (ii). Suppose that μ^n converges weakly to Q . As a $\mathcal{P}(E)$ -valued random variable, Q is constant. Hence, $\mu^n \rightarrow Q$ in probability. Take any $f \in C_b(E)$. We define a continuous map

$$\Phi : \mathcal{P}(E) \rightarrow \mathbb{R}; \quad \nu \mapsto \int_E f d\nu.$$

It follows by standard properties of convergence in probability that $\Phi(\mu^n) \rightarrow \Phi(Q)$ in probability, i.e.

$$\int_E f d\mu^n \rightarrow \int_E f dQ \quad \text{in probability.}$$

Note that $\left\{ \int_E f d\mu^n \right\}$ is uniformly bounded by $\|f\|_\infty$ and is hence uniformly integrable.

This implies that

$$\int_E f d\mu^n \rightarrow \int_E f dQ \quad \text{in } L^1.$$

(ii) \implies (iii). Since E is Polish, it is a standard result that $\mathcal{P}(E)$ (equipped with the weak topology) is also a Polish space. Let $M \subseteq C_b(\mathcal{P}(E))$ be defined by

$$M = \left\{ \Phi : \mathcal{P}(E) \rightarrow \mathbb{R} \mid \begin{array}{l} \Phi(\nu) = \sum_{i=1}^n c_i \int_E f_1^{(i)} d\nu \dots \int_E f_{\ell_i}^{(i)} d\nu, \quad \text{where } n, \ell_1, \dots, \ell_n \in \mathbb{N}, \\ c_1, \dots, c_n \in \mathbb{R}, \quad f_1^{(1)}, \dots, f_{\ell_1}^{(1)}, \dots, f_1^{(n)}, \dots, f_{\ell_n}^{(n)} \in C_b(E) \end{array} \right\}.$$

We can argue in the same way as in the implication of (ii) \implies (i) to show that

$$\mathbb{E}[\Phi(\mu^n)] \rightarrow \mathbb{E}[\Phi(Q)], \quad \forall \Phi \in M.$$

By the definition of M , it is an algebra. Moreover, by the seminorm characterisation of the weak topology, it is easy to see that M is strongly separating. Thus, by Lemma 2.3.2, M is a convergence determining set, i.e.

$$\mathbb{E}[\Phi(\mu^n)] \rightarrow \mathbb{E}[\Phi(Q)], \quad \forall \Phi \in C_b(\mathcal{P}(E)).$$

□

Let (E, d) be a Polish space, equipped with its Borel sigma-algebra and let $M \subseteq \mathcal{P}(E)$ be a collection of probability measures defined on E . Recall that the collection M is called tight if, for any $\epsilon > 0$, there is a compact subset K_ϵ of S such that

$$\sup_{\mu \in M} \mu(E \setminus K_\epsilon) < \epsilon.$$

If we equip $\mathcal{P}(E)$ with the topology of weak convergence (which is metrisable), then the Prokhorov's theorem states that for any collection of probability measures $M \subseteq \mathcal{P}(E)$,

$$M \text{ is tight} \quad \iff \quad M \text{ is precompact.}$$

We consider the system of interacting particles as described in (2.2.4) for the remaining of this section. In this situation, $Y^{1,N}, \dots, Y^{N,N}$ are C_T -valued random variables. To apply Theorem 2.3.3, we set $E = C_T$. Our goal is to prove condition (iii) in Theorem 2.3.3 in order to establish chaoticity. The Prokhorov's theorem therefore leads to the classical trilogy of arguments:

- (I) Tightness of $(\mathcal{L}(\mu^{Y,N}))_{N \in \mathbb{N}}$ in $\mathcal{P}(\mathcal{P}(C_T))$.
- (II) Identification of the limiting value of a subsequence of $(\mathcal{L}(\mu^{Y,N}))_{N \in \mathbb{N}}$ (by Prokhorov's theorem).
- (III) The use of a uniqueness argument to conclude that the limit is equal to δ_Q , where Q is defined to be the solution to some martingale problem.

Since the space $\mathcal{P}(\mathcal{P}(C_T))$ is very complicated to analyse, the following result transfers the analysis of tightness in $\mathcal{P}(\mathcal{P}(C_T))$ to a more "manageable" space.

Lemma 2.3.4. *Let E be a Polish space and (m^n) be a sequence of probability measures in the space $\mathcal{P}(\mathcal{P}(E))$. Then*

$$(m^n)_n \text{ is tight} \quad \iff \quad (I(m^n))_n \subseteq \mathcal{P}(E) \text{ is tight,}$$

where

$$\int_E f dI(m) := \int_{\mathcal{P}(E)} \left[\int_E f d\mu \right] m(d\mu), \quad \forall f \in C_b(E), \quad \forall m \in \mathcal{P}(\mathcal{P}(E)).$$

Proof. (\implies). Clearly, the map $\mathcal{P}(\mathcal{P}(E)) \rightarrow \mathcal{P}(E); m \mapsto I(m)$ is continuous w.r.t. the weak topologies. Let $a_n = I(m^n)$. Since $\{m^n \mid n \in \mathbb{N}\}$ is tight, Prokhorov's theorem implies that there exists a subsequence $(m^{n_k})_k$ such that $m^{n_k} \rightarrow m$ in the weak topology, for some $m \in \mathcal{P}(\mathcal{P}(E))$. By the continuity of I , $a_{n_k} \rightarrow I(m)$. Therefore,

$$I(m) \in \overline{\{a_{n_k} \mid k \in \mathbb{N}\}} \subseteq \overline{\{I(m^p) \mid p \in \mathbb{N}\}},$$

which shows that $\{I(m^p) \mid p \in \mathbb{N}\}$ is precompact. Prokhorov's theorem finally concludes that $(I(m^n))_n$ is tight.

(\impliedby). Suppose that $(I(m^n))_n$ is tight. Take any $\epsilon > 0$. There exists a compact subset K_ϵ of E such that

$$I(m^n)(K_\epsilon^c) < \epsilon, \quad \forall n \in \mathbb{N}.$$

By approximating the indicator function of an open set with a sequence of increasing continuous functions,

$$I(m^n)(K_{\epsilon\eta}^c) = \int_E \mathbf{1}_{K_{\epsilon\eta}^c} dI(m^n) = \int_{\mathcal{P}(E)} \mu(K_{\epsilon\eta}^c) m^n(d\mu) \geq \eta m^n(\{\mu \mid \mu(K_{\epsilon\eta}^c) \geq \eta\}),$$

which implies that

$$m^n(\{\mu \mid \mu(K_{\epsilon\eta}^c) \geq \eta\}) < \epsilon.$$

Therefore,

$$m^n\left(\bigcup_{k \geq 1} \left\{\mu \mid \mu\left(K_{\frac{\epsilon 2^{-k}}{k}}^c\right) > \frac{1}{k}\right\}\right) \leq \sum_{k \geq 1} \epsilon 2^{-k} = \epsilon.$$

Note that $\bigcap_{k \geq 1} \left\{\mu \mid \mu\left(K_{\frac{\epsilon 2^{-k}}{k}}^c\right) \leq \frac{1}{k}\right\}$ is closed, by Portmanteau's lemma. Thus, it is compact as well, by Prokhorov's theorem. \square

We now observe that by the exchangeability of $(Y^{1,N}, \dots, Y^{N,N})$, for any function $f \in C_b(C_T)$, we have

$$\begin{aligned} \int_{C_T} f d\mathcal{L}(Y^{1,N}) &= \mathbb{E}[f(Y^{1,N})] \\ &= \mathbb{E}\left[\frac{1}{N} \sum_{i=1}^N f(Y^{i,N})\right] \\ &= \mathbb{E}\left[\int_{C_T} f d\mu^{Y,N}\right] \\ &= \int_{\mathcal{P}(C_T)} \left(\int_{C_T} f d\mu\right) \mathcal{L}(\mu^{Y,N})(d\mu). \end{aligned}$$

We state this result formally in the following corollary.

Corollary 2.3.5. *The tightness of $(\mathcal{L}(\mu^{Y,N}))_{N \in \mathbb{N}}$ in $\mathcal{P}(\mathcal{P}(C_T))$ is equivalent to the tightness of $(\mathcal{L}(Y^{1,N}))_{N \in \mathbb{N}}$ in $\mathcal{P}(C_T)$.*

To show the tightness of $(\mathcal{L}(Y^{1,N}))_{N \in \mathbb{N}}$ in $\mathcal{P}(C_T)$, we first recall from Section 2.4 of [42] a general sufficient condition for tightness of measures on C_T .

Theorem 2.3.6. *Let $\{Q_t^{(m)}\}_{t \in [0,T]}$ be a sequence of continuous processes on $(\Omega, \mathcal{F}, \mathbb{P})$, taking values in \mathbb{R}^d , satisfying the following conditions:*

- (i) $\sup_{m \geq 1} \mathbb{E}[|Q_0^{(m)}|^\nu] = M < +\infty$, for some $\nu > 0$,

(ii) $\sup_{m \geq 1} \mathbb{E}[|Q_t^{(m)} - Q_s^{(m)}|^\alpha] \leq C|t-s|^{1+\beta}$, for each $0 \leq s, t \leq T$, for some positive constants α, β and C (depending on T).

Then the laws of $Q^{(m)}$ form a tight sequence of measures on $(C_T, \mathcal{B}(C_T))$.

A combination of (2.2.6), Corollary 2.3.5 and Theorem 2.3.6 gives the following result.

Theorem 2.3.7. *Assume (Lip) and (p-Int), for some $p > 1$. Then the sequence of measures $(\mathcal{L}(\mu^{Y,N}))_{N \in \mathbb{N}}$ is tight in $\mathcal{P}(\mathcal{P}(C_T))$.*

We now briefly introduce the martingale problem formulation for SDEs, introduced by Stroock and Varadhan.

Let $b_1 : [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $b_2 : [0, T] \times \mathbb{R}^d \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d$ be continuous functions with at most quadratic growth. We consider the SDE

$$d\Pi_t = b_1(t, \Pi_t) dt + b_2(t, \Pi_t) dW_t, \quad t \in [0, T], \quad (2.3.1)$$

where W is a d -dimensional Brownian motion and Π is a suitable stochastic process with continuous sample paths on $[0, T]$. A probability measure on $(C_T, \mathcal{B}(C_T))$, under which

$$\begin{aligned} & M_t^f(y) \\ := & f(y(t)) - f(y(0)) - \int_0^t \frac{1}{2} \sum_{i,j=1}^d (b_2 b_2^T)_{ij}(s, y(s)) \frac{\partial^2 f(y(s))}{\partial x_i \partial x_j} + \sum_{i=1}^d (b_1)_i(s, y(s)) \frac{\partial f(y(s))}{\partial x_i} ds, \end{aligned}$$

is a continuous martingale w.r.t. the filtration $\{\mathcal{B}(C_t)\}_{t \in [0, T]}$, for every $f \in C_0^2(\mathbb{R}^d)$, is called a *solution to the martingale problem associated to (2.3.1)*. The following result is well-known (see Proposition 4.11 and Corollary 4.9 in Section 5.4 of [42]).

Theorem 2.3.8. *The existence of a solution Q to the martingale problem associated to (2.3.1) is equivalent to the existence of a weak solution (Π, W) , $(\Omega, \mathcal{F}, \mathbb{P})$, $\{\mathcal{F}_t\}$ to (2.3.1). The two solutions are related by $Q = \mathbb{P} \circ \Pi^{-1}$. Moreover, the uniqueness of the solution Q to the martingale problem with fixed but arbitrary initial distribution*

$$Q_0(\Gamma) := Q\left\{y \in C_T \mid y(0) \in \Gamma\right\} = \mu(\Gamma), \quad \Gamma \in \mathcal{B}(\mathbb{R}^d),$$

is equivalent to uniqueness in law in (2.3.1).

Note that it is not necessary to verify the martingale problem for each function in $C_0^2(\mathbb{R}^d)$. Only a countable class of functions has to be considered. The following fact (Remark 4.12 in Section 5.4 of [42]) is crucial in subsequent discussions.

Theorem 2.3.9. *Let $\mathcal{D} := \bigcup_{1 \leq i, j \leq d} \left[\{g_i^{(k)} \mid k \in \mathbb{N}\} \cup \{g_{ij}^{(k)} \mid k \in \mathbb{N}\} \right]$, where for each $1 \leq i, j \leq d$ and $k \in \mathbb{N}$, $g_i^{(k)}$ and $g_{ij}^{(k)}$ are functions in $C_0^2(\mathbb{R}^d)$ such that*

$$g_i^{(k)}(x) = x_i, \quad g_{ij}^{(k)} = x_i x_j, \quad \text{for each } \|x\| \leq k.$$

Then Q is the solution to the martingale problem associated to (2.3.1) if $\{M_t^f\}_{t \in [0, T]}$ is a Q -continuous martingale for every $f \in \mathcal{D}$.

We now state the main result of this section. Note that it is possible to relax the assumptions, e.g. to include jumps. See Theorem 4.4 in [53] and Proposition 1.10 in [40] for further details. Note that the following theorem gives a *qualitative* result on propagation of chaos based on the definition of chaoticity given in Definition 2.3.1, whereas Theorem 2.2.6 gives a *quantitative* result of propagation of chaos by analysing the strong error.

Theorem 2.3.10. *Assume (First order) and (p-Int), for some $p > 1$. Moreover, suppose that the functions B and Σ in (First order) are bounded and satisfy (B and Σ -Lip). Then $\{\mathcal{L}((Y^{1,N}, \dots, Y^{N,N}))\}_{N \in \mathbb{N}}$ is μ^X -chaotic (up to a subsequence).*

We first state and prove a fact that gives a sufficient condition for an adapted integrable process to be a martingale.

Lemma 2.3.11. *Suppose that $\{M_t\}_{t \in [0, T]}$ is a bounded continuous adapted process defined on the filtered probability space $(C_T, \mathcal{B}(C_T), \{\mathcal{F}_t := \mathcal{B}(C_t)\}_{t \in [0, T]}, \mu)$. Then there exists a **countable** subset Λ (independent of the measure μ and the process M) of*

$$\left\{ \left((q_1, \dots, q_n, s, t), (f_1, \dots, f_n) \right) \mid n \in \mathbb{N}, 0 \leq q_1 < \dots < q_n \leq s < t \leq T, f_1, \dots, f_n \in C_b(\mathbb{R}^d) \right\}$$

such that if for each $((q_1, \dots, q_n, s, t), (f_1, \dots, f_n)) \in \Lambda$,

$$\int_{C_T} (M_t(y) - M_s(y)) f_1(y(q_1)) \dots f_n(y(q_n)) \mu(dy) = 0,$$

then M is a μ -martingale.

Proof. Fix $0 \leq s < t \leq T$. Note that $\mathcal{F}_s = \mathcal{B}(C_s)$ is generated by a countable collection \mathcal{C} of sets of the form

$$F = \left\{ z \in C_s \mid \left(z(q_1^{(F)}), \dots, z(q_{n_F}^{(F)}) \right) \in A^{(F)} \right\},$$

where $n_F \geq 1$, $q_i^{(F)} \in [0, s] \cap \mathbb{Q}$, $A^{(F)} \in \mathcal{B}(\mathbb{R}^{n_F d})$ is a product of open sets $I_1^{(F)} \times \dots \times I_{n_F}^{(F)}$, where each $I_k^{(F)} \in \mathbb{R}^d$, $k = 1, \dots, n_F$. Since $I_1^{(F)}, \dots, I_{n_F}^{(F)}$ are open, there exist sequences of functions $\{f_{1m}^{(F)}\}_{m \in \mathbb{N}}, \dots, \{f_{n_F m}^{(F)}\}_{m \in \mathbb{N}}$ in $C_b(\mathbb{R}^d)$ such that $f_{km}^{(F)} \uparrow \mathbf{1}_{I_k^{(F)}}$, as $m \rightarrow \infty$, for $k \in \{1, \dots, n_F\}$. By Dynkin's lemma and the dominated convergence theorem, it is easy to see that if for each

$$\left((q_1, \dots, q_n, s, t), (f_1, \dots, f_n) \right) \in A_{s,t} := \bigcup_{F \in \mathcal{C}} \bigcup_{m \in \mathbb{N}} \left\{ \left((q_1^{(F)}, \dots, q_{n_F}^{(F)}, s, t), (f_{1m}^{(F)}, \dots, f_{n_F m}^{(F)}) \right) \right\},$$

$$\int_{C_T} (M_t(y) - M_s(y)) f_1(y(q_1)) \dots f_n(y(q_n)) \mu(dy) = 0,$$

then $\mathbb{E}^\mu[M_t | \mathcal{F}_s] = M_s$ almost surely. Since M is continuous, we finish the proof by defining

$$\Lambda = \bigcup_{\substack{0 \leq s < t \leq T \\ s, t \in \mathbb{Q}}} A_{s,t},$$

which is clearly a countable set. □

Proof of Theorem 2.3.10. For each $\phi \in C_0^2(\mathbb{R}^d)$ and $R \in \mathcal{P}(C_T)$, we define the process

$$M_t^{\phi, R}(y) = \phi(y(t)) - \phi(y(0)) - \int_0^t \frac{1}{2} \sum_{i,j=1}^d a_{ij}(y(s), R_s) \frac{\partial^2 \phi(y(s))}{\partial x_i \partial x_j} + \sum_{i=1}^d b_i(y(s), R_s) \frac{\partial \phi(y(s))}{\partial x_i} ds. \quad (2.3.2)$$

Subsequently, we fix $\lambda = ((q_1, \dots, q_j, s, t), (f_1, \dots, f_j)) \in \Lambda$. We define a function $F^{\phi, \lambda} : \mathcal{P}(C_T) \rightarrow \mathbb{R}$ such that

$$F^{\phi, \lambda}(R) = \int_{C_T} (M_t^{\phi, R}(y) - M_s^{\phi, R}(y)) f_1(y(q_1)) \dots f_j(y(q_j)) R(dy).$$

Lemma 2.3.12. *$F^{\phi, \lambda}$ is a continuous function with respect to the weak topology and Euclidean topology.*

Proof. By Theorem 1.12.4 from [64], we recall that the weak topology on any separable metric

space (E, ρ) is metrisable by the bounded Lipschitz metric $d_{\text{BL}, E}$ given by

$$d_{\text{BL}, E}(\nu_1, \nu_2) := \sup_{f \in \text{BL}_E} \left| \int_E f d\nu_1 - \int_E f d\nu_2 \right|,$$

where

$$\text{BL}_E := \left\{ f \in C_b(E) \mid \sup_{x \in E} |f(x)| \leq 1, \sup_{x \neq y} \frac{|f(x) - f(y)|}{\rho(x, y)} \leq 1 \right\}.$$

Let $\{R^n\}_n$ be a sequence in $\mathcal{P}(C_T)$ converging to R . Then we obtain

$$\begin{aligned} |a_{ij}(y(s), R_s^n) - a_{ij}(y(s), R_s)| &= \left| \int_{\mathbb{R}^d} A_{ij}(y(s), z) R_s^n(dz) - \int_{\mathbb{R}^d} A_{ij}(y(s), z) R(dz) \right| \\ &\leq \left(\|A_{ij}\|_\infty + \|A_{ij}\|_{\text{Lip}} \right) d_{\text{BL}, \mathbb{R}^d}(R_s^n, R_s) \end{aligned}$$

and a similar result for b_i , $1 \leq i \leq d$. Therefore, since $\phi \in C_0^2(\mathbb{R}^d)$, by (2.3.2), we have

$$\sup_{y \in C_T} |M_t^{\phi, R^n}(y) - M_t^{\phi, R}(y)| \leq C \sup_{s \in [0, T]} d_{\text{BL}, \mathbb{R}^d}(R_s^n, R_s).$$

We further note that

$$\begin{aligned} \sup_{s \in [0, T]} d_{\text{BL}, \mathbb{R}^d}(R_s^n, R_s) &= \sup_{s \in [0, T]} \sup_{f \in \text{BL}_{\mathbb{R}^d}} \left| \int_{\mathbb{R}^d} f(x) R_s^n(dx) - \int_{\mathbb{R}^d} f(x) R_s(dx) \right| \\ &= \sup_{s \in [0, T]} \sup_{f \in \text{BL}_{\mathbb{R}^d}} \left| \int_{C_T} f(\omega(s)) R_s^n(d\omega) - \int_{C_T} f(\omega(s)) R(d\omega) \right| \\ &\leq d_{\text{BL}, C_T}(R^n, R), \end{aligned}$$

which implies that

$$\sup_{y \in C_T} |M_t^{\phi, R^n}(y) - M_t^{\phi, R}(y)| \leq C d_{\text{BL}, C_T}(R^n, R).$$

Finally, we conclude the result by considering the decomposition

$$\begin{aligned} &|F^{\phi, \lambda}(R_n) - F^{\phi, \lambda}(R)| \\ &\leq \left| \int_{C_T} (M_t^{\phi, R_n}(y) - M_s^{\phi, R_n}(y)) f_1(y(q_1)) \dots f_j(y(q_j)) R_n(dy) \right. \\ &\quad \left. - \int_{C_T} (M_t^{\phi, R}(y) - M_s^{\phi, R}(y)) f_1(y(q_1)) \dots f_j(y(q_j)) R_n(dy) \right| \\ &\quad + \left| \int_{C_T} (M_t^{\phi, R}(y) - M_s^{\phi, R}(y)) f_1(y(q_1)) \dots f_j(y(q_j)) R_n(dy) \right. \\ &\quad \left. - \int_{C_T} (M_t^{\phi, R}(y) - M_s^{\phi, R}(y)) f_1(y(q_1)) \dots f_j(y(q_j)) R(dy) \right| \\ &\leq C d_{\text{BL}, C_T}(R^n, R) + \left| \int_{C_T} (M_t^{\phi, R}(y) - M_s^{\phi, R}(y)) f_1(y(q_1)) \dots f_j(y(q_j)) R_n(dy) \right. \\ &\quad \left. - \int_{C_T} (M_t^{\phi, R}(y) - M_s^{\phi, R}(y)) f_1(y(q_1)) \dots f_j(y(q_j)) R(dy) \right| \xrightarrow{n \rightarrow \infty} 0. \end{aligned}$$

□

By the definition of $M^{\phi, R}$,

$$F^{\phi, \lambda}(R) = \int_{C_T} \left[\phi(y(t)) - \phi(y(s)) - \int_s^t \frac{1}{2} \sum_{i, j=1}^d a_{ij}(y(u), R_u) \frac{\partial^2 \phi(y(u))}{\partial x_i \partial x_j} \right]$$

$$+ \sum_{i=1}^d b_i(y(u), R_u) \frac{\partial \phi(y(u))}{\partial x_i} du \Big] f_1(y(q_1)) \dots f_j(y(q_j)) R(dy).$$

We then notice that

$$\mathbb{E} \left[(F^{\phi, \lambda}(\mu^{Y, N}))^2 \right] = \mathbb{E} \left[\left(\frac{1}{N} \sum_{i=1}^N (Z_t^{\phi, i, N} - Z_s^{\phi, i, N}) f_1(Y_{q_1}^{1, N}) \dots f_j(Y_{q_j}^{i, N}) \right)^2 \right],$$

where

$$\begin{aligned} & Z_t^{\phi, i, N} \\ := & \phi(Y_t^{i, N}) - \phi(\xi_i) - \int_0^t \frac{1}{2} \sum_{\ell, j=1}^d a_{\ell j}(Y_s^{i, N}, \mu_s^{Y, N}) \frac{\partial^2 \phi}{\partial x_\ell \partial x_j}(Y_s^{i, N}) + \sum_{\ell=1}^d b_\ell(Y_s^{i, N}, \mu_s^{Y, N}) \frac{\partial \phi}{\partial x_\ell}(Y_s^{i, N}) ds. \end{aligned}$$

By the exchangeability of the particle system $(Y^{1, N}, \dots, Y^{N, N})$,

$$\begin{aligned} & \mathbb{E} \left[(F^{\phi, \lambda}(\mu^{Y, N}))^2 \right] \\ = & \frac{1}{N} \mathbb{E} \left[\left((Z_t^{\phi, 1, N} - Z_s^{\phi, 1, N}) f_1(Y_{q_1}^{1, N}) \dots f_j(Y_{q_j}^{1, N}) \right)^2 \right] \\ & + \frac{N-1}{N} \mathbb{E} \left[(Z_t^{\phi, 1, N} - Z_s^{\phi, 1, N}) (Z_t^{\phi, 2, N} - Z_s^{\phi, 2, N}) f_1(Y_{q_1}^{1, N}) \dots f_j(Y_{q_j}^{1, N}) f_1(Y_{q_1}^{2, N}) \dots f_j(Y_{q_j}^{2, N}) \right]. \end{aligned}$$

Since $Z_t^{\phi, 1, N}$ and the functions f_1, \dots, f_j are all bounded, the first term converges to zero, as $N \rightarrow \infty$. By Itô's formula, for $i \in \{1, \dots, N\}$,

$$Z_t^{\phi, i, N} = \int_0^t \partial_x \phi(Y_s^{i, N})^T \sigma(Y_s^{i, N}, \mu_s^{Y, N}) dW_s^i.$$

By the assumption of the boundedness of σ and the partial derivatives of ϕ , we can see that $\{Z_t^{\phi, 1, N}\}_{t \in [0, T]}$ and $\{Z_t^{\phi, 2, N}\}_{t \in [0, T]}$ are square-integrable martingales. Moreover, since W^1 and W^2 are independent \mathbb{R}^d -valued Brownian motions, $\langle Z^{\phi, 1, N}, Z^{\phi, 2, N} \rangle = 0$. Thus, $\{Z_t^{\phi, 1, N} Z_t^{\phi, 2, N}\}_{t \in [0, T]}$ is a uniformly integrable martingale. This shows that

$$\begin{aligned} & \mathbb{E} \left[(Z_t^{\phi, 1, N} - Z_s^{\phi, 1, N}) (Z_t^{\phi, 2, N} - Z_s^{\phi, 2, N}) f_1(Y_{q_1}^{1, N}) \dots f_j(Y_{q_j}^{1, N}) f_1(Y_{q_1}^{2, N}) \dots f_j(Y_{q_j}^{2, N}) \right] \\ = & \mathbb{E} \left[f_1(Y_{q_1}^{1, N}) \dots f_j(Y_{q_j}^{1, N}) f_1(Y_{q_1}^{2, N}) \dots f_j(Y_{q_j}^{2, N}) \mathbb{E} \left[(Z_t^{\phi, 1, N} - Z_s^{\phi, 1, N}) (Z_t^{\phi, 2, N} - Z_s^{\phi, 2, N}) \middle| \mathcal{F}_s \right] \right] \\ = & \mathbb{E} \left[f_1(Y_{q_1}^{1, N}) \dots f_j(Y_{q_j}^{1, N}) f_1(Y_{q_1}^{2, N}) \dots f_j(Y_{q_j}^{2, N}) \mathbb{E} \left[Z_t^{\phi, 1, N} Z_t^{\phi, 2, N} - Z_s^{\phi, 1, N} Z_s^{\phi, 2, N} \middle| \mathcal{F}_s \right] \right] \\ = & 0, \end{aligned}$$

which implies that $F^{\phi, \lambda}(\mu^{Y, N})$ converges to 0 in L^1 . Recall that by Theorem 2.3.7, $\{\mathcal{L}(\mu^{Y, N})\}_N$ is tight. Hence, by Prokhorov's theorem, it converges through a subsequence of indices $\{n_k\}_{k \in \mathbb{N}}$ to a measure $\pi^\infty \in \mathcal{P}(\mathcal{P}(C_T))$. By the definition of weak convergence,

$$\int_{\mathcal{P}(C_T)} |F^{\phi, \lambda}| d\pi^\infty = \lim_{k \rightarrow \infty} \int_{\mathcal{P}(C_T)} |F^{\phi, \lambda}| d(\mathcal{L}(\mu^{Y, N_k})) = \lim_{k \rightarrow \infty} \mathbb{E} \left[|F^{\phi, \lambda}(\mu^{Y, N_k})| \right] = 0.$$

Consequently,

$$\pi^\infty \{R \in \mathcal{P}(C_T) \mid F^{\phi, \lambda}(R) = 0\} = 1.$$

Since ϕ and λ are arbitrary, we have

$$\pi^\infty \left(\bigcap_{\phi \in \mathcal{D}} \bigcap_{\lambda \in \Lambda} \{R \in \mathcal{P}(C_T) \mid F^{\phi, \lambda}(R) = 0\} \right) = 1,$$

where the sets \mathcal{D} and Λ are defined in Theorem 2.3.9 and Lemma 2.3.11.

We now recall that the initial law of (2.1.5) is $\nu \in \mathcal{P}_2(\mathbb{R}^d)$. Moreover, we recall that the particles in (2.2.4) are i.i.d. at time $t = 0$ with law ν . For every $\theta \in \mathbb{R}^d$, we define the map

$$\varphi_\theta : \mathcal{P}(C_T) \rightarrow \mathbb{R}; \quad \mu \mapsto \int_{\mathbb{R}^d} e^{i\theta x} \mu_0(dx).$$

As before, by the weak law of large numbers (along with uniform integrability), we deduce that

$$\begin{aligned} \int_{\mathcal{P}(C_T)} \left| \int_{\mathbb{R}^d} e^{i\theta x} \nu(dx) - \varphi_\theta \right| d\pi^\infty &= \lim_{k \rightarrow \infty} \mathbb{E} \left| \int_{\mathbb{R}^d} e^{i\theta x} \nu(dx) - \varphi_\theta(\mu^{Y, N_k}) \right| \\ &= \lim_{k \rightarrow \infty} \mathbb{E} \left| \int_{\mathbb{R}^d} e^{i\theta x} \nu(dx) - \frac{1}{N_k} \sum_{j=1}^{N_k} e^{i\theta \xi_j} \right| = 0, \end{aligned}$$

which implies that

$$\pi^\infty \left\{ R \in \mathcal{P}(C_T) \mid \int_{\mathbb{R}^d} e^{i\theta x} \nu(dx) = \int_{\mathbb{R}^d} e^{i\theta x} R_0(dx) \right\} = 1.$$

Since $\theta \in \mathbb{R}^d$ is arbitrary, by the fact that characteristic functions uniquely determine distributions, we have

$$\pi^\infty \{R \in \mathcal{P}(C_T) \mid \mathcal{L}(R_0) = \nu\} = \pi^\infty \left(\bigcap_{\theta \in \mathbb{Q}^d} \left\{ R \in \mathcal{P}(C_T) \mid \int_{\mathbb{R}^d} e^{i\theta x} \nu(dx) = \int_{\mathbb{R}^d} e^{i\theta x} R_0(dx) \right\} \right) = 1.$$

Therefore,

$$\pi^\infty \left(\bigcap_{\phi \in \mathcal{D}} \bigcap_{\lambda \in \Lambda} \{R \in \mathcal{P}(C_T) \mid F^{\phi, \lambda}(R) = 0\} \cap \{R \in \mathcal{P}(C_T) \mid \mathcal{L}(R_0) = \nu\} \right) = 1.$$

By Theorem 2.3.9 and Lemma 2.3.11,

$$\begin{aligned} &\bigcap_{\phi \in \mathcal{D}} \bigcap_{\lambda \in \Lambda} \{R \in \mathcal{P}(C_T) \mid F^{\phi, \lambda}(R) = 0\} \cap \{R \in \mathcal{P}(C_T) \mid \mathcal{L}(R_0) = \nu\} \\ &= \left\{ R \in \mathcal{P}(C_T) \mid R \text{ is the solution of the martingale problem associated to the SDE} \right. \\ &\quad \left. dX_t = b(X_t, R_t) dt + \sigma(X_t, R_t) dW_t, \quad \text{with initial law } \nu \right\}, \end{aligned}$$

which implies, by Theorem 2.1.5 and Theorem 2.3.8, that

$$\bigcap_{\phi \in \mathcal{D}} \bigcap_{\lambda \in \Lambda} \{R \in \mathcal{P}(C_T) \mid F^{\phi, \lambda}(R) = 0\} \cap \{R \in \mathcal{P}(C_T) \mid \mathcal{L}(R_0) = \nu\} = \{\mu^X\}.$$

Finally, $\pi^\infty = \delta_{\mu^X}$. We conclude the result by applying Theorem 2.3.3. \square

Chapter 3

The theory of differentiation of measures

We start this chapter by considering a classical one-dimensional SDE:

$$\mathcal{Z}_t^{s,\xi} = \xi + \int_0^t f_1(\mathcal{Z}_u^{s,\xi}) du + \int_0^t f_2(\mathcal{Z}_u^{s,\xi}) dW_u, \quad 0 \leq s \leq t \leq T,$$

where $f_1, f_2 : \mathbb{R} \rightarrow \mathbb{R}$ are Lipschitz functions. By the Yamada-Watanabe theorem (see Corollary 3.23 in Section 5.3 of [42]), we know that there exists a $(\mathcal{B}(\mathbb{R}) \otimes \mathcal{B}(C_T)) / \mathcal{B}(C_T)$ -measurable function $h : \mathbb{R} \times C_T \rightarrow C_T$ such that

$$\mathcal{Z}^{0,\xi} = h(\xi, W) \quad \text{almost surely.}$$

Therefore, we have the relation $\mathcal{Z}^{0,\xi} = \mathcal{Z}^{0,x} \big|_{x=\xi}$. The behaviour of $\mathcal{Z}^{0,\xi}$ can hence be investigated through $\mathcal{Z}^{0,x}$, at any fixed point $x \in \mathbb{R}$.

On the other hand, we consider the following McKean-Vlasov SDE:

$$\mathcal{X}_t^{s,\xi} = \xi + \int_0^t \mathbb{E}(\mathcal{X}_u^{s,\xi}) du + (W_t - W_s), \quad 0 \leq s \leq t \leq T. \quad (3.0.1)$$

Taking expectation on both sides of (3.0.1) gives

$$\mathbb{E}[\mathcal{X}_t^{0,\xi}] = \mathbb{E}[\xi]e^t, \quad t \in [0, T],$$

which gives the solution

$$\mathcal{X}_t^{0,\xi} = \xi + \mathbb{E}[\xi](e^t - 1) + W_t, \quad t \in [0, T].$$

Let $\hat{\xi}$ be a centered random variable. Then

$$\mathcal{X}_t^{0,\hat{\xi}} = \hat{\xi} + W_t.$$

However,

$$\mathcal{X}_t^{0,x} = xe^t + W_t \quad \implies \quad \mathcal{X}_t^{0,x} \big|_{x=\hat{\xi}} = \hat{\xi}e^t + W_t \neq \mathcal{X}_t^{0,\hat{\xi}}, \quad t > 0. \quad (3.0.2)$$

Equation (3.0.2) tells us that the behaviour of $\mathcal{Z}^{0,\xi}$ can no longer be investigated through $\mathcal{Z}^{0,x}$, by fixing $x \in \mathbb{R}$. Since the path of $\mathcal{Z}^{0,\xi}$ is determined by the law of ξ , this suggests that we need a machinery that enables us to deal with perturbation of probability measures, i.e. calculus on the space of probability measures.

It follows from classical theory (e.g., see Section 11 from [28]) that for smooth functions $f : \mathbb{R} \rightarrow \mathbb{R}$, the function $[0, t] \times \mathbb{R} \ni (s, x) \mapsto \mathbb{E}[f(\mathcal{Z}_t^{s,x})]$ satisfies a PDE. We shall see later

that the function $[0, t] \times \mathcal{P}_2(\mathbb{R}) \ni (s, \mathcal{L}(\xi)) \mapsto \mathbb{E}[f(\mathcal{X}_t^{s, \xi})]$ also satisfies a PDE in the sense of L-derivatives.

The work in subsequent chapters relies heavily on the calculus on $(\mathcal{P}_2(\mathbb{R}^d), W_2)$. There are many notions of differentiability for functions defined on the space of probability measures and much of the work in the literature is based on the theory of optimal transport. We shall focus on the notions of *linear functional derivatives* and *L-derivatives*. We shall also introduce higher-order versions of these derivatives (in the same spirit as [19]), as they are needed in later parts of the work.

In this chapter, we follow the approach presented by P. Lions in his course at Collège de France [49] (redacted by Cardaliaguet [10]) and the book, [14], by R. Carmona and F. Delarue, as well as the papers [9] and [11].

Sections 3.3 and 3.5 are extracted from [17].

3.1 Linear functional derivatives

A continuous function $\frac{\delta U}{\delta m} : \mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \rightarrow \mathbb{R}$ is said to be the *linear functional derivative* of $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, if

- for any bounded ¹ set $\mathcal{K} \subset \mathcal{P}_2(\mathbb{R}^d)$, $y \mapsto \frac{\delta U}{\delta m}(m, y)$ has at most quadratic growth in y uniformly in $m \in \mathcal{K}$,
- for any $m, m' \in \mathcal{P}_2(\mathbb{R}^d)$,

$$U(m') - U(m) = \int_0^1 \int_{\mathbb{R}^d} \frac{\delta U}{\delta m}((1-s)m + sm', y) (m' - m)(dy) ds. \quad (3.1.1)$$

For the purpose of our work, we need to introduce derivatives at any order $p \geq 1$.

Definition 3.1.1. For any $p \geq 1$, the p -th order linear functional derivative of the function U is a continuous function from $\frac{\delta^p U}{\delta m^p} : \mathcal{P}_2(\mathbb{R}^d) \times (\mathbb{R}^d)^{p-1} \times \mathbb{R}^d \rightarrow \mathbb{R}$ satisfying

- for any bounded set $\mathcal{K} \subset \mathcal{P}_2(\mathbb{R}^d)$, the map $(\mathbb{R}^d)^{p-1} \times \mathbb{R}^d \ni (\mathbf{y}, y') \mapsto \frac{\delta^p U}{\delta m^p}(m, \mathbf{y}, y')$ has at most quadratic growth in (\mathbf{y}, y') uniformly in $m \in \mathcal{K}$,
- for any $m, m' \in \mathcal{P}_2(\mathbb{R}^d)$, $\mathbf{y} \in (\mathbb{R}^d)^{p-1}$,

$$\frac{\delta^{p-1} U}{\delta m^{p-1}}(m', \mathbf{y}) - \frac{\delta^{p-1} U}{\delta m^{p-1}}(m, \mathbf{y}) = \int_0^1 \int_{\mathbb{R}^d} \frac{\delta^p U}{\delta m^p}((1-s)m + sm', \mathbf{y}, y') (m' - m)(dy') ds,$$

provided that the $(p-1)$ -th order derivative is well defined.

Note that $\frac{\delta U}{\delta m}$ is defined up to an additive constant via (3.1.1). Iteratively, we normalise the higher order derivatives via the convention that

$$\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_p) = 0, \quad \text{if } y_i = 0 \text{ for some } i \in \{1, \dots, p\}. \quad (3.1.2)$$

We consider an example to illustrate the theory.

Example 3.1.2. Let $G : \mathbb{R}^d \rightarrow \mathbb{R}$ be a continuous function such that

$$\int_{\mathbb{R}^d} |G(x)| \mu(dx) < +\infty, \quad \forall \mu \in \mathcal{P}_2(\mathbb{R}^d).$$

Let $F : \mathbb{R} \rightarrow \mathbb{R}$ be a C^1 function. Then the function $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ defined by

$$U(\mu) := F\left(\int_{\mathbb{R}^d} G(x) \mu(dx)\right)$$

¹A subset \mathcal{K} of $\mathcal{P}_2(\mathbb{R}^d)$ is said to be bounded if there exists $a > 0$ such that for each $\mu \in \mathcal{K}$, $\int_{\mathbb{R}^d} |x|^2 \mu(dx) \leq a$.

admits a linear functional derivative given by

$$\frac{\delta U}{\delta m}(\mu, y) = F' \left(\int_{\mathbb{R}^d} G(x) \mu(dx) \right) (G(y) - G(0)).$$

Proof. Clearly, the normalisation convention (3.1.2) holds. Let $\varphi(\mu) := \int_{\mathbb{R}^d} G(x) \mu(dx)$. Then, by the fundamental theorem of calculus,

$$\begin{aligned} U(m') - u(m) &= F(\varphi(m')) - F(\varphi(m)) \\ &= \int_0^1 F'((1-s)\varphi(m) + s\varphi(m'))(\varphi(m') - \varphi(m)) ds \\ &= \int_0^1 F'((1-s)\varphi(m) + s\varphi(m')) \left(\int_{\mathbb{R}^d} G(y) (m' - m)(dy) \right) ds \\ &= \int_0^1 \int_{\mathbb{R}^d} F' \left(\int_{\mathbb{R}^d} G(x) ((1-s)m + sm')(dx) \right) G(y) (m' - m)(dy) ds \\ &= \int_0^1 \int_{\mathbb{R}^d} F' \left(\int_{\mathbb{R}^d} G(x) ((1-s)m + sm')(dx) \right) (G(y) - G(0)) (m' - m)(dy) ds. \end{aligned}$$

□

We now state the Taylor formula for measures in terms of linear functional derivatives, which will be useful in later parts of the work.

Lemma 3.1.3. *If U admits linear functional derivatives up to order q , then the following expansion holds:*

$$\begin{aligned} U(m') - U(m) &= \sum_{p=1}^{q-1} \frac{1}{p!} \int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(m, \mathbf{y}) \{m' - m\}^{\otimes p}(\mathbf{dy}) \\ &\quad + \frac{1}{(q-1)!} \int_0^1 (1-t)^{q-1} \int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q}((1-t)m + tm', \mathbf{y}) \{m' - m\}^{\otimes q}(\mathbf{dy}) dt. \end{aligned}$$

Proof. We define

$$[0, 1] \ni t \mapsto f(t) = U((1-t)m + tm') = U(m + t(m' - m)) \in \mathbb{R} \quad (3.1.3)$$

and apply Taylor-Lagrange formula to f up to order q , namely

$$f(1) - f(0) = \sum_{p=1}^{q-1} \frac{1}{p!} f^{(p)}(0) + \frac{1}{(q-1)!} \int_0^1 (1-t)^{(q-1)} f^{(q)}(t) dt.$$

It remains to show that

$$f^{(p)}(t) = \int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(m + t(m' - m), \mathbf{y}) \{m' - m\}^{\otimes p}(\mathbf{dy}), \quad \forall p \in \{0, \dots, q\}. \quad (3.1.4)$$

by induction. Since (3.1.4) holds trivially for $p = 0$, we suppose that (3.1.4) holds for $p \in \{0, \dots, q-1\}$. Then

$$\begin{aligned} &\frac{f^{(p)}(t+h) - f^{(p)}(t)}{h} \\ &= \frac{1}{h} \left[\int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(m + (t+h)(m' - m), \mathbf{y}) \{m' - m\}^{\otimes p}(\mathbf{dy}) \right. \\ &\quad \left. - \int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(m + t(m' - m), \mathbf{y}) \{m' - m\}^{\otimes p}(\mathbf{dy}) \right] \\ &= \int_{\mathbb{R}^{pd}} \int_0^1 \int_{\mathbb{R}^d} \frac{\delta^{p+1} U}{\delta m^{p+1}}(m + (t+sh)(m' - m), \mathbf{y}, y') (m' - m)(dy') ds \{m' - m\}^{\otimes p}(\mathbf{dy}). \end{aligned}$$

Taking $h \rightarrow 0$ gives (3.1.4) for $p + 1$. This completes the proof. \square

3.2 L-derivatives

The notion of linear functional derivatives is proven to be insufficient for the analysis of the MVSEs. In this section, we introduce the notion proposed by P. Lions, which was expounded in other works in the literature (e.g. [9, 10, 14, 19]).

Suppose that the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ is atomless (i.e. there does not exist a measurable set which has positive measure and contains no set of smaller positive measure). Then for any $\mu \in \mathcal{P}(\mathbb{R}^d)$, we can always construct an \mathbb{R}^d -valued random variable on Ω with law μ (see page 376 from [14]).

Let $L^2(\mathcal{F}; \mathbb{R}^d) := L^2(\Omega, \mathcal{F}, \mathbb{P}; \mathbb{R}^d)$ be the Hilbert space of L^2 random variables, equipped with the inner product $\langle \xi, \eta \rangle = \mathbb{E}[\xi \eta]$. For any function $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, we define the lift $\tilde{U} : L^2(\mathcal{F}, \mathbb{R}^d) \rightarrow \mathbb{R}$ by

$$\tilde{U}(\theta) := U(\mathcal{L}(\theta)).$$

Recall that \tilde{U} is said to be Fréchet differentiable at θ_0 if there exists a linear continuous map $D\tilde{U}(\theta_0) : L^2(\mathcal{F}; \mathbb{R}^d) \rightarrow \mathbb{R}$ such that

$$\tilde{U}(\theta_0 + \eta) - \tilde{U}(\theta_0) = D\tilde{U}(\theta_0)(\eta) + o(\|\eta\|_{L^2}),$$

as $\|\eta\|_{L^2} \rightarrow 0$. By the Riesz representation theorem, there exists a (\mathbb{P} -a.s.) unique random variable $L_{\theta_0} \in L^2(\mathcal{F}; \mathbb{R}^d)$ such that

$$D\tilde{U}(\theta_0)(\eta) = \mathbb{E}[L_{\theta_0} \eta], \quad \forall \eta \in L^2(\mathcal{F}; \mathbb{R}^d).$$

The following theorem follows from Theorem 6.2 and Theorem 6.5 from [10] (or equivalently, Proposition 5.24 and Proposition 5.25 from [14]).

Theorem 3.2.1. *Suppose that \tilde{U} is Fréchet differentiable at θ_0 and $\hat{\theta}_0$. Suppose that $\mathcal{L}(\theta_0) = \mathcal{L}(\hat{\theta}_0) = \mu \in \mathcal{P}_2(\mathbb{R}^d)$. Then*

(i) *The joint law (θ_0, L_{θ_0}) is equal to the joint law of $(\hat{\theta}_0, L_{\hat{\theta}_0})$.*

(ii) *There exists a Borel-measurable function $h : \mathbb{R}^d \rightarrow \mathbb{R}^d$ (uniquely determined μ -a.e.) such that $\int_{\mathbb{R}^d} |h(x)|^2 \mu(dx) < +\infty$ and*

$$h(\theta_0) = L_{\theta_0}, \quad h(\hat{\theta}_0) = L_{\hat{\theta}_0}, \quad a.s.$$

We are now in a position to define L-derivatives. The previous theorem tells us that the following definition is well-defined.

Definition 3.2.2. (i) A function $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ is said to be L-differentiable at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ if there exists a random variable θ_0 with law μ such that \tilde{U} is Fréchet differentiable at θ_0 .

(ii) If $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ is L-differentiable at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, then its L-derivative² $\partial_\mu U(\mu)$ is defined to be $\partial_\mu U(\mu) := h$, where $h : \mathbb{R}^d \rightarrow \mathbb{R}^d$ is the Borel-measurable function in (ii) of Theorem 3.2.1. Moreover, we define the joint map $\partial_\mu U : \mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ by

$$\partial_\mu U(\mu, y) := [\partial_\mu U(\mu)](y).$$

Since we perform different computations with L-derivatives in later parts, it is helpful to notice some basic properties regarding arithmetic on L-derivatives.

Theorem 3.2.3. *Suppose that $U, U_1, U_2 : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ are L-differentiable at $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. Suppose that $g : \mathbb{R} \rightarrow \mathbb{R}$ is a differentiable function. Then the following properties hold for any $y \in \mathbb{R}^d$.*

²For brevity, in this work, we say *the* L-derivative, rather than a μ -version of L-derivative. Any property imposed on the L-derivatives in later parts means that it is applicable to at least one μ -version.

- (i) $\partial_\mu[U_1 + U_2](\mu)(y) = \partial_\mu U_1(\mu)(y) + \partial_\mu U_2(\mu)(y)$.
- (ii) $\partial_\mu[U_1 U_2](\mu)(y) = U_2(\mu)\partial_\mu U_1(\mu)(y) + U_1(\mu)\partial_\mu U_2(\mu)(y)$.
- (iii) $\partial_\mu[g \circ U](\mu)(y) = g'(U(\mu))\partial_\mu U(\mu)(y)$.

Proof. These statements can be verified easily by using basic properties of Fréchet differentiation. We provide a proof for (iii). Let $\Phi = g \circ U$ and let $\tilde{\Phi}, \tilde{U}$ denote the lifts of Φ and U respectively. Let θ_0 be a random variable with law μ . By the chain rule of Fréchet differentiation, we have

$$D\tilde{\Phi}(\theta_0) = Dg(\tilde{U}(\theta_0)) \circ D\tilde{U}(\theta_0) = g'(\tilde{U}(\theta_0))D\tilde{U}(\theta_0).$$

Therefore,

$$D\tilde{\Phi}(\theta_0)(\eta) = g'(\tilde{U}(\theta_0))D\tilde{U}(\theta_0)(\eta) = g'(U(\mu))\mathbb{E}[\partial_\mu U(\mu)(\theta_0)\eta] = \mathbb{E}[(g'(U(\mu))\partial_\mu U(\mu)(\theta_0))\eta],$$

which completes the proof by the definition of L-derivatives. \square

The following theorem (taken from Example 5.2.2.3 from [14]) gives the formula of the L-derivative for functions in which the measure appears both in the integrand and in the measure of the integral.

Theorem 3.2.4. *Let $v : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ be a continuous function (w.r.t. the Euclidean and Wasserstein metrics) satisfying the following conditions.*

- (i) *For fixed $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, v is differentiable w.r.t. $x \in \mathbb{R}^d$, with the spatial derivative being jointly continuous in (x, μ) , with linear growth in x , uniformly in μ for bounded subsets of $\mathcal{P}_2(\mathbb{R}^d)$.*
- (ii) *For fixed $x \in \mathbb{R}^d$, v is L-differentiable w.r.t. μ with $\partial_\mu v(x, \mu)(y)$ being jointly continuous in (x, μ, y) . The map $(x, y) \mapsto \partial_\mu v(x, \mu)(y)$ has linear growth, uniformly in μ for bounded subsets of $\mathcal{P}_2(\mathbb{R}^d)$.*

Let $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ be defined by

$$U(\mu) = \int_{\mathbb{R}^d} v(x, \mu) \mu(dx).$$

Then for every fixed $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, v has quadratic growth in x (which shows that U is well-defined). Also, U is L-differentiable with

$$\partial_\mu U(\mu)(y) = \partial_x v(y, \mu) + \int_{\mathbb{R}^d} \partial_\mu v(x, \mu)(y) \mu(dx).$$

Proof. We begin by deriving the fundamental theorem of calculus for L-derivatives. Let $\Phi = v(0, \cdot)$. Then, by the definition of L-derivatives, for any $\theta_1, \theta_2 \in L^2(\mathcal{F}; \mathbb{R}^d)$ with $\eta = \theta_1 - \theta_2$,

$$\begin{aligned} \Phi(\mathcal{L}(\theta_1)) - \Phi(\mathcal{L}(\theta_2)) &= \int_0^1 \frac{d}{d\lambda} \Phi(\mathcal{L}(\theta_2 + \lambda\eta)) d\lambda \\ &= \int_0^1 \lim_{h \rightarrow 0} \frac{\tilde{\Phi}(\theta_2 + (\lambda + h)\eta) - \tilde{\Phi}(\theta_2 + \lambda\eta)}{h} d\lambda \\ &= \int_0^1 \lim_{h \rightarrow 0} \frac{\mathbb{E}[\partial_\mu \Phi(\mathcal{L}(\theta_2 + \lambda\eta))(\theta_2 + \lambda\eta) \cdot (h\eta)] + o(\|h\eta\|_{L^2})}{h} d\lambda \\ &= \int_0^1 \mathbb{E}[\partial_\mu \Phi(\mathcal{L}(\theta_2 + \lambda\eta))(\theta_2 + \lambda\eta) \cdot \eta] d\lambda \\ &= \int_0^1 \mathbb{E}[\partial_\mu \Phi(\mathcal{L}((1 - \lambda)\theta_2 + \lambda\theta_1))((1 - \lambda)\theta_2 + \lambda\theta_1) \cdot (\theta_1 - \theta_2)] d\lambda. \end{aligned} \tag{3.2.1}$$

By (3.2.1) and the standard fundamental theorem of calculus, for $\theta \in L^2(\mathcal{F}; \mathbb{R}^d)$ with $\mathcal{L}(\theta) = \mu$, we have

$$\begin{aligned} v(z, \mu) &= v(0, \mu) + \int_0^1 \partial_x v(\lambda z, \mu) z \, d\lambda \\ &= v(0, \delta_0) + \int_0^1 \mathbb{E}[\partial_\mu v(0, \mathcal{L}(\lambda\theta))(\lambda\theta) \cdot (\theta)] \, d\lambda + \int_0^1 \partial_x v(\lambda z, \mu) z \, d\lambda, \end{aligned}$$

which implies that

$$|v(z, \mu)| \leq C_\mu(1 + |z|^2),$$

for every $z \in \mathbb{R}^d$ and $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, where C_μ depends on μ . This shows that U is well-defined.

To prove the second statement, we pick any $\theta, \eta \in L^2(\mathcal{F}; \mathbb{R}^d)$ with $\mathcal{L}(\theta) = \mu$ and $\|\eta\|_{L^2} \leq 1$. Then, by (3.2.1) and the standard fundamental theorem of calculus,

$$\begin{aligned} \tilde{U}(\theta + \eta) - \tilde{U}(\theta) &= \mathbb{E}[v(\theta + \eta, \mathcal{L}(\theta + \eta)) - v(\theta, \mathcal{L}(\theta + \eta))] + \mathbb{E}[v(\theta, \mathcal{L}(\theta + \eta)) - v(\theta, \mathcal{L}(\theta))] \\ &= \mathbb{E}[\partial_x v(\theta, \mathcal{L}(\theta))\eta] + \mathbb{E}\hat{\mathbb{E}}[\partial_\mu v(\theta, \mathcal{L}(\theta))(\hat{\theta})\hat{\eta}] + E_1 + E_2 \\ &= \hat{\mathbb{E}}\left[\left(\partial_x v(\hat{\theta}, \mathcal{L}(\theta)) + \mathbb{E}(\partial_\mu v(\theta, \mathcal{L}(\theta))(\hat{\theta}))\right)\hat{\eta}\right] + E_1 + E_2, \end{aligned} \quad (3.2.2)$$

where

$$E_1 := \int_0^1 \mathbb{E}\left[\left(\partial_x v(\theta + \lambda\eta, \mathcal{L}(\theta + \eta)) - \partial_x v(\theta, \mathcal{L}(\theta))\right)\eta\right] \, d\lambda$$

and

$$E_2 := \int_0^1 \mathbb{E}\hat{\mathbb{E}}\left[\left(\partial_\mu v(\theta, \mathcal{L}(\theta + \lambda\eta))(\hat{\theta} + \lambda\hat{\eta}) - \partial_\mu v(\theta, \mathcal{L}(\theta))(\hat{\theta})\right)\hat{\eta}\right] \, d\lambda.$$

We first estimate E_1 . We rewrite

$$\begin{aligned} |E_1| &\leq \int_0^1 \mathbb{E}\left|\left(\partial_x v(\theta + \lambda\eta, \mathcal{L}(\theta + \eta)) - \partial_x v(\theta, \mathcal{L}(\theta))\right)\eta\right| \, d\lambda \\ &\leq \int_0^1 \mathbb{E}\left|\left(\partial_x v(\theta + \lambda\eta, \mathcal{L}(\theta + \eta)) - \partial_x v(\theta, \mathcal{L}(\theta))\right)\eta \mathbf{1}_{\{|\eta| \leq \|\eta\|_{L^2}^{1/2}\}}\right| \, d\lambda \\ &\quad + \int_0^1 \mathbb{E}\left|\left(\partial_x v(\theta + \lambda\eta, \mathcal{L}(\theta + \eta)) - \partial_x v(\theta, \mathcal{L}(\theta))\right)\eta \mathbf{1}_{\{|\eta| > \|\eta\|_{L^2}^{1/2}\}}\right| \, d\lambda =: E_{11} + E_{12}. \end{aligned} \quad (3.2.3)$$

By the Cauchy-Schwarz inequality,

$$\begin{aligned} E_{11} &\leq \left(\sup_{\lambda \in [0,1]} \mathbb{E}\left|\left(\partial_x v(\theta + \lambda\eta, \mathcal{L}(\theta + \eta)) - \partial_x v(\theta, \mathcal{L}(\theta))\right)\mathbf{1}_{\{|\eta| \leq \|\eta\|_{L^2}^{1/2}\}}\right|^2\right)^{1/2} \|\eta\|_{L^2} \\ &\leq \left(\mathbb{E}\left|\sup_{|y| \leq \|\eta\|_{L^2}^{1/2}} \sup_{m \in \{m \in \mathcal{P}_2(\mathbb{R}^d) \mid W_2(\mu, m) \leq \|\eta\|_{L^2}\}} \left(\partial_x v(\theta + y, m) - \partial_x v(\theta, \mu)\right)\right|^2\right)^{1/2} \|\eta\|_{L^2}. \end{aligned}$$

By the joint continuity of $\partial_x v$, it is clear that

$$\lim_{\|\eta\|_{L^2} \downarrow 0} \left[\sup_{|y| \leq \|\eta\|_{L^2}^{1/2}} \sup_{m \in \{m \in \mathcal{P}_2(\mathbb{R}^d) \mid W_2(\mu, m) \leq \|\eta\|_{L^2}\}} \left(\partial_x v(\theta + y, m) - \partial_x v(\theta, \mu)\right) \right]^2 = 0.$$

Since $\|\eta\|_{L^2} \leq 1$ by assumption, the set $\{m \in \mathcal{P}_2(\mathbb{R}^d) \mid W_2(\mu, m) \leq \|\eta\|_{L^2}\}$ is bounded in $\mathcal{P}_2(\mathbb{R}^d)$. Therefore, by assumption, $\partial_x v$ has linear growth that is uniform in m . By the dominated convergence theorem,

$$\frac{E_{11}}{\|\eta\|_{L^2}} \leq \left(\mathbb{E}\left|\sup_{|y| \leq \|\eta\|_{L^2}^{1/2}} \sup_{m \in \{m \in \mathcal{P}_2(\mathbb{R}^d) \mid W_2(\mu, m) \leq \|\eta\|_{L^2}\}} \left(\partial_x v(\theta + y, m) - \partial_x v(\theta, \mu)\right)\right|^2\right)^{1/2} \xrightarrow{\|\eta\|_{L^2} \downarrow 0} 0. \quad (3.2.4)$$

Using again the fact that $\partial_x v$ has linear growth that is uniform in m belonging to the set $\{m \in \mathcal{P}_2(\mathbb{R}^d) \mid W_2(\mu, m) \leq 1\}$, we estimate E_{12} as

$$\begin{aligned} E_{12} &\leq \mathbb{E} \left[\left| \sup_{\lambda \in [0,1]} \sup_{m \in \{m \in \mathcal{P}_2(\mathbb{R}^d) \mid W_2(\mu, m) \leq 1\}} \left| \partial_x v(\theta + \lambda \eta, m) - \partial_x v(\theta, \mu) \right| |\eta| \mathbf{1}_{\{|\eta| > \|\eta\|_{L^2}^{1/2}\}} \right| \right] \\ &\leq C \mathbb{E} \left[(1 + |\theta| + |\eta|) |\eta| \mathbf{1}_{\{|\eta| > \|\eta\|_{L^2}^{1/2}\}} \right] = C \mathbb{E} \left[(|\eta| + |\theta| |\eta| + |\eta|^2) \mathbf{1}_{\{|\eta| > \|\eta\|_{L^2}^{1/2}\}} \right]. \end{aligned}$$

By Chebychev's inequality,

$$\mathbb{P}\{|\eta| > \|\eta\|_{L^2}^{1/2}\} \leq \|\eta\|_{L^2}.$$

Therefore, we obtain that

$$\mathbb{E} \left[|\eta| \mathbf{1}_{\{|\eta| > \|\eta\|_{L^2}^{1/2}\}} \right] \leq \|\eta\|_{L^2} (\|\eta\|_{L^2})^{1/2},$$

$$\mathbb{E} \left[|\eta|^2 \mathbf{1}_{\{|\eta| > \|\eta\|_{L^2}^{1/2}\}} \right] \leq \mathbb{E} [|\eta|^2] = \|\eta\|_{L^2}^2,$$

$$\begin{aligned} \mathbb{E} \left[|\theta| |\eta| \mathbf{1}_{\{|\eta| > \|\eta\|_{L^2}^{1/2}\}} \right] &\leq \left(\mathbb{E} [|\theta|^2 \mathbf{1}_{\{|\eta| > \|\eta\|_{L^2}^{1/2}\}}] \right)^{1/2} \left(\mathbb{E} [|\eta|^2] \right)^{1/2} \\ &\leq \|\eta\|_{L^2} \left(\sup_{A \in \mathcal{F}: \mathbb{P}(A) \leq \|\eta\|_{L^2}} \mathbb{E} [|\theta|^2 \mathbf{1}_A] \right)^{1/2}. \end{aligned}$$

This shows that

$$\frac{E_{12}}{\|\eta\|_{L^2}} \leq C \left((\|\eta\|_{L^2})^{1/2} + \|\eta\|_{L^2} + \left(\sup_{A \in \mathcal{F}: \mathbb{P}(A) \leq \|\eta\|_{L^2}} \mathbb{E} [|\theta|^2 \mathbf{1}_A] \right)^{1/2} \right) \xrightarrow{\|\eta\|_{L^2} \downarrow 0} 0. \quad (3.2.5)$$

Finally, we bound E_2 by

$$|E_2| \leq \|\eta\|_{L^2} \left(\mathbb{E} \left[\sup_{Z \in L^2(\mathcal{F}; \mathbb{R}^d): \|Z\|_{L^2} \leq \|\eta\|_{L^2}} \left| \hat{\mathbb{E}} \left[\partial_\mu v(\theta, \mathcal{L}(\theta + Z))(\hat{\theta} + \hat{Z}) - \partial_\mu v(\theta, \mathcal{L}(\theta))(\hat{\theta}) \right]^2 \right] \right)^{1/2}.$$

For every $x \in \mathbb{R}^d$, we define the function $\varphi_x : L^2(\mathcal{F}; \mathbb{R}^d) \rightarrow L^2(\mathcal{F}; \mathbb{R}^d)$ given by $\varphi_x(Z) := \partial_\mu v(x, \mathcal{L}(Z))(Z)$. We claim that φ_x is continuous. To observe this fact, we take a sequence of random variables $\{Z_n\}_n$ converging to Z in L^2 . Then $W_2(\mathcal{L}(Z_n), \mathcal{L}(Z)) \rightarrow 0$ and there exists a subsequence $\{Z_{n_k}\}_k$ such that Z_{n_k} converges to Z almost surely as $k \rightarrow \infty$. Therefore,

$$\left| \partial_\mu v(x, \mathcal{L}(Z_{n_k}))(Z_{n_k}) - \partial_\mu v(x, \mathcal{L}(Z))(Z) \right|^2 \xrightarrow{k \rightarrow \infty} 0 \quad \text{a.s.}$$

Since $W_2(\mathcal{L}(Z_n), \mathcal{L}(Z)) \rightarrow 0$, the set $\{\mathcal{L}(Z_n) \mid n \in \mathbb{N}\}$ is bounded in $\mathcal{P}_2(\mathbb{R}^d)$. Therefore, by the dominated convergence theorem and the fact that $\partial_\mu v(\cdot, m)(\cdot)$ has linear growth that is uniform in $m \in \{\mathcal{L}(Z_n) \mid n \in \mathbb{N}\}$, we have

$$\mathbb{E} \left| \partial_\mu v(x, \mathcal{L}(Z_{n_k}))(Z_{n_k}) - \partial_\mu v(x, \mathcal{L}(Z))(Z) \right|^2 \xrightarrow{k \rightarrow \infty} 0,$$

which shows that φ_x is continuous. Therefore,

$$\begin{aligned} &\sup_{Z \in L^2(\mathcal{F}; \mathbb{R}^d): \|Z\|_{L^2} \leq \|\eta\|_{L^2}} \left| \hat{\mathbb{E}} \left[\partial_\mu v(\theta, \mathcal{L}(\theta + Z))(\hat{\theta} + \hat{Z}) - \partial_\mu v(\theta, \mathcal{L}(\theta))(\hat{\theta}) \right]^2 \right| \\ &= \sup_{Z \in L^2(\mathcal{F}; \mathbb{R}^d): \|Z\|_{L^2} \leq \|\eta\|_{L^2}} \left| \hat{\mathbb{E}} \left[\varphi_\theta(\hat{\theta} + \hat{Z}) - \varphi_\theta(\hat{\theta}) \right]^2 \right| \xrightarrow{\|\eta\|_{L^2} \downarrow 0} 0. \end{aligned}$$

Finally, since $\|\eta\|_{L^2} \leq 1$, we note that the set $\{\mathcal{L}(\theta + Z) \mid Z \in L^2(\mathcal{F}; \mathbb{R}^d), \|Z\|_{L^2} \leq \|\eta\|_{L^2}\}$

is bounded in $\mathcal{P}_2(\mathbb{R}^d)$. Therefore, by the dominated convergence theorem and the fact that $\partial_\mu v(\cdot, m)(\cdot)$ has linear growth that is uniform in $m \in \{\mathcal{L}(\theta + Z) \mid Z \in L^2(\mathcal{F}; \mathbb{R}^d), \|Z\|_{L^2} \leq \|\eta\|_{L^2}\}$, we have

$$\frac{|E_2|}{\|\eta\|_{L^2}} \xrightarrow{\|\eta\|_{L^2} \downarrow 0} 0. \quad (3.2.6)$$

The proof is complete by combining (3.2.2), (3.2.3), (3.2.4), (3.2.5) and (3.2.6). \square

The next theorem (see Proposition 3.1 from [13]) connects L-derivatives with real derivatives through empirical measures. It is crucial to many subsequent results. To state the theorem, we introduce second order L-derivatives

$$\mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \ni (m, y) \mapsto \partial_v \partial_\mu U(m, y) \in \mathbb{R}^d \otimes \mathbb{R}^d$$

and

$$\mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \times \mathbb{R}^d \ni (m, y, y') \mapsto \partial_\mu^2 U(m, y, y') \in \mathbb{R}^d \otimes \mathbb{R}^d$$

defined by

$$\partial_v \partial_\mu U(m, y) := (\partial_y (\partial_\mu U(m, y)))_{1 \leq i \leq d} \quad (3.2.7)$$

and

$$\partial_\mu^2 U(m, y, y') := (\partial_\mu (\partial_\mu U(\cdot, y)))_{1 \leq i \leq d} (y'). \quad (3.2.8)$$

Theorem 3.2.5. *Let $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ be L-differentiable on $\mathcal{P}_2(\mathbb{R}^d)$. We define a function $u^N : (\mathbb{R}^d)^N \rightarrow \mathbb{R}$ by*

$$u^N(x_1, \dots, x_N) = U\left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}\right).$$

Then, for any $N \geq 1$, the function u^N is differentiable on $(\mathbb{R}^d)^N$ and

$$\mathbb{R}^d \ni \partial_{x_i} u^N(x_1, \dots, x_N) = \frac{1}{N} \partial_\mu U\left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}\right)(x_i). \quad (3.2.9)$$

If $\partial_v \partial_\mu U$ and $\partial_\mu^2 U$ exist and are jointly continuous, then u^N is twice-differentiable on $(\mathbb{R}^d)^N$ and

$$\mathbb{R}^d \otimes \mathbb{R}^d \ni \partial_{x_j x_i}^2 u^N(x_1, \dots, x_N) = \frac{1}{N} \partial_v \left[\partial_\mu U\left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}\right) \right](x_i) \delta_{i,j} + \frac{1}{N^2} \partial_\mu^2 U\left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}\right)(x_i, x_j). \quad (3.2.10)$$

Proof. Let θ be a uniform random variable taking values on $\{1, \dots, N\}$. Then the random variable x_θ has law $\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}$. Let \tilde{U} be the lift of U . Then

$$U\left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}\right) = \tilde{U}(x_\theta).$$

By Fréchet differentiation, we have

$$\tilde{U}(x_\theta + \eta) = \tilde{U}(x_\theta) + (D\tilde{U}(x_\theta))(\eta) + o(\|\eta\|_{L^2}),$$

where, by the definition of L-derivatives,

$$(D\tilde{U}(x_\theta))(\eta) = \mathbb{E} \left[\left(\partial_\mu U\left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell}\right) \right)(x_\theta) \cdot \eta \right].$$

For any $x \in (\mathbb{R}^d)^N$, define a linear function $\varphi(x) : (\mathbb{R}^d)^N \rightarrow \mathbb{R}$ given by

$$\varphi(x)(h) = \sum_{j=1}^N \frac{1}{N} \partial_\mu U \left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell} \right) (x_i) \cdot h_j.$$

Note that $(D\tilde{U}(x_\theta))(h_\theta) = \varphi(x)(h)$ and $\|h_\theta\|_{L^2}^2 = \frac{1}{N} \sum_{i=1}^N |h_i|^2 \leq |h|^2$. Therefore,

$$\begin{aligned} & \frac{1}{|h|} \left[u^N(x+h) - u^N(x) - \varphi(x)(h) \right] \\ &= \frac{1}{|h|} \left[\tilde{U}(x_\theta + h_\theta) - \tilde{U}(x_\theta) - (D\tilde{U}(x_\theta))(h_\theta) \right] \\ &\leq \frac{1}{\|h_\theta\|_{L^2}} \left[\tilde{U}(x_\theta + h_\theta) - \tilde{U}(x_\theta) - (D\tilde{U}(x_\theta))(h_\theta) \right] \xrightarrow{|h| \downarrow 0} 0. \end{aligned}$$

This shows that u^N is differentiable at $x \in (\mathbb{R}^d)^N$ with Fréchet derivative given by

$$Du^N(x) = \varphi(x).$$

Since $Du^N(x)(h) = \nabla u^N(x) \cdot h$, for every $x, h \in (\mathbb{R}^d)^N$, we conclude that

$$\partial_{x_i} u^N(x_1, \dots, x_N) = \frac{1}{N} \partial_\mu U \left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell} \right) (x_i).$$

This completes the first part of the proof. For the second part, we define a function

$$\phi : (\mathbb{R}^d)^{N+1} \rightarrow \mathbb{R}; \quad (x_1, \dots, x_N, y) \mapsto \frac{1}{N} \partial_\mu U \left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell} \right) (y).$$

Since $\partial_v \partial_\mu U$ and $\partial_\mu^2 U$ exist, we know that the partial derivatives of ϕ exist and are given by

$$\partial_y \phi(x_1, \dots, x_N, y) = \frac{1}{N} \partial_v \partial_\mu U \left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell} \right) (y)$$

and

$$\partial_{x_j} \phi(x_1, \dots, x_N, y) = \frac{1}{N^2} \partial_\mu^2 U \left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell} \right) (y, x_j).$$

For $j \neq i$, it is clear that

$$\partial_{x_j x_i}^2 u^N(x_1, \dots, x_N) = \partial_{x_j} \phi(x_1, \dots, x_N, x_i) = \frac{1}{N^2} \partial_\mu^2 U \left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell} \right) (x_i, x_j).$$

Since $\partial_v \partial_\mu U$ and $\partial_\mu^2 U$ are jointly continuous, we observe that the partial derivatives of ϕ are also continuous. Hence, we can apply the standard chain rule of differentiation to ϕ , which gives

$$\begin{aligned} \partial_{x_i x_i}^2 u^N(x_1, \dots, x_N) &= \partial_{x_i} \phi(x_1, \dots, x_i, \dots, x_N, x_i) \\ &= \partial_{x_i} \phi(x_1, \dots, y, \dots, x_N, x_i) \Big|_{y=x_i} + \partial_{x_i} \phi(x_1, \dots, x_i, \dots, x_N, y) \Big|_{y=x_i} \\ &= \frac{1}{N} \partial_v \partial_\mu U \left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell} \right) (x_i) + \frac{1}{N^2} \partial_\mu^2 U \left(\frac{1}{N} \sum_{\ell=1}^N \delta_{x_\ell} \right) (x_i, x_i). \end{aligned}$$

□

For the theory in subsequent chapters, we define higher order derivatives of measure functionals by iterating the definitions of second order L-derivatives in (3.2.7) and (3.2.8). Inspired by the work [19], for any $k \in \mathbb{N}$, we formally define higher order derivatives in measures through the

following iteration (provided that they actually exist): for any $k \geq 2$, $(i_1, \dots, i_k) \in \{1, \dots, d\}^k$ and $x_1, \dots, x_k \in \mathbb{R}^d$, the function $\partial_\mu^k f : \mathcal{P}_2(\mathbb{R}^d) \times (\mathbb{R}^d)^k \rightarrow (\mathbb{R}^d)^{\otimes k}$ is defined by

$$\left(\partial_\mu^k f(\mu, x_1, \dots, x_k) \right)_{(i_1, \dots, i_k)} := \left(\partial_\mu \left(\left(\partial_\mu^{k-1} f(\cdot, x_1, \dots, x_{k-1}) \right)_{(i_1, \dots, i_{k-1})} \right) (\mu, x_k) \right)_{i_k}, \quad (3.2.11)$$

and its corresponding mixed derivatives in space $\partial_{v_k}^{\ell_k} \dots \partial_{v_1}^{\ell_1} \partial_\mu^k f : \mathcal{P}_2(\mathbb{R}^d) \times (\mathbb{R}^d)^k \rightarrow (\mathbb{R}^d)^{\otimes (k+\ell_1+\dots+\ell_k)}$ are defined by

$$\left(\partial_{v_k}^{\ell_k} \dots \partial_{v_1}^{\ell_1} \partial_\mu^k f(\mu, x_1, \dots, x_k) \right)_{(i_1, \dots, i_k)} := \frac{\partial^{\ell_k}}{\partial x_k^{\ell_k}} \dots \frac{\partial^{\ell_1}}{\partial x_1^{\ell_1}} \left[\left(\partial_\mu^k f(\mu, x_1, \dots, x_k) \right)_{(i_1, \dots, i_k)} \right], \quad (3.2.12)$$

for $\ell_1 \dots \ell_k \in \mathbb{N} \cup \{0\}$. Since this notation for higher order derivatives in measure is quite cumbersome, we introduce the following multi-index notation for brevity. This notation was first proposed in [19].

Definition 3.2.6 (Multi-index notation). Let n, ℓ be non-negative integers. Also, let $\beta = (\beta_1, \dots, \beta_n)$ be an n -dimensional vector of non-negative integers. Then we call any ordered tuple of the form (n, ℓ, β) or (n, β) a *multi-index*. For any function $f : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, the derivative $D^{(n, \ell, \beta)} f(x, \mu, v_1, \dots, v_n)$ is defined as

$$D^{(n, \ell, \beta)} f(x, \mu, v_1, \dots, v_n) := \partial_{v_n}^{\beta_n} \dots \partial_{v_1}^{\beta_1} \partial_x^\ell \partial_\mu^n f(x, \mu, v_1, \dots, v_n),$$

if this derivative is well-defined. For any function $\Phi : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, we define

$$D^{(n, \beta)} \Phi(\mu, v_1, \dots, v_n) := \partial_{v_n}^{\beta_n} \dots \partial_{v_1}^{\beta_1} \partial_\mu^n \Phi(\mu, v_1, \dots, v_n),$$

if this derivative is well-defined. Finally, we also define the *order*³ $|(n, \ell, \beta)|$ (resp. $|(n, \beta)|$) by

$$|(n, \ell, \beta)| := n + \beta_1 + \dots + \beta_n + \ell, \quad |(n, \beta)| := n + \beta_1 + \dots + \beta_n. \quad (3.2.13)$$

3.3 Connection between linear functional derivatives and L-derivatives

Recall the function U defined in Example 3.1.2. A combination of Theorem 3.2.3 and Theorem 3.2.4 gives

$$\partial_\mu U(\mu, y) = F' \left(\int_{\mathbb{R}^d} G(x) \mu(dx) \right) G'(y),$$

which implies that

$$\partial_\mu U(\mu, y) = \partial_y \frac{\delta U}{\delta m}(\mu, y).$$

It turns out that this is in fact a special case of a more general result, by which we can even deduce the existence of the corresponding linear functional derivative, given the existence of the L-derivative. The following theorem comes from Proposition 5.51 in [14].

Theorem 3.3.1. *Suppose that $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ is L-differentiable on $\mathcal{P}_2(\mathbb{R}^d)$. Moreover, suppose that the L-derivative of U is Lipschitz continuous, i.e. there exists a constant $C > 0$ such that*

$$\left| \partial_\mu U(\mu_1, x_1) - \partial_\mu U(\mu_2, x_2) \right| \leq C(W_2(\mu_1, \mu_2) + |x_1 - x_2|),$$

for each $\mu_1, \mu_2 \in \mathcal{P}_2(\mathbb{R}^d)$, $x_1, x_2 \in \mathbb{R}^d$, for some $C > 0$. Then the linear functional derivative of U exists and satisfies the relation

$$\partial_\mu U(\mu, y) = \partial_y \frac{\delta U}{\delta m}(\mu, y).$$

³We do not consider ‘zeroth’ order derivatives in our definition, i.e. at least one of $n, \beta_1, \dots, \beta_n$ and ℓ must be non-zero, for every multi-index $(n, \ell, (\beta_1, \dots, \beta_n))$.

The following theorem is a straightforward generalisation of Theorem 3.3.1.

Theorem 3.3.2. Consider $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$. Suppose that, for every $j \in \{1, \dots, k\}$, $\partial_\mu^j U$ exists and is Lipschitz continuous. Then the k th order linear functional derivative of U exists and satisfies the relation

$$\partial_\mu^k U(\mu, y_1, \dots, y_k) = \partial_{y_1} \dots \partial_{y_k} \frac{\delta^k U}{\delta m^k}(\mu, y_1, \dots, y_k).$$

Proof. The proof is presented in dimension one, for simplicity of notations. We proceed by induction in k . The case corresponding to $k = 1$ is established in Theorem 3.3.1. Suppose that the theorem holds for $k - 1$. Then, by induction hypothesis, we know that

$$\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(\cdot, y_1, \dots, y_{k-1}) = \partial_\mu^{k-1} U(\cdot, y_1, \dots, y_{k-1}) \quad (3.3.1)$$

is L-differentiable with Lipschitz continuous L-derivative. Therefore, by Theorem 3.3.1, $\frac{\delta}{\delta m}(\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(\cdot, y_1, \dots, y_{k-1}))$ exists and satisfies

$$\begin{aligned} & \left[\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(m', y_1, \dots, y_{k-1}) \right] - \left[\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(m, y_1, \dots, y_{k-1}) \right] \\ &= \int_0^1 \int_{\mathbb{R}} \left[\frac{\delta}{\delta m} \left(\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(\cdot, y_1, \dots, y_{k-1}) \right) ((1-s)m + sm', y_k) \right] (m' - m)(dy_k) ds. \end{aligned}$$

By integrating each of y_1, \dots, y_{k-1} from 0 to x_1, \dots, x_{k-1} respectively and applying the normalisation convention (3.1.2), we obtain that

$$\begin{aligned} & \left[\frac{\delta^{k-1} U}{\delta m^{k-1}}(m', x_1, \dots, x_{k-1}) \right] - \left[\frac{\delta^{k-1} U}{\delta m^{k-1}}(m, x_1, \dots, x_{k-1}) \right] \\ &= \int_0^{x_{k-1}} \dots \int_0^{x_1} \left[\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(m', y_1, \dots, y_{k-1}) \right] \\ & \quad - \left[\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(m, y_1, \dots, y_{k-1}) \right] dy_1 \dots dy_{k-1} \\ &= \int_0^1 \int_{\mathbb{R}} \left[\int_0^{x_{k-1}} \dots \int_0^{x_1} \frac{\delta}{\delta m} \left(\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(\cdot, y_1, \dots, y_{k-1}) \right) ((1-s)m + sm', y_k) \right. \\ & \quad \left. dy_1 \dots dy_{k-1} \right] (m' - m)(dy_k) ds. \end{aligned}$$

This shows that $\frac{\delta^k U}{\delta m^k}$ exists and is given by

$$\begin{aligned} & \frac{\delta^k U}{\delta m^k}(\mu, x_1, \dots, x_{k-1}, y_k) \\ &= \int_0^{x_{k-1}} \dots \int_0^{x_1} \left[\frac{\delta}{\delta m} \left(\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(\cdot, y_1, \dots, y_{k-1}) \right) (\mu, y_k) \right] dy_1 \dots dy_{k-1}, \end{aligned}$$

which implies that

$$\frac{\delta}{\delta m} \left(\partial_{x_1} \dots \partial_{x_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(\cdot, x_1, \dots, x_{k-1}) \right) (\mu, y_k) = \partial_{x_1} \dots \partial_{x_{k-1}} \frac{\delta^k U}{\delta m^k}(\mu, x_1, \dots, x_{k-1}, y_k). \quad (3.3.2)$$

Finally,

$$\begin{aligned} \partial_\mu^k U(\mu, y_1, \dots, y_k) &= \partial_\mu \left[\partial_\mu^{k-1} U(\cdot, y_1, \dots, y_{k-1}) \right] (\mu, y_k) \\ &= \partial_{y_k} \left[\frac{\delta}{\delta m} \left(\partial_\mu^{k-1} U(\cdot, y_1, \dots, y_{k-1}) \right) (\mu, y_k) \right] \end{aligned}$$

$$\begin{aligned}
&= \partial_{y_k} \left[\frac{\delta}{\delta m} \left(\partial_{y_1} \dots \partial_{y_{k-1}} \frac{\delta^{k-1} U}{\delta m^{k-1}}(\cdot, y_1, \dots, y_{k-1}) \right) (\mu, y_k) \right] \\
&= \partial_{y_1} \dots \partial_{y_k} \frac{\delta^k U}{\delta m^k}(\mu, y_1, \dots, y_k),
\end{aligned}$$

where the second equality follows from Theorem 3.3.1 and the third and final equalities follow from (3.3.1) and (3.3.2) respectively. \square

Theorem 3.3.2 is crucial, as it follows us to only work with L-derivatives as conditions (the main strategy), whilst obtaining existential results on the corresponding linear functional derivatives.

By imposing the additional assumption that the p th order L-derivative is uniformly bounded, we can in fact conclude that the p th order linear functional derivative has p th order polynomial growth in space, uniform in measure. Before introducing this result, we first introduce a convenient class of functionals of measure that will serve as a hypothesis in many results of this work.

Definition 3.3.3. A function $f : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ belongs to class $\mathcal{M}_k(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$, if the derivatives $D^{(n, \ell, \beta)} f(x, \mu, v_1, \dots, v_n)$ exist for every multi-index (n, ℓ, β) such that $|(n, \ell, \beta)| \leq k$ and satisfy

$$(i) \quad |D^{(n, \ell, \beta)} f(x, \mu, v_1, \dots, v_n)| \leq C, \quad (3.3.3)$$

(ii)

$$\begin{aligned}
&\left| D^{(n, \ell, \beta)} f(x, \mu, v_1, \dots, v_n) - D^{(n, \ell, \beta)} f(x', \mu', v'_1, \dots, v'_n) \right| \\
&\leq C \left(|x - x'| + \sum_{i=1}^n |v_i - v'_i| + W_2(\mu, \mu') \right), \quad (3.3.4)
\end{aligned}$$

for any $x, x', v_1, v'_1, \dots, v_n, v'_n \in \mathbb{R}^d$ and $\mu, \mu' \in \mathcal{P}_2(\mathbb{R}^d)$, for some constant $C > 0$.

Remark 3.3.4. By the mean-value theorem and equality (3.2.1), assumption (3.3.4) automatically holds for any $|(n, \ell, \beta)| < k$, by assumption (3.3.3).

For the time-dependent case, we extend the previous definition as follows.

Definition 3.3.5. Let $t \in [0, T]$. A function $\mathcal{V} : [0, t] \times \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ is said to be in $\mathcal{M}_k([0, t] \times \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$, if

- (i) $s \mapsto \mathcal{V}(s, x, \mu)$ is continuously differentiable on $[0, t]$.
- (ii) $\mathcal{V}(s, \cdot, \cdot) \in \mathcal{M}_k(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$, for each $s \in [0, t]$, where the constant C in (3.3.3) and (3.3.4) is uniform in $s \in [0, t]$.
- (iii) All derivatives in measure (including the zeroth order derivative) of $\mathcal{V}(\cdot, \cdot, \cdot)$ up to the k th order are jointly continuous in time, measure and space.

By convention, any function f defined only on $\mathcal{P}_2(\mathbb{R}^d)$ will be extended to $\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d)$ naturally by $(x, \mu) \mapsto f(\mu)$, for all $x \in \mathbb{R}^d$. Similarly, any function \mathcal{V} defined only on $[0, t] \times \mathcal{P}_2(\mathbb{R}^d)$ will be extended to $[0, t] \times \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d)$ naturally by $(s, x, \mu) \mapsto \mathcal{V}(s, \mu)$, for all $x \in \mathbb{R}^d$. For any function with a codomain in a higher dimensional space, these definitions are applied to each component. When it is clear from context, we will just use the notation \mathcal{M}_k for the two definitions above.

Note that, by (3.2.1), any function in $\mathcal{M}_1(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ is automatically (jointly) Lipschitz in space and measure.

It is worth noting that these definitions are extensions of the framework in [9] to higher-order derivatives corresponding to $k \geq 3$. Since we mainly work with functions in the class \mathcal{M}_k , here we give some examples of functions in $\mathcal{M}_k(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$, taken from [19].

Example 3.3.6. The following functions $F : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ belong to $\mathcal{M}_k(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$. This is a direct consequence of Theorem 3.2.3 and Theorem 3.2.4.

(i) p th-degree interaction:

$$F(x, \mu) = \int_{\mathbb{R}^d} \dots \int_{\mathbb{R}^d} \varphi(x, y_1, \dots, y_p) \mu(dy_1) \dots \mu(dy_p),$$

where $\varphi \in C_{b, \text{Lip}}^k((\mathbb{R}^d)^{p+1})$.

(ii) p th-degree polynomial on the Wasserstein space:

$$F(x, \mu) = \prod_{i=1}^p \int_{\mathbb{R}^d} \varphi_i(x, y) \mu(dy),$$

where $\varphi_i \in C_{b, \text{Lip}}^k((\mathbb{R}^d)^2)$ is *uniformly bounded*, for each $i \in \{1, \dots, p\}$. Note that the requirement of uniform boundedness comes from an application of Theorem 3.2.3 (ii).

Theorem 3.3.7. Let $p \geq 1$ and assume that $U \in \mathcal{M}_p(\mathcal{P}_2(\mathbb{R}^d))$. Then

$$\left| \frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_p) \right| \leq \frac{(\sqrt{d})^p}{p} \|\partial_\mu^p U\|_\infty (|y_1|^p + \dots + |y_p|^p).$$

Proof. We present the main argument of the proof by induction in dimension one, for ease of notation. First, we compute that

$$\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_p) = \frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_{p-1}, 0) + \int_0^1 \partial_{t_p} \left[\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, t_p y_p) \right] dt_p.$$

Let ∂_{x_p} denote the derivative w.r.t. the p th component of the spatial variables. From the convention of normalisation (3.1.2), we simply obtain that

$$\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_p) = y_p \int_0^1 \partial_{x_p} \left[\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, t_p y_p) \right] dt_p.$$

We now show that, for every $k < p$, we have

$$\begin{aligned} \frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_p) &= \\ y_{p-k} \dots y_p \int_{[0,1]^{k+1}} \partial_{x_{p-k}} \dots \partial_{x_p} \left[\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_{p-k-1}, t_{p-k} y_{p-k}, \dots, t_p y_p) \right] dt_{p-k} \dots dt_p. \end{aligned} \quad (3.3.5)$$

Suppose that this holds for some $k \leq p-2$. Then, observing that

$$\partial_{x_{p-k}} \dots \partial_{x_p} \left[\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_{p-k-2}, 0, t_{p-k} y_{p-k}, \dots, t_p y_p) \right] = 0,$$

we recover

$$\begin{aligned} \frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_p) &= \\ y_{p-k-1} \dots y_p \int_{[0,1]^{k+2}} \partial_{x_{p-k-1}} \dots \partial_{x_p} \left[\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_{p-k-2}, t_{p-k-1} y_{p-k-1}, \dots, t_p y_p) \right] dt_{p-k-1} \dots dt_p. \end{aligned}$$

Setting $k = p-1$ in (3.3.5), we then obtain

$$\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_p) = y_1 \dots y_p \int_{[0,1]^p} \partial_\mu^p U(m, t_1 y_1, \dots, t_p y_p) dt_1 \dots dt_p.$$

The proof is concluded for dimension one by invoking the boundedness assumption of $\partial_\mu^p U$ along

with Young's inequality. For higher dimensional cases where $d > 1$, we simply note that

$$\frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_p) = \sum_{k_1=1}^d \dots \sum_{k_p=1}^d y_1^{(k_1)} \dots y_p^{(k_p)} \int_{[0,1]^p} \left(\partial_\mu^p U(m, t_1 y_1, \dots, t_p y_p) \right)_{(k_1, \dots, k_p)} dt_1 \dots dt_p.$$

Therefore, by Hölder and Young's inequalities,

$$\begin{aligned} \left| \frac{\delta^p U}{\delta m^p}(m, y_1, \dots, y_p) \right| &\leq \|\partial_\mu^p U\|_\infty \left(\sum_{k_1=1}^d |y_1^{(k_1)}| \right) \dots \left(\sum_{k_p=1}^d |y_p^{(k_p)}| \right) \\ &\leq (\sqrt{d})^p \|\partial_\mu^p U\|_\infty |y_1| \dots |y_p| \\ &\leq \frac{(\sqrt{d})^p}{p} \|\partial_\mu^p U\|_\infty (|y_1|^p + \dots + |y_p|^p). \end{aligned}$$

□

3.4 Itô's formula along flows of marginals and the master equation on the space of measures

We start by defining the class $\mathcal{D}_0([0, t])$, which gives a minimal set of assumptions required for the Itô's formula in measure to hold.

Definition 3.4.1. Let $t \in [0, T]$. A function $U : [0, t] \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ is of class $\mathcal{D}_0([0, t])$ if the following conditions hold:

- i) U is jointly continuous on $[0, t] \times \mathcal{P}_2(\mathbb{R}^d)$.
- ii) For all $s \in [0, t]$, the mappings $\mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \ni (m, y) \mapsto \partial_\mu U(s, m)(y)$ and $\mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \ni (m, y) \mapsto \partial_v \partial_\mu U(s, m)(y)$ are well-defined and continuous in the product topologies.
- iii) There exists $L > 0$ such that for all $s \in [0, t]$ and $\xi \in L^2(\mathbb{R}^d)$,

$$\mathbb{E}[|\partial_\mu U(s, \mathcal{L}(\xi))(\xi)|^2 + |\partial_v \partial_\mu U(s, \mathcal{L}(\xi))(\xi)|^2] \leq L.$$

- iv) There exists $C > 0$ such that for all $s \in [0, t]$ and $\xi_1, \xi_2 \in L^2(\mathbb{R}^d)$,

$$|U(s, \mathcal{L}(\xi_1)) - U(s, \mathcal{L}(\xi_2))| \leq CW_2(\mathcal{L}(\xi_1), \mathcal{L}(\xi_2)),$$

$$\left(\mathbb{E}[|\partial_\mu U(s, \mathcal{L}(\xi_1))(\xi_1) - \partial_\mu U(s, \mathcal{L}(\xi_2))(\xi_2)|^2] \right)^{1/2} \leq CW_2(\mathcal{L}(\xi_1), \mathcal{L}(\xi_2)),$$

$$\left(\mathbb{E}[|\partial_v \partial_\mu U(s, \mathcal{L}(\xi_1))(\xi_1) - \partial_v \partial_\mu U(s, \mathcal{L}(\xi_2))(\xi_2)|^2] \right)^{1/2} \leq CW_2(\mathcal{L}(\xi_1), \mathcal{L}(\xi_2)).$$

- v) The map $s \mapsto U(s, \mu)$ is continuously differentiable on $[0, t]$.

- vi) The functions

$$\begin{aligned} [0, t] \times L^2(\mathbb{R}^d) \ni (s, \xi) &\mapsto \partial_t U(s, \mathcal{L}(\xi))(\xi) \in L^2(\mathbb{R}^d) \\ [0, t] \times L^2(\mathbb{R}^d) \ni (s, \xi) &\mapsto \partial_\mu U(s, \mathcal{L}(\xi))(\xi) \in L^2(\mathbb{R}^d) \\ [0, t] \times L^2(\mathbb{R}^d) \ni (s, \xi) &\mapsto \partial_v \partial_\mu U(s, \mathcal{L}(\xi))(\xi) \in L^2(\mathbb{R}^d \otimes \mathbb{R}^d) \end{aligned}$$

are continuous.

Note that for any $U \in \mathcal{D}_0([0, t])$, $\partial_\mu^2 U$ might not necessarily be well-defined. In Chapter 4, we will define a more restrictive class \mathcal{D} that includes regularity properties of $\partial_\mu^2 U$. Also, note that any element of \mathcal{M}_2 also belongs to \mathcal{D}_0 .

The following comes from Proposition 3.9 in [16].

Theorem 3.4.2. *Suppose that $\Gamma = (\Gamma_s)_{s \in [0, t]}$ is an Itô process defined by*

$$\Gamma_s = \Gamma_0 + \int_0^s b_u du + \int_0^s \sigma_u dW_u, \quad s \in [0, t],$$

where $(b_s)_{s \in [0, t]}$ and $(\sigma_s)_{s \in [0, t]}$ are progressively-measurable processes with values in \mathbb{R}^d and $\mathbb{R}^d \otimes \mathbb{R}^d$ respectively, with respect to the filtration generated by W , such that

$$\mathbb{E} \left[\int_0^t |b_s|^2 + |\sigma_s|^4 ds \right] < +\infty. \quad (3.4.1)$$

Let $U \in \mathcal{D}_0([0, t])$ and $\mu_s := \mathcal{L}(\Gamma_s)$. Then

$$U(t, \mu_t) = U(0, \mu_0) + \int_0^t \partial_t U(s, \mu_s) + \mathbb{E} \left[\partial_\mu U(s, \mu_s, \Gamma_s) b_s + \frac{1}{2} \text{Tr} \left(\partial_v \partial_\mu U(s, \mu_s, \Gamma_s) \sigma_s \sigma_s^T \right) \right] ds. \quad (3.4.2)$$

Note that the more general version that is stated in Proposition 3.9 of [16] involves a space variable in the function U as well. However, we only work with time-dependent measure functionals our subsequent analysis. Furthermore, the definition of \mathcal{D}_0 becomes tedious when the space variable is included. Therefore, we restrict ourselves to the special case without the space variable.

The main argument in the proof of Theorem 3.4.2 in [16] is done by first restricting our consideration to functions $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ with bounded and uniformly continuous $\partial_\mu U$, $\partial_v \partial_\mu U$ and $\partial_\mu^2 U$, along with bounded b_t and σ_t . Then, for i.i.d. copies $\{\Gamma_s^i\}$ of $\{\Gamma_s\}$, we compute $\mathbb{E}[U(\frac{1}{N} \sum_{i=1}^N \delta_{\Gamma_s^i})]$, which is just the expectation of a twice-differentiable function of $(\Gamma_s^1, \dots, \Gamma_s^N)$. Hence, we can apply the standard Itô's formula to compute $\mathbb{E}[U(\frac{1}{N} \sum_{i=1}^N \delta_{\Gamma_s^i})]$, and subsequently converting real derivatives into L-derivatives via the projection formula (Theorem 3.2.5). The argument is complete for this special case by taking N to ∞ , via the result that

$$\lim_{N \rightarrow \infty} \mathbb{E} \left[\sup_{0 \leq s \leq t} W_2^2 \left(\frac{1}{N} \sum_{i=1}^N \delta_{\Gamma_s^i}, \mathcal{L}(\Gamma_s) \right) \right] = 0,$$

by Theorem 10.2.7 of [58]. The general case of $U \in \mathcal{D}_0([0, t])$ is done via smoothing and approximation arguments.

An alternative proof is presented in [9], for the McKean-Vlasov flow (2.1.1), under the assumption that $b, \sigma \in \mathcal{M}_2(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and $U \in \mathcal{M}_2([0, t] \times \mathcal{P}_2(\mathbb{R}^d))$. We first consider functions $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ in $\mathcal{M}_2(\mathcal{P}_2(\mathbb{R}^d))$. The key idea involves rewriting the difference $U(\mathcal{L}(X_t^{s, \xi})) - U(\mathcal{L}(\xi))$ as

$$U(\mathcal{L}(X_t^{s, \xi})) - U(\mathcal{L}(\xi)) = \sum_{i=0}^{2^n - 1} \left[U(\mathcal{L}(X_{t_n^{i+1}}^{s, \xi})) - U(\mathcal{L}(X_{t_n^i}^{s, \xi})) \right],$$

where $t_n^i := s + i(t - s)2^{-n}$, $0 \leq i \leq 2^n$, $i \in \mathbb{N}$. Each difference is expanded up to second-order L-derivatives (by re-expanding (3.2.1) once more). This yields the Itô's formula for $U \in \mathcal{M}_2(\mathcal{P}_2(\mathbb{R}^d))$ upon taking n to ∞ . The general case for $U \in \mathcal{M}_2([0, t] \times \mathcal{P}_2(\mathbb{R}^d))$ is obtained by applying the multivariate chain rule in time.

The next theorem is the Feynman-Kac formula in the space of probability measures.

Theorem 3.4.3. *Let $t \in [0, T]$. Let $\Phi : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ be a measurable function. Define $\mathcal{V} : [0, t] \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ by*

$$\mathcal{V}(s, \mathcal{L}(\xi)) = \Phi(\mathcal{L}(X_t^{s, \xi})).$$

Suppose that (Lip) holds and that one of the following holds:

- (i) σ is uniformly bounded.
- (ii) The initial law ν is in $\mathcal{P}_4(\mathbb{R}^d)$.

Also, suppose that $\mathcal{V} \in \mathcal{D}_0([0, t])$, then \mathcal{V} satisfies on $(0, t) \times \mathcal{P}_2(\mathbb{R}^d)$ the PDE (also called the master equation)

$$\partial_s \mathcal{V}(s, \mu) + \int_{\mathbb{R}^d} [\partial_\mu \mathcal{V}(s, \mu)(y) b(y, \mu) + \frac{1}{2} \text{Tr}(\partial_v \partial_\mu \mathcal{V}(s, \mu)(y) a(y, \mu))] \mu(dy) = 0, \quad (3.4.3)$$

with terminal condition $\mathcal{V}(t, \cdot) = \Phi(\cdot)$, where $a = (a_{i,k})_{1 \leq i, k \leq d} : \mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d$ is defined as in (2.2.1).

Proof. It is clear that (3.4.1) is satisfied under the assumption. By the flow property, we observe that the function $[0, t] \ni s \mapsto \mathcal{V}(s, \mathcal{L}(X_s^{0, \xi})) \in \mathbb{R}$ is constant. Indeed, $\mathcal{V}(s, \mathcal{L}(X_s^{0, \xi})) = \Phi(\mathcal{L}(X_t^{s, X_s^{0, \xi}})) = \Phi(\mathcal{L}(X_t^{0, \xi}))$. By Theorem 3.4.2, we have

$$\begin{aligned} 0 &= \int_0^h \partial_t \mathcal{V}(s, \mathcal{L}(X_s^{0, \xi})) + \mathbb{E} \left[\partial_\mu \mathcal{V}(s, \mathcal{L}(X_s^{0, \xi}))(X_s^{0, \xi}) b(X_s^{0, \xi}, \mathcal{L}(X_s^{0, \xi})) \right. \\ &\quad \left. + \frac{1}{2} \text{Tr} [a(X_s^{0, \xi}, \mathcal{L}(X_s^{0, \xi})) \partial_v \partial_\mu \mathcal{V}(s, \mathcal{L}(X_s^{0, \xi}))(X_s^{0, \xi})] \right] ds. \end{aligned}$$

Dividing by h and letting $h \rightarrow 0$, fundamental theorem of calculus gives

$$\begin{aligned} 0 &= \partial_t \mathcal{V}(s, \mathcal{L}(X_0^{0, \xi})) + \mathbb{E} \left[\partial_\mu \mathcal{V}(s, \mathcal{L}(X_0^{0, \xi}))(X_0^{0, \xi}) b(X_0^{0, \xi}, \mathcal{L}(X_0^{0, \xi})) \right. \\ &\quad \left. + \frac{1}{2} \text{Tr} [a(X_0^{0, \xi}, \mathcal{L}(X_0^{0, \xi})) \partial_v \partial_\mu \mathcal{V}(s, \mathcal{L}(X_0^{0, \xi}))(X_0^{0, \xi})] \right] \\ &= \partial_t \mathcal{V}(s, \mathcal{L}(\xi)) + \mathbb{E} \left[\partial_\mu \mathcal{V}(s, \mathcal{L}(\xi))(\xi) b(\xi, \mathcal{L}(\xi)) + \frac{1}{2} \text{Tr} [a(\xi, \mathcal{L}(\xi)) \partial_v \partial_\mu \mathcal{V}(s, \mathcal{L}(\xi))(\xi)] \right]. \end{aligned}$$

□

The theorem is extremely useful, but with a clear drawback: it requires \mathcal{V} to be in $\mathcal{D}_0([0, t])$, a condition that is not easy to verify. The next section is thus dedicated to the regularity of \mathcal{V} .

3.5 Smoothness of the map $(s, \mathcal{L}(\xi)) \mapsto \Phi(\mathcal{L}(X_t^{s, \xi}))$

Let $\Phi : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ be a Borel-measurable function. In this section, we study the smoothness of the function $\mathcal{V} : [0, t] \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ defined by

$$\mathcal{V}(s, \mu) = \Phi(\mathcal{L}(X_t^{s, \mu})). \quad (3.5.1)$$

There are various methods of establishing smoothness of functions of this form in the literature.

One way involves considering PDE (3.4.3) and proving regularity properties of the solution to this PDE ([11]).

The method of Malliavin calculus is adopted in [19]. This paper proves smoothness of \mathcal{V} , for Φ being in the form

$$\Phi(\mu) = \int_{\mathbb{R}^d} \zeta(y) \mu(dy),$$

where $\zeta : \mathbb{R}^d \rightarrow \mathbb{R}$ is infinitely differentiable with bounded partial derivatives.

Article [20] considers the method of parametrix. We represent \mathcal{V} in terms of the transition density $p(s, \mu; t', y'; t, y)$ of $X_t^{s, x; \mu}$ (defined below in (3.5.3)). This method is applied to the case in which b and σ are of the form

$$b(x, \mu) = \int_{\mathbb{R}^d} B(x, y) \mu(dy), \quad \sigma(x, \mu) = \int_{\mathbb{R}^d} \Sigma(x, y) \mu(dy),$$

for some functions $B : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d$ and $\Sigma : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d$. Nonetheless, it is not clear whether this method can be applied to b and σ with more general forms.

We follow here a different route.

Framework of analysis. We adopt the ‘variational’ approach employed in [9]. The core idea is to prove smoothness of \mathcal{V} by viewing the lift of \mathcal{V} as a composition of the map $\xi \mapsto X_t^{s,\xi}$ and the lift of Φ .

Theorem 7.2 of [9] already proves smoothness of derivatives in measure up to the second order:

Theorem 3.5.1. *Let \mathcal{V} be defined by (3.5.1). Suppose that $b, \sigma \in \mathcal{M}_2(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and $\Phi \in \mathcal{M}_2(\mathcal{P}_2(\mathbb{R}^d))$. Then $\mathcal{V} \in \mathcal{M}_2([0, t] \times \mathcal{P}_2(\mathbb{R}^d))$ and satisfies PDE (3.4.3).*

Note that the conclusion that $\mathcal{V} \in \mathcal{M}_2([0, t] \times \mathcal{P}_2(\mathbb{R}^d))$ implies that $\mathcal{V} \in \mathcal{D}_0([0, t])$, which automatically implies PDE (3.4.3). However, for the analysis in subsequent chapters, we need to generalise that result to an arbitrary order as follows.

Theorem 3.5.2. *Let \mathcal{V} be defined by (3.5.1) and $k \geq 2$. Suppose that $b, \sigma \in \mathcal{M}_k(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and $\Phi \in \mathcal{M}_k(\mathcal{P}_2(\mathbb{R}^d))$. Then $\mathcal{V} \in \mathcal{M}_k([0, t] \times \mathcal{P}_2(\mathbb{R}^d))$.*

The proof of Theorem 3.5.2 would be the main goal of this section. We follow closely the techniques in the proof of Theorem 7.2 in [9].

The analysis of variational derivatives of solutions to classical SDEs is rather well-understood in the literature ([27], [45]). As differentiation in the direction of measure leads to rather complicated expressions, we restrict ourselves to the following special case in this section. This captures the key difficulty of this approach. The general case can be handled in an analogous way.

We consider the forward system $(\{X_t^{s,\xi}\}_{t \in [s,T]}, \{X_t^{s,x,\mu}\}_{t \in [s,T]})$, $\xi \sim \mu$, which takes the form

$$\begin{cases} X_t^{s,\xi} &= \xi + \int_s^t \sigma(\mathcal{L}(X_r^{s,\xi})) dW_r, & t \in [s, T], \\ X_t^{s,x,\mu} &= x + \int_s^t \sigma(\mathcal{L}(X_r^{s,\mu})) dW_r, & t \in [s, T], \quad x \in \mathbb{R}, \end{cases} \quad (3.5.2)$$

for some Borel-measurable function $\sigma : \mathcal{P}_2(\mathbb{R}) \rightarrow \mathbb{R}$ and one-dimensional Brownian motion W . $\{X_t^{s,x,\mu}\}_{t \in [s,T]}$ is also called the decoupled process, as it no longer depends on the law of itself.

Let $\{\mathcal{F}_t\}_{t \in [0,T]}$ (resp. $\{\mathcal{F}_t^{(n)}\}_{t \in [0,T]}$) denote the filtration generated by Brownian motion $W = \{W_t\}_{t \in [0,T]}$ (resp. $\{W_t^{(n)}\}_{t \in [0,T]}$). Let ξ be a random variable in $L^2(\mathcal{F}_s)$.

For brevity, in the following calculations of this section, we shall denote the law $\mathcal{L}(\xi)$ by $[\xi]$.

First order derivative of $[\xi] \mapsto X_t^{s,x,[\xi]}$. We start our analysis by analysing the smoothness of the map $[\xi] \mapsto X_t^{s,x,[\xi]}$. Suppose that the lift of $[\xi] \mapsto X_t^{s,x,[\xi]}$ with values in L^2

$$L^2(\mathcal{F}_s) \rightarrow L^2(\mathcal{F}_t); \quad \xi \mapsto X_t^{s,x,[\xi]}$$

is Fréchet differentiable with its Fréchet derivative given by

$$L^2(\mathcal{F}_s) \rightarrow L(L^2(\mathcal{F}_s), L^2(\mathcal{F}_t)); \quad \xi \mapsto \left(\eta \mapsto \hat{\mathbb{E}}[U_t^{s,x,[\xi]}(\hat{\xi})\hat{\eta}] \right),$$

for some real-valued process $\{U_t^{s,x,[\xi]}(y)\}_{t \in [s,T]}$ that is adapted to $\{\mathcal{F}_t\}_{t \in [s,T]}$. Then we define the derivative of $X_t^{s,x,[\xi]}$ with respect to the measure component by

$$\partial_\mu X_t^{s,x,[\xi]}(y) := U_t^{s,x,[\xi]}(y), \quad t \in [s, T], \quad x, y \in \mathbb{R}. \quad (3.5.4)$$

The next theorem computes $\partial_\mu X_t^{s,x,[\xi]}(y)$ explicitly.

Theorem 3.5.3. *Suppose that $\sigma \in \mathcal{M}_1(\mathcal{P}_2(\mathbb{R}))$. Then $\partial_\mu X_t^{s,x,[\xi]}(y)$ exists and is the unique solution of the SDE*

$$\partial_\mu X_t^{s,x,[\xi]}(y) = \int_s^t \mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,y,[\xi]} \right) \right]$$

$$+ (\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,\xi^{(1)}} \right) \partial_\mu (X^{(1)})_r^{s,x,[\xi]}(y) \Big] dW_r.$$

Proof. The proof is done in [9], but is included for completeness. We first define the L^2 -directional derivative $D_\xi(X_t^{s,x,[\xi]})(\eta)$ of $X_t^{s,x,[\xi]}$ in direction $\eta \in L^2(\mathcal{F}_s)$, given by

$$D_\xi(X_t^{s,x,[\xi]})(\eta) := \lim_{h \rightarrow 0} \frac{1}{h} \left(X_t^{s,x,[\xi+h\eta]} - X_t^{s,x,[\xi]} \right), \quad (3.5.5)$$

where the limit is interpreted in the L^2 sense, i.e.

$$\lim_{h \rightarrow 0} \mathbb{E} \left[\left(\frac{1}{h} \left(X_t^{s,x,[\xi+h\eta]} - X_t^{s,x,[\xi]} \right) - D_\xi(X_t^{s,x,[\xi]})(\eta) \right)^2 \right] = 0.$$

Similarly, the L^2 -directional derivative of $X_t^{s,\xi}$ in direction $\eta \in L^2(\mathcal{F}_s)$ is given by

$$\lim_{h \rightarrow 0} \frac{1}{h} \left(X_t^{s,\xi+h\eta} - X_t^{s,\xi} \right) = \partial_h X_t^{s,\xi+h\eta} \Big|_{h=0}, \quad (3.5.6)$$

where both the limit and the derivative are interpreted in the L^2 sense. We proceed by formal differentiation and obtain that

$$\begin{aligned} \partial_h X_t^{s,\xi+h\eta} &= \partial_h \left(X_t^{s,x,[\xi+h\eta]} \Big|_{x=\xi+h\eta} \right) \\ &= \left(\partial_x X_t^{s,x,[\xi+h\eta]} \Big|_{x=\xi+h\eta} \right) \eta + \left(\lim_{\nu \rightarrow 0} \frac{1}{\nu} \left(X_t^{s,x,[\xi+(h+\nu)\eta]} - X_t^{s,x,[\xi+h\eta]} \right) \right) \Big|_{x=\xi+h\eta}. \end{aligned}$$

Hence,

$$D_\xi(X_t^{s,\xi})(\eta) = \partial_h X_t^{s,\xi+h\eta} \Big|_{h=0} = \eta + D_\xi(X_t^{s,x,[\xi]})(\eta) \Big|_{x=\xi}. \quad (3.5.7)$$

Recall that the lift of σ , i.e. $\tilde{\sigma} : L^2(\mathcal{F}) \rightarrow \mathbb{R}$, is defined by $\tilde{\sigma}(\theta) := \sigma([\theta])$. By (3.5.5), (3.5.6), and (3.5.7), formal differentiation of (3.5.3) with respect to ξ in the direction η gives

$$D_\xi(X_t^{s,x,[\xi]})(\eta) = \int_s^t (D_\theta \tilde{\sigma})(X_r^{s,\xi}) \left(\eta + D_\xi(X_r^{s,x,[\xi]})(\eta) \Big|_{x=\xi} \right) dW_r. \quad (3.5.8)$$

By the definition of derivative in measure of σ , we can further rewrite (3.5.8) as

$$D_\xi(X_t^{s,x,[\xi]})(\eta) = \int_s^t \mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,\xi^{(1)}} \right) \left(\eta^{(1)} + D_\xi \left((X^{(1)})_r^{s,x,[\xi]} \right) (\eta^{(1)}) \Big|_{x=\xi^{(1)}} \right) \right] dW_r. \quad (3.5.9)$$

It is then verified rigorously in Lemma 4.2 of [9] that $D_\xi(X_t^{s,x,[\xi]})(\eta)$ is indeed the directional derivative of $X_t^{s,x,[\xi]}$ in direction $\eta \in L^2(\mathcal{F}_s)$, by using the fact that σ is in \mathcal{M}_1 .

The next step involves the consideration of a process $\{U_t^{s,x,[\xi]}\}_{t \in [s,T]}$ satisfying the SDE

$$\begin{aligned} U_t^{s,x,[\xi]}(y) &= \int_s^t \mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,y,[\xi]} \right) \right. \\ &\quad \left. + (\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,\xi^{(1)}} \right) (U_r^{(1)})_r^{s,x,[\xi]}(y) \Big|_{x=\xi^{(1)}} \right] dW_r. \end{aligned} \quad (3.5.10)$$

We write

$$\begin{aligned} &\hat{\mathbb{E}} \left[U_t^{s,x,[\xi]}(\hat{\xi}) \hat{\eta} \right] \\ &= \int_s^t \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,y,[\xi]} \right) \Big|_{y=\hat{\xi}} \right] \hat{\eta} \right] dW_r \end{aligned}$$

$$+ \int_s^t \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,\xi^{(1)}} \right) (U^{(1)})_r^{s,x,[\xi]}(y) \Big|_{x=\xi^{(1)}} \right] \Big|_{y=\hat{\xi}} \hat{\eta} \right] dW_r$$

and notice that

$$\begin{aligned} & \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,y,[\xi]} \right) \right] \Big|_{y=\hat{\xi}} \hat{\eta} \right] \\ &= \mathbb{E}^{(1)} \left[\mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,y,[\xi]} \right) \right] \Big|_{y=\xi^{(1)}} \eta^{(1)} \right] \\ &= \mathbb{E}^{(1)} \left[\mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,y,[\xi]} \right) \right] \Big|_{y=\xi^{(1)}} \eta^{(1)} \Big| \mathcal{F}_s^{(1)} \right] \\ &= \mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,\xi^{(1)}} \right) \eta^{(1)} \right], \end{aligned} \quad (3.5.11)$$

where the second equality uses the fact that $(X^{(1)})_r^{s,y,[\xi]}$ is $\sigma\{W_r^{(1)} - W_s^{(1)} \mid r \in [s, t]\}$ -adapted and is therefore independent of $\mathcal{F}_s^{(1)}$, whereas $\xi^{(1)}$ and $\eta^{(1)}$ are both $\mathcal{F}_s^{(1)}$ -measurable. The final equality uses the fact that $(X^{(1)})_r^{s,y,[\xi]} \Big|_{y=\xi^{(1)}} = (X^{(1)})_r^{s,\xi^{(1)}}$. We also notice by the Fubini's theorem that

$$\begin{aligned} & \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,\xi^{(1)}} \right) (U^{(1)})_r^{s,x,[\xi]}(y) \Big|_{x=\xi^{(1)}} \right] \Big|_{y=\hat{\xi}} \hat{\eta} \right] \\ &= \mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,\xi^{(1)}} \right) \hat{\mathbb{E}} \left[(U^{(1)})_r^{s,x,[\xi]}(\hat{\xi}) \hat{\eta} \right] \Big|_{x=\xi^{(1)}} \right]. \end{aligned} \quad (3.5.12)$$

Therefore, by (3.5.11) and (3.5.12), we observe that $D_\xi(X^{s,x,[\xi]})(\eta)$ and $\hat{\mathbb{E}}[U^{s,x,[\xi]}(\hat{\xi})\hat{\eta}]$ satisfy the same SDE and hence

$$D_\xi(X_t^{s,x,[\xi]})(\eta) = \hat{\mathbb{E}}[U_t^{s,x,[\xi]}(\hat{\xi})\hat{\eta}], \quad t \in [s, T], \quad \eta \in L^2(\mathcal{F}_s). \quad (3.5.13)$$

We then observe that $U_t^{s,x,[\xi]}(y)$ satisfies the same SDE for any $x \in \mathbb{R}$. Therefore, there is no dependence on x and hence (3.5.10) can be rewritten as

$$U_t^{s,x,[\xi]}(y) = \int_s^t \mathbb{E}^{(1)} \left[(\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,y,[\xi]} \right) + (\partial_\mu \sigma) \left([X_r^{s,\xi}], (X^{(1)})_r^{s,\xi^{(1)}} \right) (U^{(1)})_r^{s,x,[\xi]}(y) \right] dW_r. \quad (3.5.14)$$

Moreover, by the fact that σ is in \mathcal{M}_1 , we establish that

$$(i) \quad \mathbb{E} \left[\sup_{t \in [s, T]} |U_t^{s,x,[\xi]}(y)|^2 \right] \leq C, \quad (3.5.15)$$

$$(ii) \quad \mathbb{E} \left[\sup_{t \in [s, T]} |U_t^{s,x,[\xi]}(y) - U_t^{s,x,[\xi']}(y')|^2 \right] \leq C \left(|y - y'|^2 + W_2([\xi], [\xi'])^2 \right), \quad (3.5.16)$$

for any $s \in [0, T]$, $x, y, y' \in \mathbb{R}$ and $\xi, \xi' \in L^2(\mathcal{F}_s)$, for some constant $C > 0$. Indeed, (3.5.15) follows from the boundedness of $\partial_\mu \sigma$ and Gronwall's inequality. (3.5.16) follows from the Lipschitz property of $\partial_\mu \sigma$ and Gronwall's inequality, along with the bounds

$$\begin{cases} \mathbb{E} \left[\sup_{t \in [s, T]} |X_t^{s,\xi} - X_t^{s,\xi'}|^2 \right] \leq C\mathbb{E}|\xi - \xi'|^2, \\ \sup_{t \in [s, T]} W_2([X_t^{s,\xi}], [X_t^{s,\xi'}])^2 \leq CW_2([\xi], [\xi'])^2, \\ \mathbb{E} \left[\sup_{t \in [s, T]} |X_t^{s,x,[\xi]} - X_t^{s,x',[\xi']}|^2 \right] \leq C(|x - x'|^2 + W_2([\xi], [\xi'])^2), \end{cases}$$

for some constant $C > 0$. Finally, the bounds (3.5.15), (3.5.16) and connection (3.5.13) allow

us to establish that the Gâteaux derivative

$$L^2(\mathcal{F}_s) \rightarrow L(L^2(\mathcal{F}_s), L^2(\mathcal{F}_t)); \quad \xi \mapsto \left(\eta \mapsto D_\xi(X_t^{s,x,[\xi]})(\eta) \right) \quad (3.5.17)$$

is continuous (where the space $L(L^2(\mathcal{F}_s), L^2(\mathcal{F}_t))$ is equipped with the corresponding operator norm), which proves that (3.5.17) is indeed the Fréchet derivative of $X_t^{s,x,[\xi]}$ with respect to ξ . By (3.5.13), it follows from the definition of $\partial_\mu X_t^{s,x,[\xi]}(y)$ that

$$\partial_\mu X_t^{s,x,[\xi]}(y) = U_t^{s,x,[\xi]}(y), \quad t \in [s, T]. \quad (3.5.18)$$

□

Higher order derivatives of $[\xi] \mapsto X^{s,x,[\xi]}$. We recall that $\partial_\mu X_t^{s,x,[\xi]}(y)$ does not depend on x and hence we define

$$\partial_\mu X_t^{s,[\xi]}(y) := \partial_\mu X_t^{s,x,[\xi]}(y). \quad (3.5.19)$$

Subsequently, we define inductively as in (3.2.11) and (3.2.12), the n th order derivative in measure of $X_t^{s,x,[\xi]}$ by

$$\partial_\mu^n X_t^{s,[\xi]}(v_1, \dots, v_n) := \partial_\mu \left(\partial_\mu^{n-1} X_t^{s,[\xi]}(v_1, \dots, v_{n-1}) \right)(v_n), \quad t \in [s, T], v_1, \dots, v_n \in \mathbb{R},$$

and its corresponding mixed derivatives by

$$\partial_{v_n}^{\beta_n} \dots \partial_{v_1}^{\beta_1} \partial_\mu^n X_t^{s,[\xi]}(v_1, \dots, v_n), \quad \ell, \beta_1, \dots, \beta_n \in \mathbb{N} \cup \{0\},$$

provided that these derivatives actually exist, where each derivative in v_i is interpreted in the L^2 sense. (See Lemma 4.1 in [9] for its precise meaning.)

Next, we generalise the multi-index notation and the class \mathcal{M}_k to include derivatives of $X_t^{s,x,[\xi]}$.

Definition 3.5.4 (Multi-index notation for derivatives of $X_t^{s,x,[\xi]}$). Let (n, β) be a multi-index. Then $D^{(n,\beta)} X_t^{s,[\xi]}(v_1, \dots, v_n)$ is defined by

$$D^{(n,\beta)} X_t^{s,[\xi]}(v_1, \dots, v_n) := \partial_{v_n}^{\beta_n} \dots \partial_{v_1}^{\beta_1} \partial_\mu^n X_t^{s,[\xi]}(v_1, \dots, v_n),$$

if this derivative is well-defined.

Definition 3.5.5 (Class \mathcal{M}_k^X of k th order differentiable functions).

The process $X^{s,x,[\xi]} = \{X_t^{s,x,[\xi]}\}_{t \in [s, T]}$ belongs to class \mathcal{M}_k^X , if $D^{(n,\beta)} X_t^{s,[\xi]}(v_1, \dots, v_n)$ exists for every multi-index (n, β) such that $|(n, \beta)| \leq k$ and

$$(a) \quad \mathbb{E} \left[\sup_{t \in [s, T]} |D^{(n,\beta)} X_t^{s,[\xi]}(v_1, \dots, v_n)|^2 \right] \leq C, \quad (3.5.20)$$

$$(b) \quad \mathbb{E} \left[\sup_{t \in [s, T]} |D^{(n,\beta)} X_t^{s,[\xi]}(v_1, \dots, v_n) - D^{(n,\beta)} X_t^{s,[\xi']}(v'_1, \dots, v'_n)|^2 \right] \leq C \left(\sum_{i=1}^n |v_i - v'_i|^2 + W_2([\xi], [\xi'])^2 \right), \quad (3.5.21)$$

for any $s \in [0, T]$, $v_1, v'_1, \dots, v_n, v'_n \in \mathbb{R}^d$ and $\xi, \xi' \in L^2(\mathcal{F}_s)$, for some constant $C > 0$.

The following theorem extends Theorem 3.5.3 to higher order derivatives. It uses the notations

$$\Lambda_{i,k} := \left\{ \theta : \{1, \dots, i\} \rightarrow \{1, \dots, k\} \mid \theta \text{ is a strictly increasing function} \right\}, \quad i \in \{1, \dots, k\},$$

and

$$R_k := \left\{ y = (y_{(j,\ell)})_{1 \leq j, \ell \leq k} \mid y_{(j,\ell)} \in \mathbb{R} \right\}, \quad T_k := \left\{ z = (z_{(j,i,\theta)})_{\substack{1 \leq j, i \leq k \\ \theta \in \Lambda_{i,k}}} \mid z_{(j,i,\theta)} \in \mathbb{R} \right\}.$$

For any function $F_k : \mathcal{P}_2(\mathbb{R}) \times \mathbb{R}^k \times R_k \times T_k \rightarrow \mathbb{R}$, $\partial_{x_j} F_k$ denotes the corresponding partial derivative with respect to the second component of F_k . $\partial_{y_{(j,\ell)}} F_k$ denotes the corresponding partial derivative with respect to the third component of F_k . $\partial_{z_{(j,i,\theta)}} F_k$ denotes the corresponding partial derivative with respect to the fourth component of F_k .

Theorem 3.5.6. *Suppose that σ is $\mathcal{M}_K(\mathcal{P}_2(\mathbb{R}))$. Then, for any $k \in \{1, \dots, K\}$, $t \in [s, T]$, the k th order derivative in measure $\partial_\mu^k X_t^{s, [\xi]}(v_1, \dots, v_k)$ exists and satisfies (3.5.20) and (3.5.21). In particular, it is the unique solution of an SDE given by*

$$\begin{aligned} & \partial_\mu^k X_t^{s, [\xi]}(v_1, \dots, v_k) \\ = & \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k)} \left[F_k \left([X_r^{s, \xi}]_r, \left((X^{(j)})_r^{s, \xi^{(j)}} \right)_{1 \leq j \leq k}, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{1 \leq j, \ell \leq k}, \right. \right. \\ & \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{\substack{1 \leq j, i \leq k \\ \theta \in \Lambda_{i,k}}} \right) \right] dW_r, \end{aligned} \quad (3.5.22)$$

where $F_k : \mathcal{P}_2(\mathbb{R}) \times \mathbb{R}^k \times R_k \times T_k \rightarrow \mathbb{R}$ is defined by the recurrence relation, $k \in \{1, \dots, K-1\}$,

$$\begin{aligned} & F_{k+1} \left(\mu, (x_j)_{1 \leq j \leq k+1}, (y_{(j,\ell)})_{1 \leq j, \ell \leq k+1}, (z_{(j,i,\theta)})_{\substack{1 \leq j, i \leq k+1 \\ \theta \in \Lambda_{i,k+1}}} \right) \\ = & \partial_\mu F_k \left(\mu, (x_j)_{1 \leq j \leq k}, (y_{(j,\ell)})_{1 \leq j, \ell \leq k}, (z_{(j,i,\theta)})_{\substack{1 \leq j, i \leq k \\ \theta \in \Lambda_{i,k}}} \right) \\ & + \partial_\mu F_k \left(\mu, (x_j)_{1 \leq j \leq k}, (y_{(j,\ell)})_{1 \leq j, \ell \leq k}, (z_{(j,i,\theta)})_{\substack{1 \leq j, i \leq k \\ \theta \in \Lambda_{i,k}}}, x_{k+1} \right) \mathcal{Z}_{(k+1,1, P_{k+1})} \\ & + \sum_{j=1}^k \partial_{x_j} F_k \left(\mu, (x_1, \dots, x_{j-1}, y_{(j,k+1)}, x_{j+1}, \dots, x_k), (y_{(j,\ell)})_{1 \leq j, \ell \leq k}, (z_{(j,i,\theta)})_{\substack{1 \leq j, i \leq k \\ \theta \in \Lambda_{i,k}}} \right) \\ & + \sum_{j=1}^k \partial_{x_j} F_k \left(\mu, (x_j)_{1 \leq j \leq k}, (y_{(j,\ell)})_{1 \leq j, \ell \leq k}, (z_{(j,i,\theta)})_{\substack{1 \leq j, i \leq k \\ \theta \in \Lambda_{i,k}}} \right) \mathcal{Z}_{(j,1, P_{k+1})} \\ & + \sum_{j,\ell=1}^k \partial_{y_{(j,\ell)}} F_k \left(\mu, (x_j)_{1 \leq j \leq k}, (y_{(j,\ell)})_{1 \leq j, \ell \leq k}, (z_{(j,i,\theta)})_{\substack{1 \leq j, i \leq k \\ \theta \in \Lambda_{i,k}}} \right) \mathcal{Z}_{(j,1, P_{k+1})} \\ & + \sum_{j,i=1}^k \sum_{\theta \in \Lambda_{i,k}} \partial_{z_{(j,i,\theta)}} F_k \left(\mu, (x_j)_{1 \leq j \leq k}, (y_{(j,\ell)})_{1 \leq j, \ell \leq k}, (z_{(j,i,\theta)})_{\substack{1 \leq j, i \leq k \\ \theta \in \Lambda_{i,k}}} \right) \mathcal{Z}_{(j,i+1, \theta_{i+1,k+1})}, \end{aligned} \quad (3.5.23)$$

where $P_{k+1} \in \Lambda_{1,k+1}$ is defined by $P_{k+1}(1) = k+1$ and for each $\theta \in \Lambda_{i,k}$, the function $\theta_{i+1,k+1} \in \Lambda_{i+1,k+1}$ is defined such that $\theta_{i+1,k+1}|_{\{1, \dots, i\}} = \theta$ and $\theta_{i+1,k+1}(i+1) = k+1$. Moreover, F_1 is given by

$$F_1(\mu, x, y, z) = \partial_\mu \sigma(\mu, y) + \partial_\mu \sigma(\mu, x) z. \quad (3.5.24)$$

Proof. We remark that the functions F_k , $k \in \{1, \dots, K\}$, are well-defined, since $\sigma \in \mathcal{M}_K$. We proceed by strong induction on $k \in \{1, \dots, K\}$. The base step $k = 1$ is done in Theorem 3.5.3. In particular, (3.5.14) verifies (3.5.24). The main arguments in the induction step are the same as the base step. Suppose that the statement holds for all $k \in \{1, \dots, k^*\}$, where

$k^* \in \{1, \dots, K-1\}$. Then, in particular, $\partial_\mu^{k^*} X_t^{s, [\xi]}(v_1, \dots, v_{k^*})$ satisfies the SDE

$$\begin{aligned} & \partial_\mu^{k^*} X_t^{s, [\xi]}(v_1, \dots, v_{k^*}) \\ = & \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[F_{k^*} \left([X_r^{s, \xi}], \left((X^{(j)})_r^{s, \xi^{(j)}} \right)_{1 \leq j \leq k^*}, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{1 \leq j, \ell \leq k^*}, \right. \right. \\ & \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{\substack{1 \leq j, i \leq k^* \\ \theta \in \Lambda_{i, k^*}}} \right) \right] dW_r. \end{aligned} \quad (3.5.25)$$

Let \tilde{F}_{k^*} be the lift of F_{k^*} . In the following expression, $\partial_x \tilde{F}_{k^*}$ denotes the partial derivative with respect to the lifted component of \tilde{F}_k . As in (3.5.7) and (3.5.8), we formally differentiate (3.5.25) with respect to ξ in the direction η to obtain the directional derivative

$$\begin{aligned} & D_\xi (\partial_\mu^{k^*} X_t^{s, [\xi]}(v_1, \dots, v_{k^*}))(\eta) \\ = & \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_x \tilde{F}_{k^*} \left([X_r^{s, \xi}], \left((X^{(j)})_r^{s, \xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{j, \ell}, \right. \right. \\ & \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j, i, \theta} \right) \left(\eta + D_\xi (X_r^{s, x, [\xi]})(\eta) \Big|_{x=\xi} \right) \right] dW_r \\ & + \sum_{j=1}^{k^*} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{x_j} \tilde{F}_{k^*} \left([X_r^{s, \xi}], \left((X^{(j)})_r^{s, \xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{j, \ell}, \right. \right. \\ & \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j, i, \theta} \right) \left(\eta^{(j)} + D_\xi \left((X^{(j)})_r^{s, x, [\xi]}(\eta^{(j)}) \Big|_{x=\xi^{(j)}} \right) \right) \right] dW_r \\ & + \sum_{j, \ell=1}^{k^*} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{y_{(j, \ell)}} \tilde{F}_{k^*} \left([X_r^{s, \xi}], \left((X^{(j)})_r^{s, \xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{j, \ell}, \right. \right. \\ & \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j, i, \theta} \right) D_\xi \left((X^{(j)})_r^{s, v_\ell, [\xi]}(\eta^{(j)}) \right) \right] dW_r \\ & + \sum_{j, i=1}^{k^*} \sum_{\theta \in \Lambda_{i, k^*}} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{z_{(j, i, \theta)}} \tilde{F}_{k^*} \left([X_r^{s, \xi}], \left((X^{(j)})_r^{s, \xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{j, \ell}, \right. \right. \\ & \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j, i, \theta} \right) D_\xi \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) (\eta^{(j)}) \right) \right] dW_r. \end{aligned}$$

We then recall that the following directional derivatives can be represented as

$$\begin{aligned} D_\xi (X_r^{s, x, [\xi]})(\eta) \Big|_{x=\xi} &= \hat{\mathbb{E}} \left[\partial_\mu X_r^{s, [\xi]}(\hat{\xi}) \hat{\eta} \right], \quad D_\xi \left((X^{(j)})_r^{s, v_\ell, [\xi]}(\eta^{(j)}) \right) = \hat{\mathbb{E}} \left[\partial_\mu (X^{(j)})_r^{s, [\xi]}(\hat{\xi}) \hat{\eta} \right], \\ D_\xi \left((X^{(j)})_r^{s, x, [\xi]}(\eta^{(j)}) \Big|_{x=\xi^{(j)}} \right) &= \hat{\mathbb{E}} \left[\partial_\mu (X^{(j)})_r^{s, [\xi]}(\hat{\xi}) \hat{\eta} \right] \end{aligned}$$

and

$$D_\xi \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) (\eta^{(j)}) \right) = \hat{\mathbb{E}} \left[\partial_\mu^{i+1} (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}, \hat{\xi}) \hat{\eta} \right], \quad i \in \{1, \dots, k^*-1\}.$$

We can therefore rewrite (3.5.26) as

$$\begin{aligned} & D_\xi (\partial_\mu^{k^*} X_t^{s, [\xi]}(v_1, \dots, v_{k^*}))(\eta) \\ = & \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \mathbb{E}^{(k^*+1)} \left[\partial_\mu F_{k^*} \left([X_r^{s, \xi}], \left((X^{(j)})_r^{s, \xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{j, \ell}, \right. \right. \\ & \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j, i, \theta}, (X^{(k^*+1)})_r^{s, \xi^{(k^*+1)}} \right) \right. \\ & \left. \times \left(\eta^{(k^*+1)} + \hat{\mathbb{E}} \left[\partial_\mu (X^{(k^*+1)})_r^{s, [\xi]}(\hat{\xi}) \hat{\eta} \right] \right) \right] dW_r \end{aligned}$$

$$\begin{aligned}
& + \sum_{j=1}^{k^*} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{x_j} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell}, \right. \right. \\
& \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j,i,\theta} \right) \left(\eta^{(j)} + \hat{\mathbb{E}} \left[\partial_\mu (X^{(j)})_r^{s, [\xi]} (\hat{\xi}) \hat{\eta} \right] \right) \right] dW_r \\
& + \sum_{j,\ell=1}^{k^*} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{y_{(j,\ell)}} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell}, \right. \right. \\
& \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j,i,\theta} \right) \hat{\mathbb{E}} \left[\partial_\mu (X^{(j)})_r^{s, [\xi]} (\hat{\xi}) \hat{\eta} \right] \right] dW_r \\
& + \sum_{j=1}^{k^*} \sum_{i=1}^{k^*-1} \sum_{\theta \in \Lambda_{i,k^*}} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{z_{(j,i,\theta)}} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell}, \right. \right. \\
& \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j,i,\theta} \right) \hat{\mathbb{E}} \left[\partial_\mu^{i+1} (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}, \hat{\xi}) \hat{\eta} \right] \right] dW_r \\
& + \sum_{j=1}^{k^*} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{z_{(j,k^*, \mathbf{1}_{k^*})}} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell}, \right. \right. \\
& \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j,i,\theta} \right) D_\xi \left(\partial_\mu^{k^*} (X^{(j)})_t^{s, [\xi]} (v_1, \dots, v_{k^*}) \right) (\eta) \right] dW_r,
\end{aligned} \tag{3.5.26}$$

where, on the second last line, $\mathbf{1}_{k^*}$ denotes the identity function from $\{1, \dots, k^*\}$ to itself. We now define a process $\{(U_{k^*+1})_t^{s, [\xi]}(v_1, \dots, v_{k^*+1})\}_{t \in [s, T]}$ that satisfies the SDE

$$\begin{aligned}
& (U_{k^*+1})_t^{s, [\xi]}(v_1, \dots, v_{k^*+1}) \\
= & \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \mathbb{E}^{(k^*+1)} \left[\partial_\mu F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell}, \right. \right. \\
& \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j,i,\theta}, (X^{(k^*+1)})_r^{s, v_{k^*+1}, [\xi]} \right) \right] dW_r \\
& + \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \mathbb{E}^{(k^*+1)} \left[\partial_\mu F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell}, \right. \right. \\
& \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j,i,\theta}, (X^{(k^*+1)})_r^{s, \xi^{(k^*+1)}} \right) \partial_\mu (X^{(k^*+1)})_r^{s, [\xi]} (v_{k^*+1}) \right] dW_r \\
& + \sum_{j=1}^{k^*} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{x_j} F_{k^*} \left([X_r^{t,\xi}], \left((X^{(1)})_r^{s,\xi^{(1)}}, \dots, (X^{(j-1)})_r^{s,\xi^{(j-1)}}, (X^{(j)})_r^{s, v_{k^*+1}, [\xi]}, \right. \right. \right. \\
& \left. \left. \left(X^{(j+1)}_r^{s, \xi^{(j+1)}}, \dots, (X^{(k^*)})_r^{s, \xi^{(k^*)}} \right), \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{j,\ell}, \right. \right. \\
& \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j,i,\theta} \right) \right] dW_r \\
& + \sum_{j=1}^{k^*} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{x_j} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{j,\ell}, \right. \right. \\
& \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j,i,\theta} \right) \partial_\mu (X^{(j)})_r^{s, [\xi]} (v_{k^*+1}) \right] dW_r \\
& + \sum_{j,\ell=1}^{k^*} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{y_{(j,\ell)}} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{j,\ell}, \right. \right. \\
& \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{j,i,\theta} \right) \partial_\mu (X^{(j)})_r^{s, [\xi]} (v_{k^*+1}) \right] dW_r
\end{aligned}$$

$$\begin{aligned}
& + \sum_{j=1}^{k^*} \sum_{i=1}^{k^*-1} \sum_{\theta \in \Lambda_{i,k^*}} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{z_{(j,i,\theta)}} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell} \right), \right. \\
& \left. \left(\partial_\mu^i \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right) \right)_{j,i,\theta} \right] \partial_\mu^{i+1} \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}, v_{k^*+1}) \right) dW_r \\
& + \sum_{j=1}^{k^*} \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{z_{(j,k^*, \mathbf{I}_{k^*})}} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell} \right), \right. \\
& \left. \left(\partial_\mu^i \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right) \right)_{j,i,\theta} \right] \left(U_{k^*+1}^{(j)} \right)_t^{s, [\xi]} (v_1, \dots, v_{k^*+1}) dW_r. \tag{3.5.27}
\end{aligned}$$

Then we write

$$\begin{aligned}
& \hat{\mathbb{E}} \left[\left(U_{k^*+1} \right)_t^{s, [\xi]} (v_1, \dots, v_{k^*}, \hat{\xi}) \hat{\eta} \right] \\
= & \int_s^t \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \mathbb{E}^{(k^*+1)} \left[\partial_\mu F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell} \right), \right. \right. \\
& \left. \left. \left(\partial_\mu^i \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right) \right)_{j,i,\theta}, \left(X^{(k^*+1)} \right)_r^{s, v_{k^*+1}, [\xi]} \right] \right] \Big|_{v_{k^*+1} = \hat{\xi}} \hat{\eta} dW_r \\
& + \int_s^t \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \mathbb{E}^{(k^*+1)} \left[\partial_\mu F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell} \right), \right. \right. \\
& \left. \left. \left(\partial_\mu^i \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right) \right)_{j,i,\theta}, \left(X^{(k^*+1)} \right)_r^{s, \xi^{(k^*+1)}} \right) \right. \\
& \left. \times \partial_\mu \left(X^{(k^*+1)} \right)_r^{s, [\xi]} (v_{k^*+1}) \right] \Big|_{v_{k^*+1} = \hat{\xi}} \hat{\eta} dW_r \\
& + \sum_{j=1}^{k^*} \int_s^t \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{x_j} F_{k^*} \left([X_r^{t,\xi}], \right. \right. \\
& \left. \left. \left((X^{(1)})_r^{s,\xi^{(1)}}, \dots, (X^{(j-1)})_r^{s,\xi^{(j-1)}}, (X^{(j)})_r^{s, v_{k^*+1}, [\xi]}, (X^{(j+1)})_r^{s,\xi^{(j+1)}}, \dots, (X^{(k^*)})_r^{s,\xi^{(k^*)}} \right), \right. \right. \\
& \left. \left. \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{j,\ell}, \left(\partial_\mu^i \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right) \right)_{j,i,\theta} \right] \right] \Big|_{v_{k^*+1} = \hat{\xi}} \hat{\eta} dW_r \\
& + \sum_{j=1}^{k^*} \int_s^t \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{x_j} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell} \right), \right. \right. \\
& \left. \left. \left(\partial_\mu^i \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right) \right)_{j,i,\theta} \right] \partial_\mu \left((X^{(j)})_r^{s, [\xi]} (v_{k^*+1}) \right) \right] \Big|_{v_{k^*+1} = \hat{\xi}} \hat{\eta} dW_r \\
& + \sum_{j,\ell=1}^{k^*} \int_s^t \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{y_{(j,\ell)}} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell} \right), \right. \right. \\
& \left. \left. \left(\partial_\mu^i \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right) \right)_{j,i,\theta} \right] \partial_\mu \left((X^{(j)})_r^{s, [\xi]} (v_{k^*+1}) \right) \right] \Big|_{v_{k^*+1} = \hat{\xi}} \hat{\eta} dW_r \\
& + \sum_{j=1}^{k^*} \sum_{i=1}^{k^*-1} \sum_{\theta \in \Lambda_{i,k^*}} \int_s^t \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{z_{(j,i,\theta)}} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell} \right), \right. \right. \\
& \left. \left. \left(\partial_\mu^i \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right) \right)_{j,i,\theta} \right] \partial_\mu^{i+1} \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}, v_{k^*+1}) \right) \right] \Big|_{v_{k^*+1} = \hat{\xi}} \hat{\eta} dW_r \\
& + \sum_{j=1}^{k^*} \int_s^t \hat{\mathbb{E}} \left[\mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*)} \left[\partial_{z_{(j,k^*, \mathbf{I}_{k^*})}} F_{k^*} \left([X_r^{s,\xi}], \left((X^{(j)})_r^{s,\xi^{(j)}} \right)_j, \left((X^{(j)})_r^{s,v_\ell, [\xi]} \right)_{j,\ell} \right), \right. \right. \\
& \left. \left. \left(\partial_\mu^i \left((X^{(j)})_r^{s, [\xi]} (v_{\theta(1)}, \dots, v_{\theta(i)}) \right) \right)_{j,i,\theta} \right] \left(U_{k^*+1}^{(j)} \right)_t^{s, [\xi]} (v_1, \dots, v_{k^*+1}) \right] \Big|_{v_{k^*+1} = \hat{\xi}} \hat{\eta} dW_r.
\end{aligned}$$

As in the proof of Theorem 3.5.3, we deduce that $D_\xi(\partial_\mu^{k^*} X_t^{s, [\xi]}(v_1, \dots, v_{k^*}))(\eta)$ satisfies the same SDE as $\hat{\mathbb{E}}\left[(U_{k^*+1})_t^{s, [\xi]}(v_1, \dots, v_{k^*}, \hat{\xi})\hat{\eta}\right]$. (Note that equality of the first and third terms follows from the same argument as (3.5.11) and equality of the other terms follows from the same argument as (3.5.12).) Consequently,

$$D_\xi(\partial_\mu^{k^*} X_t^{s, [\xi]}(v_1, \dots, v_{k^*}))(\eta) = \hat{\mathbb{E}}\left[(U_{k^*+1})_t^{s, [\xi]}(v_1, \dots, v_{k^*}, \hat{\xi})\hat{\eta}\right]. \quad (3.5.28)$$

By the induction hypothesis, we can again establish that (as in the proof of Theorem 3.5.3)

(i)

$$\mathbb{E}\left[\sup_{t \in [s, T]} |(U_{k^*+1})_t^{s, [\xi]}(v_1, \dots, v_{k^*+1})|^2\right] \leq C,$$

(ii)

$$\begin{aligned} & \mathbb{E}\left[\sup_{t \in [s, T]} |(U_{k^*+1})_t^{s, [\xi]}(v_1, \dots, v_{k^*+1}) - (U_{k^*+1})_t^{s, [\xi']}(v'_1, \dots, v'_{k^*+1})|^2\right] \\ & \leq C\left(\sum_{i=1}^{k^*+1} |v_i - v'_i|^2 + W_2([\xi], [\xi'])^2\right), \end{aligned}$$

for any $s \in [0, T]$, $v_1, \dots, v_{k^*+1}, v'_1, \dots, v'_{k^*+1} \in \mathbb{R}$ and $\xi, \xi' \in L^2(\mathcal{F}_s)$, for some constant $C > 0$. Subsequently, it follows from the same reasoning as in the proof of Theorem 3.5.3 and (3.5.28) that

$$\partial_\mu^{k^*+1} X_t^{s, [\xi]}(v_1, \dots, v_{k^*+1}) = (U_{k^*+1})_t^{s, [\xi]}(v_1, \dots, v_{k^*+1}).$$

Finally, by the recurrence relation (3.5.23) and the expression of $(U_{k^*+1})_t^{s, [\xi]}$ in (3.5.27), it is clear that $\partial_\mu^{k^*+1} X_t^{s, [\xi]}(v_1, \dots, v_{k^*+1})$ satisfies the SDE

$$\begin{aligned} & \partial_\mu^{k^*+1} X_t^{s, [\xi]}(v_1, \dots, v_{k^*+1}) \\ & = \int_s^t \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(k^*+1)} \left[F_{k^*+1} \left([X_r^{s, \xi}], \left((X^{(j)})_r^{s, \xi^{(j)}} \right)_{1 \leq j \leq k^*+1}, \left((X^{(j)})_r^{s, v_\ell, [\xi]} \right)_{1 \leq j, \ell \leq k^*+1}, \right. \right. \\ & \quad \left. \left. \left(\partial_\mu^i (X^{(j)})_r^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{\substack{1 \leq j, i \leq k^*+1 \\ \theta \in \Lambda_{i, k^*+1}}} \right) \right] dW_r. \end{aligned}$$

□

Corollary 3.5.7. *Suppose that σ is in $\mathcal{M}_k(\mathcal{P}_2(\mathbb{R}))$. Then $X^{s, x, [\xi]} \in \mathcal{M}_k^X$.*

Proof. For any multi-index (n, β) such that $|(n, \beta)| \leq k$, we have an SDE representation of $\partial_\mu^n X_t^{s, [\xi]}(v_1, \dots, v_n)$, by (3.5.22) in Theorem 3.5.6. By (3.5.23) and (3.5.24), we know that the function F_n in (3.5.22) is differentiable in the spatial components for at most $k - n$ times. This is exactly what we need, since $|\beta| = \beta_1 + \dots + \beta_n \leq k - n$. Hence, we formally differentiate β_i times with respect to each variable v_i , $1 \leq i \leq n$, and then use a standard Gronwall argument to establish bounds (3.5.20) and (3.5.21). (See Theorem 5.5.3 in [27] or Proposition 4.10 in [45] for details.) □

We are now in a position to prove Theorem 3.5.2, via the smoothness of σ and $X^{s, x, [\xi]}$.

Proof of Theorem 3.5.2. By combining (3.5.7), (3.5.13), (3.5.18) and (3.5.19), we deduce that

$$\chi : L^2(\mathcal{F}_s) \rightarrow L^2(\mathcal{F}_t); \quad \xi \mapsto X_t^{s, \xi}$$

is Fréchet differentiable with Fréchet derivative given by

$$D\chi(\xi)(\eta) = \eta + \hat{\mathbb{E}}[\partial_\mu X_t^{s, [\xi]}(\hat{\xi})\hat{\eta}].$$

Next, for any fixed $s \in [0, t]$, we define the lifts $\tilde{\Phi} : L^2(\mathcal{F}_t) \rightarrow \mathbb{R}$ and $\tilde{\mathcal{V}}(s, \cdot) : L^2(\mathcal{F}_s) \rightarrow \mathbb{R}$ for functions Φ and $\mathcal{V}(s, \cdot)$ respectively, given by

$$\tilde{\Phi}(\theta_1) = \Phi([\theta_1]), \quad \tilde{\mathcal{V}}(s, \theta_2) = \mathcal{V}(s, [\theta_2]), \quad \text{for } \theta_1 \in L^2(\mathcal{F}_t), \quad \theta_2 \in L^2(\mathcal{F}_s).$$

Then, we notice from equation (3.5.1) that

$$\tilde{\mathcal{V}}(s, \cdot) = \tilde{\Phi} \circ \chi.$$

By the chain rule of Fréchet differentiation, we obtain that

$$D\tilde{\mathcal{V}}(s, \xi) = D\tilde{\Phi}(\chi(\xi)) \circ D\chi(\xi),$$

which implies that

$$\begin{aligned} D\tilde{\mathcal{V}}(s, \xi)(\eta) &= D\tilde{\Phi}(\chi(\xi))(D\chi(\xi)(\eta)) \\ &= \mathbb{E}[\partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, \xi}) D\chi(\xi)(\eta)] \\ &= \mathbb{E}[\partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, \xi})(\eta + \hat{\mathbb{E}}[\partial_\mu X_t^{s, [\xi]}(\hat{\xi}) \hat{\eta}])], \end{aligned} \quad (3.5.29)$$

for any $\xi, \eta \in \mathcal{F}_s$. Note that the first term can be rewritten as

$$\mathbb{E}[\partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, \xi}) \eta] = \mathbb{E}[\mathbb{E}(\partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, x, [\xi]})) |_{x=\xi} \eta] \quad (3.5.30)$$

and the second term can be rewritten by the Fubini's theorem as

$$\mathbb{E}[\partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, \xi}) \hat{\mathbb{E}}[(\partial_\mu X_t^{s, [\xi]}(\hat{\xi})) \hat{\eta}]] = \hat{\mathbb{E}}[\mathbb{E}[\partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, \xi}) \partial_\mu X_t^{s, [\xi]}(\hat{\xi}) \hat{\eta}]]. \quad (3.5.31)$$

Consequently, by combining (3.5.30) and (3.5.31), equation (3.5.29) becomes

$$D\tilde{\mathcal{V}}(s, \xi)(\eta) = \mathbb{E}[\mathbb{E}(\partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, x, [\xi]})) |_{x=\xi} \eta] + \hat{\mathbb{E}}[\mathbb{E}[\partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, \xi}) \partial_\mu X_t^{s, [\xi]}(\hat{\xi}) \hat{\eta}]],$$

which implies that

$$\partial_\mu \mathcal{V}(s, [\xi])(y) = \mathbb{E}[\partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, y, [\xi]}) + \partial_\mu \Phi([X_t^{s, \xi}], X_t^{s, \xi}) \partial_\mu X_t^{s, [\xi]}(y)], \quad y \in \mathbb{R}.$$

By our assumption, we know that $\partial_\mu \Phi$ satisfies (3.3.3) and (3.3.4), and the process $\partial_\mu X_t^{s, [\xi]}(v_1)$ satisfies (3.5.20) and (3.5.21). It follows that $\partial_\mu \mathcal{V}$ also satisfies (3.3.3) and (3.3.4), with the constant bound C uniform in time.

By iterating this procedure, we can show that for any $n \leq k$,

$$\begin{aligned} &\partial_\mu^n \mathcal{V}(s, [\xi])(v_1, \dots, v_n) \\ &= \mathbb{E}^{(1)} \mathbb{E}^{(2)} \dots \mathbb{E}^{(n)} \left[F_n \left([X_t^{s, \xi}], \left((X^{(j)})_t^{s, \xi^{(j)}} \right)_{1 \leq j \leq n}, \left((X^{(j)})_t^{s, v_\ell, [\xi]} \right)_{1 \leq j, \ell \leq n}, \right. \right. \\ &\quad \left. \left. \left(\partial_\mu^i (X^{(j)})_t^{s, [\xi]}(v_{\theta(1)}, \dots, v_{\theta(i)}) \right)_{\substack{1 \leq j, i \leq n \\ \theta \in \Lambda_{i, n}}} \right) \right], \end{aligned} \quad (3.5.32)$$

where F_n satisfies the same recurrence relation as (3.5.23) and F_1 is defined by

$$F_1(\mu, x, y, z) = \partial_\mu \Phi(\mu, y) + \partial_\mu \Phi(\mu, x)z.$$

The computation is almost identical to the proof of Theorem 3.5.6.

Next, we proceed with the same argument as the proof of Corollary 3.5.7. Take any multi-index (n, β) such that $|(n, \beta)| \leq k$. We know that the function F_n is differentiable in the spatial components for at most $k-n$ times. This is exactly what we need, since $|\beta| = \beta_1 + \dots + \beta_n \leq k-n$. Hence, we formally differentiate (3.5.32) β_i times with respect to each variable v_i , $1 \leq i \leq n$, which, along with recurrence relation (3.5.23), allows us to establish bounds (3.3.3) and (3.3.4)

for $D^{(n,\beta)}\mathcal{V}(s,\mu)(v_1,\dots,v_n)$, uniform in s . This shows that $\mathcal{V}(s,\cdot)$ is in $\mathcal{M}_k(\mathcal{P}_2(\mathbb{R}))$ and that all derivatives $D^{(n,\beta)}\mathcal{V}(s,\mu)(v_1,\dots,v_n)$ with $|(n,\beta)| \leq k$ are jointly continuous in time, space and measure.

Finally, we know from Theorem 3.5.1 (i.e. Theorem 7.2 in [9]) that $\mathcal{V}(\cdot,\mu) \in C^1([0,t])$, for every $\mu \in \mathcal{P}_2(\mathbb{R})$. This concludes that $\mathcal{V} \in \mathcal{M}_k$. \square

Chapter 4

Weak error expansion

The content of this chapter is extracted from [17].

In this chapter, we provide an exact weak error expansion between a (nonlinear) functional $\Phi : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ of the empirical measure $\mu_N \in \mathcal{P}_2(\mathbb{R}^d)$ and its deterministic limit $\Phi(\mu)$, $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. We investigate the following two cases:

- (a) μ_N is the empirical measure of a sample of N i.i.d. random variables from μ ;
- (b) μ is the marginal law of the McKean-Vlasov process X at some time and μ_N is the empirical measure of the marginal laws of the corresponding particle system $\{Y^{i,N}\}_{1 \leq i \leq N}$ at the same time.

In the first case where μ_N is the empirical measure of N -samples from μ , the only interesting case is when the functional Φ is non-linear. Assume that Φ is Lipschitz continuous with respect to the W_2 -Wasserstein distance, then one could bound $|\Phi(\mu) - \mathbb{E}\Phi(\mu_N)|$ by $\mathbb{E}W_2(\mu, \mu_N)$. Consequently, following [26] or [23], the rate of convergence in the number of samples N deteriorates as the dimension d increases. On the other hand, recently, authors from [21] made a remarkable observation (Lemma 5.10 of [21]) that if the functional Φ is twice-differentiable with respect to the linear functional derivative with uniformly bounded $\frac{\delta\Phi}{\delta m}$ and $\frac{\delta^2\Phi}{\delta m^2}$, along with W_1 -Lipschitz continuous $\frac{\delta^2\Phi}{\delta m^2}$, then one can obtain a dimension-independent bound for the strong error $\mathbb{E}|\Phi(\mu) - \Phi(\mu_N)|^4$, which is of order $O(N^{-1/2})$ (as expected by CLT). A slight generalisation of this result is presented in Lemma 5.2.2. Here, we study the weak error and show that (see Theorem 4.2.10), if $\mu \in \mathcal{P}_{2k+1}(\mathbb{R}^d)$ and Φ is $(2k+1)$ -times differentiable with respect to the linear functional derivative, then indeed we have

$$|\Phi(\mu) - \mathbb{E}\Phi(\mu_N)| = \sum_{j=1}^{k-1} \frac{C_j}{N^j} + O\left(\frac{1}{N^k}\right),$$

for some real constants C_1, \dots, C_{k-1} that do not depend on N . The result is of independent interest, but is also needed to obtain a complete expansion for the error in particle approximations of McKean-Vlasov SDEs.

The second case concerns estimates of propagation-of-chaos type between X and $Y^{i,N}$. We saw in Theorem 2.3.3 that the property of propagation of chaos is equivalent to weak convergence of measure-valued random variables $\mu_t^{Y^{i,N}}$ to μ^X , which in turns allows us to show that $\{(Y^{1,N}, \dots, Y^{N,N})\}_N$ is μ^X -chaotic. However, this approach does not reveal quantitative bounds. A new direction of research has been put forward very recently by independent works [3], [44, Ch. 9] and [56, Th. 2.1]. The authors presented novel weak estimates of propagation of chaos for linear functions in measure, i.e. $\Phi(\mu) := \int_{\mathbb{R}^d} F(x)\mu(dx)$ with $F : \mathbb{R}^d \rightarrow \mathbb{R}$ being smooth. This gives the rate of convergence $O(1/N)$, plus the error due to approximation of the functional of the initial law (see [56, Lem. 4.6] for a discussion of a dimensional-dependent case). While the aim of [56] is to establish quantitative propagation of chaos for the Boltzmann's equation, in a spirit of Kac's programme [41, 52], Theorem 6.1 in [56, Th. 6.1] specialises their result to McKV-SDEs studied here, but only for elliptic diffusion coefficients that do not

depend on measure and symmetric Lipschitz drifts with linear measure dependence. The key idea behind both results is to work with the semigroup that acts on the space of functions of measure, sometimes called the lifted semigroup, which can be viewed as a dual space of probability measures on $\mathcal{P}(\mathbb{R}^d)$ as presented in [55]. In [3], the weak error $|\mathbb{E}\Phi(\mathcal{L}(X_T^{0,\xi})) - \mathbb{E}\Phi(\mu_T^{Y,N})|$ is also shown to converge to zero in the rate $O(1/N)$, under the assumption of linearity in measure (i.e. $\Phi(\mu) := \int_{\mathbb{R}^d} F(x)\mu(dx)$), as well as non-interacting diffusion, i.e. for b and σ of the form

$$b(x, \mu) = B\left(x, \int_{\mathbb{R}^d} \alpha(y) \mu(dy)\right), \quad \sigma(x, \mu) = \Sigma\left(x, \int_{\mathbb{R}^d} \alpha(y) \mu(dy)\right),$$

where $B : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}^d$, $\Sigma : \mathbb{R}^d \times \mathbb{R} \rightarrow \mathbb{R}^d \otimes \mathbb{R}^d$ and $\alpha : \mathbb{R}^d \rightarrow \mathbb{R}$ are functions satisfying certain regularity assumptions on the smoothness. The proof is based on the more classical approach by using the Feynman-Kac PDE on $[0, T] \times \mathbb{R}^d$.

Our method of expansion, on the other hand, relies heavily on the calculus on $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ and, in particular, the Feynman-Kac PDE on $[0, T] \times \mathcal{P}_2(\mathbb{R}^d)$. We first identify minimal assumptions for the expansion in number of particles N to hold. This is presented in terms of class \mathcal{D} (see Definition 4.2.2). Next, we verify these assumptions for McKean-Vlasov SDEs with general drift and (possibly non-elliptic) diffusion coefficients, along with non-linear functionals of measure. This is presented in terms of class \mathcal{M}_k (see Definition 3.3.3). In order for the expansion to work, we need certain smoothness properties on the functions $\mathcal{V}^{(m)}$ (see Definition 4.2.3), which are defined in a recursive manner. Nonetheless, Theorem 3.5.2 gives us information about higher-order smoothness, which in turn allows us to show the smoothness properties on the functions $\mathcal{V}^{(m)}$ (see Theorems 4.3.2 and 4.3.3). The main theorem in this chapter, Theorem 4.3.3, states that given sufficient regularity of b , σ and Φ , we have

$$\mathbb{E}\left[\Phi(\mu_T^{Y,N})\right] - \Phi(\mathcal{L}(X_T^{0,\xi})) = \sum_{j=1}^{k-1} \frac{C_j}{N^j} + O\left(\frac{1}{N^k}\right),$$

where C_1, \dots, C_{k-1} are constants that do not depend on N .

The immediate consequence of the weak expansion is that it allows us to use Romberg extrapolation to obtain an estimator of X with weak error being in the order of $O(\frac{1}{N^k})$, for each $k \in \mathbb{N}$. For sufficiently smooth McKean-Vlasov SDEs, the order of interactions (see Definition 4.1.1) in estimating $\mathbb{E}[F(X_T)]$ can be reduced to the order $O(\epsilon^{-2-p/k})$, for a mean-square error of $O(\epsilon^2)$, where k corresponds to the degree of smoothness and p corresponds to the degree of interactions. This is the theme of the first section.

4.1 Romberg extrapolation, ensembles of particles and complexity analysis

In this section, we construct an ensemble particle system in the spirit of Richardson's extrapolation method [59] that has been studied in the context of time-discretisation of SDEs in [63] and in the context of discretisation of SPDEs in [31].

Let $F : \mathbb{R}^d \rightarrow \mathbb{R}$ satisfy $F \in C_{b, \text{Lip}}^{2k+1}(\mathbb{R}^d)$ and define $\Phi(\mu) := \int_{\mathbb{R}^d} F(x)\mu(dx) \in \mathcal{M}_{2k+1}(\mathcal{P}_2(\mathbb{R}^d))$. Assume that b and σ satisfy the relevant regularity requirements of Theorem 4.3.3. Observe that

$$\mathbb{E}[\Phi(\mu_T^{Y,N})] = \mathbb{E}\left[\frac{1}{N} \sum_{i=1}^N F(Y_T^{i,N})\right] = \mathbb{E}[F(Y_T^{1,N})].$$

Hence, the weak error reads $|\mathbb{E}[F(X_T^{0,\xi})] - \mathbb{E}[F(Y_T^{1,N})]|$. By the result of Theorem 4.3.3, we can apply the technique of Romberg extrapolation to construct an estimator which approximates $\mathbb{E}[F(X_T^{0,\xi})]$ such that the weak error is of the order of $O(1/N^k)$. More precisely, for $k = 2$, since C_1 is independent of N ,

$$\mathbb{E}F(Y_T^{i,N}) - \mathbb{E}[F(X_T^{0,\xi})] = \frac{C_1}{N} + O\left(\frac{1}{N^2}\right)$$

and

$$\mathbb{E}F(Y_T^{i,2N}) - \mathbb{E}[F(X_T^{0,\xi})] = \frac{C_1}{2N} + O\left(\frac{1}{N^2}\right).$$

Hence,

$$\left| \left(2\mathbb{E}F(Y_T^{i,2N}) - \mathbb{E}F(Y_T^{i,N}) \right) - \mathbb{E}[F(X_T^{0,\xi})] \right| = O\left(\frac{1}{N^2}\right).$$

For general k , we can use a similar method to show that

$$\left| \sum_{m=1}^k \alpha_m \mathbb{E}F(Y_T^{i,mN}) - \mathbb{E}[F(X_T^{0,\xi})] \right| = O\left(\frac{1}{N^k}\right),$$

where

$$\alpha_m = (-1)^{k-m} \frac{m^k}{m!(k-m)!}, \quad 1 \leq m \leq k.$$

To motivate the study of weak error expansion, we first define the notions of *order of interactions* and *computational complexity*.

Definition 4.1.1 (Order of interactions and complexity for p th-degree interactions). Suppose that b and σ take the forms

$$b_i(x, \mu) = \int_{\mathbb{R}^d} \dots \int_{\mathbb{R}^d} \mathcal{I}_{1,i}(x, y_1, \dots, y_p) \mu(dy_1) \dots \mu(dy_p), \quad (4.1.1)$$

$$\sigma_{i,j}(x, \mu) = \int_{\mathbb{R}^d} \dots \int_{\mathbb{R}^d} \mathcal{I}_{2,i,j}(x, y_1, \dots, y_p) \mu(dy_1) \dots \mu(dy_p), \quad (4.1.2)$$

where $\mathcal{I}_{1,i}, \mathcal{I}_{2,i,j} : (\mathbb{R}^d)^{p+1} \rightarrow \mathbb{R}$ are continuous functions, for each $i, j \in \{1, \dots, d\}$. Then the order of interactions ¹ of the standard particle system (with N particles) with b and σ given by (4.1.1) and (4.1.2) is defined to be a quantity that satisfies

$$\text{Order of interactions of the particle system} = O(N^{p+1}).$$

The order of interactions of an estimator composed of particle systems S_1, S_2, \dots, S_i is defined by

$$\text{Order of interactions of estimator} := \sum_{i'=1}^i \left[\text{Order of interactions of particle system } S_{i'} \right].$$

For an estimator involving an Euler numerical scheme with discretisation step h , its *computational complexity* is defined by

$$\text{Computational complexity} := h^{-1} \left(\text{Order of interactions of estimator} \right).$$

The goal of this section is to construct an estimator that uses M ensembles of particles, which achieves a reduction in the order of interactions. Suppose that

$$\mathcal{I}_{1,i}, \mathcal{I}_{2,i,j} \in C_{b, \text{Lip}}^{2k+1}((\mathbb{R}^d)^{p+1}) \quad \text{and} \quad \mathcal{I}_{2,i,j} \text{ is uniformly bounded.}$$

Then, clearly, b and σ satisfy the relevant regularity requirements of Theorem 4.3.3. Fix $M \geq 1$. The ensembles are indexed by θ . For $\theta \in \{1, \dots, M\}$, consider

$$Y_t^{i,N,(\theta)} = \xi_{(i,\theta)} + \int_0^t b\left(Y_r^{i,N,(\theta)}, \mu_r^{Y,N,(\theta)}\right) dr + \int_0^t \sigma\left(Y_r^{i,N,(\theta)}, \mu_r^{Y,N,(\theta)}\right) dW_r^{(i,\theta)}, \quad (4.1.3)$$

¹This is a reasonable assumption, as the replacement of μ by the empirical measure gives rise to p averages for each particle. Note that each average is taken over N particles. Hence, the number of interactions required to simulate each particle should have the order $O(N^p)$. Since there are N particles in total, it is reasonable to define the order of interactions for the entire system to be $O(N^{p+1})$.

$1 \leq i \leq N$, where $\mu_r^{Y,N,(\theta)} := \frac{1}{N} \sum_{j=1}^N \delta_{Y_r^{j,N,(\theta)}}$ denotes the empirical measure for each θ ; $\{W^{(i,\theta)} : 1 \leq i \leq N\}_{1 \leq \theta \leq M}$ are M independent ensembles each consisting of N d -dimensional Brownian motions; and $\{\xi^{(i,\theta)} : 1 \leq i \leq N\}_{1 \leq \theta \leq M}$ are M independent ensembles each consisting of N i.i.d. random variables with the same distribution as ξ . We consider the following estimator

$$\frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \Phi(\mu_T^{Y,mN,(\theta)}) = \frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} F(Y_T^{i,mN,(\theta)}). \quad (4.1.4)$$

Next, we analyse the mean-square error of this estimator:

$$\begin{aligned} & \mathbb{E} \left[\left(\mathbb{E}[F(X_T)] - \frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} F(Y_T^{i,mN,(\theta)}) \right)^2 \right] \\ & \leq 2 \left[\left(\mathbb{E}[F(X_T)] - \sum_{m=1}^k \alpha_m \mathbb{E}F(Y_T^{1,mN}) \right)^2 \right] \\ & \quad + 2\mathbb{E} \left[\left(\mathbb{E} \left[\sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} F(Y_T^{i,mN}) \right] - \frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} F(Y_T^{i,mN,(\theta)}) \right)^2 \right]. \end{aligned}$$

The first term on the right-hand side is studied in Theorem 4.3.3 and, provided that the coefficients of (2.1.1) are sufficiently smooth, it converges with order $\mathcal{O}(N^{-2k})$. Control of the second term follows from strong propagation of chaos. Indeed, we write

$$\begin{aligned} & \mathbb{V}ar \left[\frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} F(Y_T^{i,mN,(\theta)}) \right] \\ & \leq 2\mathbb{V}ar \left[\frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} F(X_T^{(i,\theta)}) \right] \\ & \quad + 2\mathbb{V}ar \left[\frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} \left(F(Y_T^{i,mN,(\theta)}) - F(X_T^{(i,\theta)}) \right) \right], \end{aligned}$$

where $X^{(i,\theta)}$ denotes the solution of (2.1.1) driven by $W^{(i,\theta)}$ with initial data $\xi^{(i,\theta)}$ (an analogue of the coupling defined in (2.2.5)). Hence, independence implies that

$$\mathbb{V}ar \left[\frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} F(X_T^{(i,\theta)}) \right] \leq \frac{2^{k-1}}{M} \sum_{m=1}^k \alpha_m^2 \frac{1}{mN} \mathbb{E}|F(X_T^{(1,1)})|^2,$$

where we used the fact that

$$\mathbb{V}ar \left[\sum_{i=1}^k \zeta_i \right] \leq 2^{k-1} \sum_{i=1}^k \mathbb{V}ar[\zeta_i], \quad (4.1.5)$$

for square-integrable random variables ζ_1, \dots, ζ_N . On the other hand, by (4.1.5),

$$\begin{aligned} & \mathbb{V}ar \left[\frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} \left(F(Y_T^{i,mN,(\theta)}) - F(X_T^{(i,\theta)}) \right) \right] \\ & \leq \frac{2^{k-1}}{M} \sum_{m=1}^k \alpha_m^2 \mathbb{E} \left[\left| \frac{1}{mN} \sum_{i=1}^{mN} F(Y_T^{i,mN,(1)}) - F(X_T^{(i,1)}) \right|^2 \right] \\ & \leq \frac{2^{k-1}}{M} \sum_{m=1}^k \alpha_m^2 \frac{1}{mN} \sum_{i=1}^{mN} \mathbb{E} \left[|F(Y_T^{i,mN,(1)}) - F(X_T^{(i,1)})|^2 \right], \end{aligned}$$

where Jensen's inequality is used in the final inequality. Using the fact we have a dimension-free bound for strong propagation of chaos, established in Theorem 5.2.5, there exists a constant

$C > 0$ with no dependence on N such that

$$\mathbb{E}[|F(Y_T^{i,mN,(1)}) - F(X_T^{(i,1)})|^2] \leq \frac{C}{mN}.$$

Consequently, we have

$$\mathbb{E} \left[\left(\mathbb{E}[F(X_T)] - \frac{1}{M} \sum_{\theta=1}^M \sum_{m=1}^k \alpha_m \frac{1}{mN} \sum_{i=1}^{mN} F(Y_T^{i,mN,(\theta)}) \right)^2 \right] \leq C(N^{-2k} + \frac{1}{M} \sum_{m=1}^k \alpha_m^2 \frac{1}{mN}).$$

Since there are M ensembles corresponding to the estimator and each ensemble has k sub-particle systems with mN particles each, $m \in \{1, \dots, k\}$, it follows from Definition 4.1.1 that the order of interactions is $O(M \sum_{m=1}^k (mN)^{p+1})$. When we take $N = \epsilon^{-1/k}$ and $M = \epsilon^{-2+1/k}$, the mean-square error is of the order $O(\epsilon^2)$ (since $\sum_{m=1}^k \alpha_m^2 m^{-1}$ is a constant). The corresponding order of interactions is $O(\epsilon^{-2-p/k})$. The message here is that as the smoothness increases, less interactions among particles are needed when approximating the law of McKean-Vlasov SDE (2.1.1). We would like to stress out again that the dimension of the system does not deteriorate the rate of convergence, in contrast to results presented in the literature [14, 26, 55].

For ensembles of particles without Romberg extrapolation, the estimator becomes

$$\frac{1}{M} \sum_{\theta=1}^M \Phi(\mu_T^{Y,N,(\theta)}) = \frac{1}{M} \sum_{\theta=1}^M \frac{1}{N} \sum_{i=1}^N F(Y_T^{i,N,(\theta)}). \quad (4.1.6)$$

This corresponds to the case $k = 1$. Therefore, by the above calculations, the order of interactions is $O(\epsilon^{-2-p})$.

It is instructive to compare the above computation with a usual mean-square analysis to the Monte-Carlo estimator (without ensembles of particles)

$$\begin{aligned} & \mathbb{E} \left[\left(\mathbb{E}[F(X_T)] - \frac{1}{N} \sum_{i=1}^N F(Y_T^{i,N}) \right)^2 \right] \\ &= \left(\mathbb{E}[F(X_T)] - \mathbb{E}[F(Y_T^{1,N})] \right)^2 + \mathbb{E} \left[\left(\mathbb{E}[F(Y_T^{1,N})] - \frac{1}{N} \sum_{i=1}^N F(Y_T^{i,N}) \right)^2 \right]. \end{aligned}$$

As above, invoking strong propagation of chaos, one can show that the second term is of order $O(N^{-1})$. This means that there would be no gain to go beyond what we can obtain from the strong propagation of chaos analysis to control the first term. Taking $N = \epsilon^{-2}$ results in mean-square error being of the order $O(\epsilon^2)$ and order of interactions being $O(N^{-2(p+1)})$. This clearly demonstrates that working with ensembles of particles leads to an improvement in quantitative properties of propagation of chaos, which is interesting on its own but can also be explored when simulating particle systems on the computer.

4.2 Method of weak error expansion

In this chapter, we adopt the assumption of uniform boundedness on σ .

Assumption 4.2.1.

There exists $L > 0$ such that $|\sigma(x, \mu)| \leq L$, for every $x \in \mathbb{R}^d$ and $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. (UB)

It will become apparent from the proofs that when working only with (Lip), higher order integrability conditions (i.e. fourth order moments) would need to be stated in Definition 4.2.2 (see below). We refrain from this extension and assume (UB) to improve readability, but encourage a curious reader to perform this simple extension.

4.2.1 Weak error expansion along dynamics

We work over a simplex in time in our expansion. For every $m \in \mathbb{N}$, we define

$$\Delta_T^m := \{(t_1, \dots, t_m) \in [0, T]^m \mid 0 \leq t_m \leq t_{m-1} \leq \dots \leq t_1 \leq T\}, \quad m \geq 1. \quad (4.2.1)$$

We often denote $(t_1, \dots, t_m) = \mathbf{t}$ and $(t_1, \dots, t_{m-1}) = \tau$.

We first perform the weak error expansion under minimal assumptions. Since the Feynman-Kac PDE is used at each step of the expansion, it is natural to require the functions at each step of the expansion to be in the class \mathcal{D}_0 (see Definition 3.4.1). However, in order for the recursive definitions (see Definition 4.2.3) in this section to be well-defined, we require the second-order L-derivative to be well-defined and to satisfy certain regularity properties. This leads to the definition of a sub-class \mathcal{D} of \mathcal{D}_0 , whose time-variable is defined over Δ_T^m .

Definition 4.2.2. Let m be a positive integer. A function $U : \Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ is of class $\mathcal{D}(\Delta_T^m)$ if the following conditions hold:

- i) U is jointly continuous on $\Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d)$.
- ii) For all $\mathbf{t} \in \Delta_T^m$, the mappings $\mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \ni (m, y) \mapsto \partial_\mu U(\mathbf{t}, m)(y)$, $\mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \ni (m, y) \mapsto \partial_v \partial_\mu U(\mathbf{t}, m)(y)$ and $\mathcal{P}_2(\mathbb{R}^d) \times \mathbb{R}^d \times \mathbb{R}^d \ni (m, y_1, y_2) \mapsto \partial_\mu^2 U(\mathbf{t}, m)(y_1, y_2)$ are well-defined and continuous in the product topologies.
- iii) There exists $L > 0$ such that for all $\mathbf{t} \in \Delta_T^m$ and $\xi \in L^2(\mathbb{R}^d)$,

$$\mathbb{E}[|\partial_\mu U(\mathbf{t}, \mathcal{L}(\xi))(\xi)|^2 + |\partial_v \partial_\mu U(\mathbf{t}, \mathcal{L}(\xi))(\xi)|^2 + |\partial_\mu^2 U(\mathbf{t}, \mathcal{L}(\xi))(\xi, \xi)|^2] \leq L.$$

- iv) There exists $C > 0$ such that for all $\mathbf{t} \in \Delta_T^m$ and $\xi_1, \xi_2 \in L^2(\mathbb{R}^d)$,

$$|U(\mathbf{t}, \mathcal{L}(\xi_1)) - U(\mathbf{t}, \mathcal{L}(\xi_2))| \leq CW_2(\mathcal{L}(\xi_1), \mathcal{L}(\xi_2)),$$

$$\left(\mathbb{E}[|\partial_\mu U(\mathbf{t}, \mathcal{L}(\xi_1))(\xi_1) - \partial_\mu U(\mathbf{t}, \mathcal{L}(\xi_2))(\xi_2)|^2] \right)^{1/2} \leq CW_2(\mathcal{L}(\xi_1), \mathcal{L}(\xi_2)),$$

$$\left(\mathbb{E}[|\partial_v \partial_\mu U(\mathbf{t}, \mathcal{L}(\xi_1))(\xi_1) - \partial_v \partial_\mu U(\mathbf{t}, \mathcal{L}(\xi_2))(\xi_2)|^2] \right)^{1/2} \leq CW_2(\mathcal{L}(\xi_1), \mathcal{L}(\xi_2)).$$

- v)
 - $m = 1$: $s \mapsto U(s, \mu)$ is continuously differentiable on $[0, T]$.
 - $m > 1$: for all $(\tau_1, \dots, \tau_{m-1}) \in \Delta_T^{m-1}$ with $\tau_{m-1} > 0$ and for all $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, the function

$$[0, \tau_{m-1}] \ni s \mapsto U((\tau_1, \dots, \tau_{m-1}, s), \mu) \in \mathbb{R}$$

is continuously differentiable on $[0, \tau_{m-1}]$.

- vi) The functions

$$\Delta_T^m \times L^2(\mathbb{R}^d) \ni (\mathbf{t}, \xi) \mapsto \partial_t U(\mathbf{t}, \mathcal{L}(\xi))(\xi) \in L^2(\mathbb{R}^d)$$

$$\Delta_T^m \times L^2(\mathbb{R}^d) \ni (\mathbf{t}, \xi) \mapsto \partial_\mu U(\mathbf{t}, \mathcal{L}(\xi))(\xi) \in L^2(\mathbb{R}^d)$$

$$\Delta_T^m \times L^2(\mathbb{R}^d) \ni (\mathbf{t}, \xi) \mapsto \partial_v \partial_\mu U(\mathbf{t}, \mathcal{L}(\xi))(\xi) \in L^2(\mathbb{R}^d \otimes \mathbb{R}^d)$$

$$\Delta_T^m \times L^2(\mathbb{R}^d) \ni (\mathbf{t}, \xi) \mapsto \partial_\mu^2 U(\mathbf{t}, \mathcal{L}(\xi))(\xi, \xi) \in L^2(\mathbb{R}^d \otimes \mathbb{R}^d)$$

are continuous.

We define recursively the functions $\Phi^{(m)}$, $\mathcal{V}^{(m)}$, $1 \leq m \leq k$, that are used to prove the expansion.

Definition 4.2.3. i) For $m = 1$, we set $\Phi^{(0)} = \Phi$ and define $\mathcal{V}^{(1)} : [0, T] \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ by

$$\mathcal{V}^{(1)}(t, \mu) := \mathcal{V}(t, \mu) = \Phi^{(0)}(\mathcal{L}(X_T^{t, \mu})) = \Phi(\mathcal{L}(X_T^{t, \mu})).$$

Assuming that $\mathcal{V}^{(1)}$ belongs to the class $\mathcal{D}(\Delta_T^1)$, we set $\Phi^{(1)} : [0, T] \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ as

$$\Phi^{(1)}(t, \mu) := \int_{\mathbb{R}^d} \text{Tr} \left[\partial_\mu^2 \mathcal{V}^{(1)}(t, \mu)(x, x) a(x, \mu) \right] \mu(dx). \quad (4.2.2)$$

ii) For $1 < m \leq k$, we define $\mathcal{V}^{(m)} : \Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ by

$$\mathcal{V}^{(m)}((\tau, t), \mu) := \Phi^{(m-1)}(\tau, \mathcal{L}(X_{\tau_{m-1}}^{t, \mu})), \quad \tau \in \Delta_T^{m-1}.$$

Assuming that $\mathcal{V}^{(m)}$ belongs to the class $\mathcal{D}(\Delta_T^m)$, we set $\Phi^{(m)} : \Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ as

$$\Phi^{(m)}(\mathbf{t}, \mu) := \int_{\mathbb{R}^d} \text{Tr} \left[\partial_\mu^2 \mathcal{V}^{(m)}(\mathbf{t}, \mu)(x, x) a(x, \mu) \right] \mu(dx).$$

A key point in our work is to show that the previous definition is licit under some assumptions on the coefficient functions b, σ and Φ (Theorem 4.3.2 and Theorem 4.3.3).

We begin with the following technical lemma for our expansion.

Lemma 4.2.4. *Assume (Lip) and (UB). Let m be a positive integer and $f : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ be a continuous function. For any $\tau \in \Delta_T^{m-1}$, we define a function $U_\tau : [0, \tau_{m-1}] \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ such that $U_\tau(t, \mu) := f(\mathcal{L}(X_{\tau_{m-1}}^{t, \mu}))$. We also define a function $U : \Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ such that $U((\tau, t), \mu) := U_\tau(t, \mu)$. Suppose that $\tau_{m-1} > 0$. If U is of class $\mathcal{D}(\Delta_T^m)$, then U_τ can be expanded along the flow of empirical measure associated to the particle system (2.2.4) as follows, for all $0 \leq t \leq \tau_{m-1}$,*

$$\begin{aligned} U_\tau(t, \mu_t^{Y, N}) &= U_\tau(0, \mu_0^{Y, N}) + \frac{1}{2N} \int_0^t \int_{\mathbb{R}^d} \text{Tr} [a(v, \mu_s^{Y, N}) \partial_\mu^2 U_\tau(s, \mu_s^{Y, N})(v, v)] \mu_s^{Y, N}(dv) ds \\ &\quad + \frac{1}{N} \sum_{i=0}^N \int_0^t \sigma(Y_s^i, \mu_s^{Y, N})^T \partial_\mu U_\tau(s, \mu_s^{Y, N})(Y_s^i) \cdot dW_s^i. \end{aligned} \quad (4.2.3)$$

Proof. The proof relies on the strategy of considering the finite dimensional projection of U_τ . For a fixed number of particles N , we define

$$u(t, x_1, \dots, x_N) := U_\tau \left(t, \frac{1}{N} \sum_{i=1}^N \delta_{x_i} \right).$$

From Definition 4.2.2(ii), (v) and (vi), along with Theorem 3.2.5, we observe that $u \in C^{1,2}([0, \tau_{m-1}] \times (\mathbb{R}^d)^N)$. Applying the classical Itô's formula to $U_\tau(t, \mu_t^{Y, N}) = u(t, Y_t^{1, N}, \dots, Y_t^{N, N})$, along with formulae (3.2.9) and (3.2.10) in Theorem 3.2.5, we obtain that

$$\begin{aligned} U_\tau(t, \mu_t^{Y, N}) &= U_\tau(0, \mu_0^{Y, N}) + \frac{1}{N} \sum_{i=0}^N \int_0^t \sigma(Y_s^i, \mu_s^{Y, N})^T \partial_\mu U_\tau(s, \mu_s^{Y, N})(Y_s^i) \cdot dW_s^i + A_t \\ &\quad + \frac{1}{2N} \int_0^t \int_{\mathbb{R}^d} \text{Tr} [a(v, \mu_s^{Y, N}) \partial_\mu^2 U_\tau(s, \mu_s^{Y, N})(v, v)] \mu_s^{Y, N}(dv) ds, \end{aligned} \quad (4.2.4)$$

where

$$\begin{aligned} A_t &:= \int_0^t \left[\partial_t U_\tau(s, \mu_s^{Y, N}) + \int_{\mathbb{R}^d} \left(\partial_\mu U_\tau(s, \mu_s^{Y, N})(v) b(v, \mu_s^{Y, N}) \right. \right. \\ &\quad \left. \left. + \frac{1}{2} \text{Tr} [a(v, \mu_s^{Y, N}) \partial_v \partial_\mu U_\tau(s, \mu_s^{Y, N})(v)] \right) \mu_s^{Y, N}(dv) \right] ds. \end{aligned} \quad (4.2.5)$$

By the definitions of the classes \mathcal{D}_0 and \mathcal{D} , since U belongs to $\mathcal{D}(\Delta_T^m)$, it follows that U_τ belongs to $\mathcal{D}_0([0, \tau_{m-1}])$. Therefore, by Theorem 3.4.3, U_τ satisfies PDE (3.4.3) on $(0, \tau_{m-1})$. Evaluating PDE (3.4.3) at $(s, \mu_s^{Y, N})$ allows us to conclude that A_t is equal to zero, which completes the proof. \square

A special case of Lemma 4.2.4 is useful for subsequent chapters.

Lemma 4.2.5. *Let \mathcal{V} be defined by (3.5.1). Suppose that $b, \sigma \in \mathcal{M}_2(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and $\Phi \in \mathcal{M}_2(\mathcal{P}_2(\mathbb{R}^d))$. Then \mathcal{V} can be expanded along the flow of empirical measure associated to the particle system (2.2.4) as follows,*

$$\begin{aligned} \mathcal{V}(t, \mu_t^{Y,N}) &= \mathcal{V}(0, \mu_0^{Y,N}) + \frac{1}{2N} \int_0^t \int_{\mathbb{R}^d} \text{Tr}[a(v, \mu_s^{Y,N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y,N})(v, v)] \mu_s^{Y,N}(dv) ds \\ &\quad + \frac{1}{N} \sum_{i=0}^N \int_0^t \sigma(Y_s^i, \mu_s^{Y,N})^T \partial_\mu \mathcal{V}(s, \mu_s^{Y,N})(Y_s^i) \cdot dW_s^i. \end{aligned} \quad (4.2.6)$$

Proof. The proof is basically identical to that of Lemma 4.2.4: we apply the standard Itô's formula to the finite dimensional projection of \mathcal{V} , followed by a cancellation in terms, due to the fact that \mathcal{V} satisfies PDE (3.4.3), by Theorem 3.5.1. \square

Theorem 4.2.6 (Weak error expansion: dynamic case). *Assume (Lip) and (UB). Suppose that Definition 4.2.3 is well-posed for $m \in \{1, \dots, k\}$. Then the weak error in the particle approximation can be expressed as*

$$\mathbb{E}[\Phi(\mu_T^{Y,N})] - \Phi(\mathcal{L}(X_T^{0,\xi})) = \sum_{j=0}^{k-1} \frac{1}{N^j} (C_j + \mathcal{I}_{j+1}^N) + O\left(\frac{1}{N^k}\right), \quad (4.2.7)$$

where $C_0 := 0$ and

$$C_m := \frac{1}{2^m} \int_{\Delta_T^m} \Phi^{(m)}(\mathbf{t}, \mathcal{L}(X_{t_m}^{0,\xi})) dt, \quad m \in \{1, \dots, k-1\},$$

$\mathcal{I}_1^N := \mathbb{E}[\mathcal{V}(0, \mu_0^{Y,N})] - \mathcal{V}(0, \mathcal{L}(\xi))$ and

$$\mathcal{I}_m^N := \int_{\Delta_T^{m-1}} \left(\mathbb{E}[\mathcal{V}^{(m)}((\tau, 0), \mu_0^{Y,N})] - \mathcal{V}^{(m)}((\tau, 0), \mathcal{L}(\xi)) \right) d\tau, \quad m \in \{2, \dots, k\}.$$

Proof. Part 1: We first check that the constants $(C_m, \mathcal{I}_{m+1}^N)_{0 \leq m \leq k-1}$ are well defined. For $1 \leq m \leq k-1$, we first show that the function

$$\Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d) \ni (\mathbf{t}, \mu) \mapsto \Phi^{(m)}(\mathbf{t}, \mu) \in \mathbb{R}$$

is continuous. Indeed, let $(\mathbf{t}_n, \mu_n)_n$ be a sequence converging to (\mathbf{t}, μ) in the product topology. Then there exists a sequence (ξ_n) of random variable such that $\mathcal{L}(\xi_n) = \mu_n$ converging to ξ with law μ in L^2 . By continuity of σ , Definition 4.2.3 and Definition 4.2.2(vi),

$$\Gamma_n := \text{Tr} \left[\partial_\mu^2 \mathcal{V}^{(m)}(\mathbf{t}_n, \mathcal{L}(\xi_n))(\xi_n, \xi_n) a(\xi_n, \mathcal{L}(\xi_n)) \right] \rightarrow \text{Tr} \left[\partial_\mu^2 \mathcal{V}^{(m)}(\mathbf{t}, \mathcal{L}(\xi))(\xi, \xi) a(\xi, \mathcal{L}(\xi)) \right] =: \Gamma$$

in probability. Next, since σ is bounded,

$$\mathbb{E} \left[\left| \text{Tr} \left[\partial_\mu^2 \mathcal{V}^{(m)}(\mathbf{t}_n, \mathcal{L}(\xi_n))(\xi_n, \xi_n) a(\xi_n, \mathcal{L}(\xi_n)) \right] \right|^2 \right] \leq C \mathbb{E} \left[\left| \partial_\mu^2 \mathcal{V}^{(m)}(\mathbf{t}_n, \mathcal{L}(\xi_n))(\xi_n, \xi_n) \right|^2 \right] \leq C,$$

where the last inequality follows from the fact that $\mathcal{V}^{(m)}$ is of class $\mathcal{D}(\Delta_T^m)$, by Definition 4.2.2(iii). By de La Vallée Poussin Theorem, the previous computation shows that (Γ_n) is uniformly integrable and thus $\Phi^{(m)}(\mathbf{t}_n, \mu_n) = \mathbb{E}[\Gamma_n] \rightarrow \mathbb{E}[\Gamma] = \Phi^{(m)}(\mathbf{t}, \mu)$. Observing that $\Delta_T^m \ni \mathbf{t} \mapsto (\mathbf{t}, \mathcal{L}(X_{t_m}^{0,\xi})) \in \Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d)$ is continuous, we conclude that $\Delta_T^m \ni \mathbf{t} \mapsto \Phi^{(m)}(\mathbf{t}, \mathcal{L}(X_{t_m}^{0,\xi})) \in \mathbb{R}$ is also continuous (hence measurable) and therefore C_m is well-defined.

Hence, by the definition of $\mathcal{V}^{(m)}$, for each $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, the function

$$\Delta_T^{m-1} \ni \tau \mapsto \mathcal{V}^{(m)}((\tau, 0), \mu) \in \mathbb{R}$$

is continuous. Also, by the previous argument along with Definition 4.2.2(iii), we can see that

$\Phi^{(m)}$ is uniformly bounded. Therefore, the function

$$(\tau, \mu) \mapsto \mathcal{V}^{(m)}((\tau, 0), \mu) \in \mathbb{R}$$

is also uniformly bounded. By the dominated convergence theorem, the function

$$\Delta_T^{m-1} \ni \tau \mapsto \mathbb{E}\left[\mathcal{V}^{(m)}((\tau, 0), \mu_0^{Y,N})\right] \in \mathbb{R}$$

is continuous. This shows that \mathcal{I}_m^N is well-defined.

Part 2: We now proceed with the proof of the expansion, which is done by induction on m .

Base step: We decompose the weak error as

$$\mathbb{E}\left[\Phi(\mu_T^{Y,N})\right] - \Phi(\mathcal{L}(X_T^{0,\xi})) = \mathbb{E}\left[\mathcal{V}(T, \mu_T^{Y,N}) - \mathcal{V}(0, \mu_0^{Y,N})\right] + (\mathbb{E}\left[\mathcal{V}(0, \mu_0^{Y,N})\right] - \mathcal{V}(0, \mathcal{L}(\xi))). \quad (4.2.8)$$

Applying Lemma 4.2.4 to the first term in the right-hand side and taking expectation on both side, we obtain that

$$\begin{aligned} \mathbb{E}\left[\Phi(\mu_T^{Y,N})\right] - \Phi(\mathcal{L}(X_T^{0,\xi})) &= \mathbb{E}\left[\mathcal{V}(0, \mu_0^{Y,N}) - \mathcal{V}(0, \mathcal{L}(\xi))\right] \\ &\quad + \frac{1}{2N} \int_0^T \int_{\mathbb{R}^d} \text{Tr}\left[a(v, \mu_s^{Y,N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y,N})(v, v)\right] \mu_s^{Y,N}(dv) ds. \end{aligned}$$

Recalling the definition of $\Phi^{(1)}$ in (4.2.2), we get

$$\mathbb{E}\left[\Phi(\mu_T^{Y,N}) - \Phi(\mathcal{L}(X_T^{0,\xi}))\right] = \mathbb{E}\left[\mathcal{V}(0, \mu_0^{Y,N}) - \mathcal{V}(0, \mathcal{L}(\xi))\right] + \frac{1}{2N} \int_0^T \mathbb{E}\left[\Phi^{(1)}(t_1, \mu_{t_1}^{Y,N})\right] dt_1.$$

From Part 1, we know that $\Phi^{(1)}$ is uniformly bounded and thus $\int_0^T \mathbb{E}\left[\Phi^{(1)}(t_1, \mu_{t_1}^{Y,N})\right] dt_1 < C$, where $C > 0$ does not depend on N . This proves the induction for the base step.

Induction step: Assume that for $1 \leq m < k$,

$$\mathbb{E}\left[\Phi(\mu_T^{Y,N}) - \Phi(\mathcal{L}(X_T^{0,\xi}))\right] = \sum_{j=0}^{m-1} \frac{1}{N^j} (\mathcal{I}_{j+1}^N + C_j) + \frac{1}{(2N)^m} \int_{\Delta_T^m} \mathbb{E}\left[\Phi^{(m)}(\mathbf{t}, \mu_{t_m}^{Y,N})\right] d\mathbf{t}.$$

Then, we observe that

$$\begin{aligned} &\mathbb{E}\left[\Phi^{(m)}(\mathbf{t}, \mu_{t_m}^{Y,N}) - \Phi^{(m)}(\mathbf{t}, \mathcal{L}(X_{t_m}^{0,\xi}))\right] \\ &= \mathbb{E}\left[\mathcal{V}^{(m+1)}((\mathbf{t}, t_m), \mu_{t_m}^{Y,N}) - \mathcal{V}^{(m+1)}((\mathbf{t}, 0), \mu_0^{Y,N}) + \mathcal{V}^{(m+1)}((\mathbf{t}, 0), \mu_0^{Y,N}) - \mathcal{V}^{(m+1)}((\mathbf{t}, 0), \mathcal{L}(\xi))\right], \end{aligned}$$

which leads to

$$\begin{aligned} &\mathbb{E}\left[\Phi(\mu_T^{Y,N}) - \Phi(\mathcal{L}(X_T^{0,\xi}))\right] \\ &= \sum_{j=0}^m \frac{1}{N^j} \mathcal{I}_{j+1}^N + \sum_{j=0}^m \frac{1}{N^j} C_j + \frac{1}{(2N)^m} \int_{\Delta_T^m} \mathbb{E}\left[\mathcal{V}^{(m+1)}((\mathbf{t}, t_m), \mu_{t_m}^{Y,N}) - \mathcal{V}^{(m+1)}((\mathbf{t}, 0), \mu_0^{Y,N})\right] d\mathbf{t}. \end{aligned} \quad (4.2.9)$$

Fix $\mathbf{t} \in \Delta_T^m$ such that $t_m > 0$. Applying Lemma 4.2.4(ii) to $\mathcal{V}^{(m+1)}(\mathbf{t}, \cdot)$, we obtain that

$$\begin{aligned} &\mathbb{E}\left[\mathcal{V}^{(m+1)}((\mathbf{t}, t_m), \mu_{t_m}^{Y,N}) - \mathcal{V}^{(m+1)}((\mathbf{t}, 0), \mu_0^{Y,N})\right] \\ &= \frac{1}{2N} \mathbb{E}\left[\int_0^{t_m} \int_{\mathbb{R}^d} \text{Tr}\left[\partial_\mu^2 \mathcal{V}^{(m+1)}((\mathbf{t}, t_{m+1}), \mu_{t_{m+1}}^{Y,N})(v, v) a(v, \mu_{t_{m+1}}^{Y,N})\right] \mu_{t_{m+1}}^{Y,N}(dv) dt_{m+1}\right]. \end{aligned}$$

Inserting this back into (4.2.9), we get

$$\mathbb{E}\left[\Phi(\mu_T^{Y,N}) - \Phi(\mathcal{L}(X_T^{0,\xi}))\right] = \sum_{j=0}^m \frac{1}{N^j} (\mathcal{I}_{j+1}^N + C_j) + \frac{1}{(2N)^{m+1}} \int_{\Delta_T^{m+1}} \mathbb{E}\left[\Phi^{(m+1)}(\mathbf{t}, \mu_{t_{m+1}}^{Y,N})\right] d\mathbf{t}.$$

The proof is concluded by observing that $\int_{\Delta_T^{m+1}} \mathbb{E}\left[\Phi^{(m+1)}(\mathbf{t}, \mu_{t_{m+1}}^{Y,N})\right] d\mathbf{t} < C$, due to the uniform boundedness of $\Phi^{(m+1)}$ given in Part 1. \square

4.2.2 Weak error expansion for the initial condition

Assuming enough smoothness of the functions $\mathcal{V}^{(m)}$, we can take care of the terms \mathcal{I}_m^N appearing in the previous theorem, which are error made at time 0. The following weak error analysis relies on the notion of linear functional derivatives. We first start by studying the weak error generated between the evaluation of the function at a measure and its empirical measure counterparts. We prove two results: one dealing mainly with expansion of low orders and the other one at an arbitrary order.

The main assumption we work with relates to the couple (U, m) , where U is a function with domain $\mathcal{P}_2(\mathbb{R}^d)$.

Assumption 4.2.7.

The p th order linear derivative of U exists and is continuous. The following holds: for any family $(\xi_i)_{1 \leq i \leq p}$ of random variable identically distributed with law m ,

$$\mathbb{E}\left[\sup_{\nu \in \mathcal{P}_2(\mathbb{R}^d)} \left| \frac{\delta^p U}{\delta m^p}(\nu, \xi_1, \dots, \xi_p) \right|\right] \leq L_{(U,m)},$$

for some positive constant $L_{(U,m)}$.

(p-LFD)

We first make the following observation regarding assumption (p-LFD), that will be of later use.

Remark 4.2.8. (i) Lemma 3.3.7 states that

$$\left| \frac{\delta^p U}{\delta m^p}(m)(y_1, \dots, y_p) \right| \leq C(|y_1|^p + \dots + |y_p|^p), \quad (4.2.10)$$

for every $m \in \mathcal{P}_2(\mathbb{R}^d)$, for every $y_1, \dots, y_p \in \mathbb{R}^d$, and for some $C > 0$. This means that for any $\mu \in \mathcal{P}_p(\mathbb{R}^d)$, the couple (U, μ) satisfies (p-LFD). This polynomial growth condition is motivated by our example of application, stated in Section 4.3, that relies on the smoothness of the coefficients.

(ii) The following simple example of measure functional shows that the above condition is reasonable to consider: For any bounded smooth function $b : \mathbb{R} \rightarrow \mathbb{R}$, we set $\Psi(m) := b\left(\int x dm(x)\right)$. An iteration of Example 3.1.2 gives ²

$$\frac{\delta^p \Psi}{\delta m^p}(m, y_1, \dots, y_p) = y_1 \dots y_p b^{(p)}\left(\int x dm(x)\right),$$

which relates to (4.2.10) easily.

Theorem 4.2.9. Let $(\xi_i)_{1 \leq i \leq N}$ be i.i.d. random variables with law $\mu \in \mathcal{P}_2(\mathbb{R}^d)$. The following statements hold:

²Note that $\frac{\delta^p \Psi}{\delta m^p}$ has an explicit product form, due to the special structure of Ψ . However, for general functionals $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, e.g. $U := \mathcal{V}(0, \cdot)$, Assumption 4.2.7 provides the necessary control in the general case.

(i) Let **(p-LFD)** hold with $p \in \{1, 2\}$ for (U, μ) . Then

$$\mathbb{E}\left[U\left(\frac{1}{N}\sum_{i=1}^N\delta_{\xi_i}\right)\right] - U(\mu) = O\left(\frac{1}{N}\right).$$

(ii) Let **(p-LFD)** hold with $p \in \{1, 2, 3, 4\}$ for (U, μ) . Suppose that $\mu \in \mathcal{P}_4(\mathbb{R}^d)$. Then

$$\mathbb{E}\left[U\left(\frac{1}{N}\sum_{i=1}^N\delta_{\xi_i}\right)\right] - U(\mu) = \frac{1}{2N}\mathbb{E}\left[\int_{\mathbb{R}^d}\frac{\delta^2U}{\delta m^2}(\mu)(\tilde{\xi}_1, y)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy)\right] + O\left(\frac{1}{N^2}\right),$$

where $\tilde{\xi}_1 \sim \mu$ and is independent of $(\xi_i)_{1 \leq i \leq N}$.

Proof. Let $\mu_N = \frac{1}{N}\sum_{i=1}^N\delta_{\xi_i}$ and $m_t^N = \mu + t(\mu_N - \mu)$, $t \in [0, 1]$. We also consider i.i.d. random variables $(\tilde{\xi}_i)$ with law μ that are also independent of (ξ_i) .

(i) By the definition of linear functional derivatives, we have

$$\begin{aligned}\mathbb{E}[U(\mu_N)] - U(\mu) &= \mathbb{E}\left[\int_0^1\int_{\mathbb{R}^d}\frac{\delta U}{\delta m}(m_t^N)(v)(\mu_N - \mu)(dv)dt\right] \\ &= \int_0^1\frac{1}{N}\sum_{i=1}^N\left(\mathbb{E}\left[\frac{\delta U}{\delta m}(m_t^N)(\xi_i)\right] - \mathbb{E}\left[\frac{\delta U}{\delta m}(m_t^N)(\tilde{\xi}_1)\right]\right)dt \\ &= \int_0^1\mathbb{E}\left[\frac{\delta U}{\delta m}(m_t^N)(\xi_1) - \frac{\delta U}{\delta m}(m_t^N)(\tilde{\xi}_1)\right]dt.\end{aligned}$$

We introduce measures

$$\tilde{m}_t^N := m_t^N + \frac{t}{N}(\delta_{\tilde{\xi}_1} - \delta_{\xi_1}) \quad \text{and} \quad m_{t,t_1}^N := (\tilde{m}_t^N - m_t^N)t_1 + m_t^N, \quad t, t_1 \in [0, 1],$$

and notice that

$$\mathbb{E}\left[\frac{\delta U}{\delta m}(\tilde{m}_t^N)(\tilde{\xi}_1)\right] = \mathbb{E}\left[\frac{\delta U}{\delta m}(m_t^N)(\xi_1)\right].$$

Therefore,

$$\begin{aligned}\mathbb{E}[U(\mu_N)] - U(\mu) &= \int_0^1\mathbb{E}\left[\frac{\delta U}{\delta m}(\tilde{m}_t^N)(\tilde{\xi}_1) - \frac{\delta U}{\delta m}(m_t^N)(\tilde{\xi}_1)\right]dt \\ &= \int_0^1\mathbb{E}\left[\int_0^1\int_{\mathbb{R}^d}\frac{\delta^2U}{\delta m^2}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1)(\tilde{m}_t^N - m_t^N)(dy_1)dt_1\right]dt \\ &= \frac{1}{N}\mathbb{E}\left[\int_0^1\int_0^1\int_{\mathbb{R}^d}t\frac{\delta^2U}{\delta m^2}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)dt_1dt\right].\end{aligned}\tag{4.2.11}$$

To conclude part (i), we observe that

$$\begin{aligned}\mathbb{E}\left[\frac{\delta^2U}{\delta m^2}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)\right] &\leq \mathbb{E}\left[\sup_{\nu \in \mathcal{P}_2(\mathbb{R}^d)}\left|\frac{\delta^2U}{\delta m^2}(\nu)(\tilde{\xi}_1, \tilde{\xi}_1)\right| + \left|\frac{\delta^2U}{\delta m^2}(\nu)(\tilde{\xi}_1, \xi_1)\right|\right] \\ &\leq 2L_{(U, \mu)},\end{aligned}$$

by assumption **(p-LFD)** with $p = 2$.

(ii) We continue the expansion of (4.2.11). To avoid a further interpolation in measure between

m_{t,t_1}^N and μ , we proceed via integration by parts. Let

$$g(t) := \int_0^1 \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1) dt_1, \quad t \in [0, 1],$$

and note that $m_{t,t_1}^N := \frac{tt_1}{N}(\delta_{\tilde{\xi}_1} - \delta_{\xi_1}) + \mu + t(\mu_N - \mu)$. Then, by a similar method as the derivation of (3.1.4),

$$g'(t) = \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1) \left(\frac{t_1}{N}(\delta_{\tilde{\xi}_1} - \delta_{\xi_1}) + (\mu_N - \mu) \right)(dy_2) dt_1.$$

Therefore, by integration by parts,

$$\begin{aligned} & \mathbb{E} \left[\int_0^1 \int_0^1 \int_{\mathbb{R}^d} t \frac{\delta^2 U}{\delta m^2}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1) dt_1 dt \right] \\ &= \mathbb{E} \left[\int_0^1 t g(t) dt \right] = \mathbb{E} \left[\int_0^1 (1-t)g(1-t) dt \right] = \mathbb{E} \left[\frac{1}{2}g(0) + \int_0^1 \left(t - \frac{t^2}{2}\right)g'(1-t) dt \right] \\ &= \mathbb{E} \left[\frac{1}{2}g(0) + \int_0^1 \left(\frac{1-t^2}{2}\right)g'(t) dt \right] \\ &= \frac{1}{2} \mathbb{E} \left[\int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(\mu)(\tilde{\xi}_1, y_1)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1) \right] \\ &\quad + \frac{1}{2N} \mathbb{E} \left[\int_0^1 \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (1-t^2)t_1 \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2) \right. \\ &\quad \quad \left. (\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_2) dt_1 dt \right] \\ &\quad + \frac{1}{2} \mathbb{E} \left[\int_0^1 \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (1-t^2) \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2) \right. \\ &\quad \quad \left. (\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\mu_N - \mu)(dy_2) dt_1 dt \right]. \end{aligned} \tag{4.2.12}$$

For the final term in (4.2.12), by exchangeability, we rewrite

$$\begin{aligned} & \mathbb{E} \left[\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\mu_N - \mu)(dy_2) \right] \\ &= \frac{1}{N} \mathbb{E} \left[\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\xi_1} - \delta_{\tilde{\xi}_2})(dy_2) \right] \\ &\quad + \frac{1}{N} \sum_{i=2}^N \mathbb{E} \left[\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\xi_i} - \delta_{\tilde{\xi}_2})(dy_2) \right] \\ &= \frac{1}{N} \mathbb{E} \left[\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\xi_1} - \delta_{\tilde{\xi}_2})(dy_2) \right] \\ &\quad + \frac{N-1}{N} \mathbb{E} \left[\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\xi_2} - \delta_{\tilde{\xi}_2})(dy_2) \right]. \end{aligned} \tag{4.2.13}$$

As before, we introduce measures

$$\tilde{m}_{t,t_1}^N := m_{t,t_1}^N + \frac{t}{N}(\delta_{\tilde{\xi}_2} - \delta_{\xi_2}) \quad \text{and} \quad \tilde{m}_{t,t_1,t_2}^N := (\tilde{m}_{t,t_1}^N - m_{t,t_1}^N)t_2 + m_{t,t_1}^N, \quad t, t_1, t_2 \in [0, 1].$$

Then

$$\mathbb{E} \left[\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\xi_2} - \delta_{\tilde{\xi}_2})(dy_2) \right]$$

$$\begin{aligned}
&= \mathbb{E} \left[\int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, \xi_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1) \right] \\
&\quad - \mathbb{E} \left[\int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, \tilde{\xi}_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1) \right] \\
&= \mathbb{E} \left[\int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(\tilde{m}_{t,t_1}^N)(\tilde{\xi}_1, y_1, \tilde{\xi}_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1) \right] \\
&\quad - \mathbb{E} \left[\int_{\mathbb{R}^d} \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, \tilde{\xi}_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1) \right] \\
&= \frac{t}{N} \mathbb{E} \left[\int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^4 U}{\delta m^4}(m_{t,t_1,t_2}^N)(\tilde{\xi}_1, y_1, \tilde{\xi}_2, y_2)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\tilde{\xi}_2} - \delta_{\xi_2})(dy_2) dt_2 \right].
\end{aligned} \tag{4.2.14}$$

Combining (4.2.11), (4.2.12), (4.2.13) and (4.2.14) gives

$$\begin{aligned}
&\mathbb{E}[U(\mu_N)] - U(\mu) \\
&= \frac{1}{2N} \mathbb{E} \left[\int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(\mu)(\tilde{\xi}_1, y_1)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1) \right] \\
&\quad + \frac{1}{2N^2} \mathbb{E} \left[\int_0^1 \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (1-t^2)t_1 \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2) \right. \\
&\quad \quad \left. (\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_2) dt_1 dt \right] \\
&\quad + \frac{1}{2N^2} \mathbb{E} \left[\int_0^1 \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} (1-t^2) \frac{\delta^3 U}{\delta m^3}(m_{t,t_1}^N)(\tilde{\xi}_1, y_1, y_2) \right. \\
&\quad \quad \left. (\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\xi_1} - \delta_{\tilde{\xi}_2})(dy_2) dt_1 dt \right] \\
&\quad + \frac{N-1}{2N^3} \mathbb{E} \left[\int_0^1 \int_0^1 \int_0^1 \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} t(1-t^2) \frac{\delta^4 U}{\delta m^4}(m_{t,t_1,t_2}^N)(\tilde{\xi}_1, y_1, \tilde{\xi}_2, y_2) \right. \\
&\quad \quad \left. (\delta_{\tilde{\xi}_1} - \delta_{\xi_1})(dy_1)(\delta_{\tilde{\xi}_2} - \delta_{\xi_2})(dy_2) dt_2 dt_1 dt \right].
\end{aligned}$$

Using the fact that (U, μ) satisfies assumption (p-LFD) with $p \in \{3, 4\}$, the statement for part (ii) is established. \square

In principle, we can continue the above expansion to higher orders. However, in the next theorem we present a simplified argument that allows for complete weak error expansion. The simplification is at the cost of requiring one extra order of regularity in the assumption. However, we believe the argument is of independent interest.

Theorem 4.2.10 (Weak error expansion: static case). *Let q be a positive integer and $\mu \in \mathcal{P}_{2q-1}(\mathbb{R}^d)$. Suppose that assumption (p-LFD) holds for $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, for each $p \in \{1, \dots, 2q-1\}$. Then, for i.i.d. random variables $\{\xi_i\}_{i \in \mathbb{N}}$ with law μ ,*

$$\mathbb{E} \left[U \left(\frac{1}{N} \sum_{i=1}^N \delta_{\xi_i} \right) \right] - U(\mu) = \sum_{p=2}^{q-1} \frac{C_p}{N^{p-1}} + O\left(\frac{1}{N^{q-1}}\right),$$

where

$$C_p = \mathbb{E} \left[\int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(\mu)(\mathbf{y}) \bigotimes_{k=1}^p (\delta_{\xi} - \delta_{\tilde{\xi}^k})(dy_k) \right],$$

for some i.i.d. random variables $(\tilde{\xi}^k)_{1 \leq k \leq q}$ with law μ that are also independent of $(\xi_i)_{i \in \mathbb{N}}$.

Proof. Let $\mu_N = \frac{1}{N} \sum_{i=1}^N \delta_{\xi_i}$. By Lemma 3.1.3, we have

$$\mathbb{E}[U(\mu_N)] - U(\mu) = \sum_{p=1}^{q-1} \frac{1}{p!} \mathbb{E} \left[\int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(\mu)(\mathbf{y}) (\mu_N - \mu)^{\otimes p}(d\mathbf{y}) \right] + \frac{1}{(q-1)!} \int_0^1 (1-t)^{(q-1)} R(q, N, t) dt \quad (4.2.15)$$

with

$$R(q, N, t) := \mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q}(m_t^N)(\mathbf{y}) (\mu_N - \mu)^{\otimes q}(d\mathbf{y}) \right],$$

where $m_t^N := (1-t)\mu + t\mu_N$. Observe that by assumption (**p-LFD**) all the terms in the expansion are well defined. We study them now. For $p = 1$, we have

$$\mathbb{E} \left[\int_{\mathbb{R}^d} \frac{\delta U}{\delta m}(\mu)(y) (\mu_N - \mu)(dy) \right] = 0.$$

Now let $p \in \{2, \dots, q-1\}$ and observe that

$$\mathbb{E} \left[\int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(\mu)(\mathbf{y}) (\mu_N - \mu)^{\otimes p}(d\mathbf{y}) \right] = \frac{1}{N^p} \sum_{1 \leq i_1, \dots, i_p \leq N} \mathbb{E} \left[\int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(\mu)(\mathbf{y}) \bigotimes_{k=1}^p (\delta_{\xi_{i_k}} - \delta_{\hat{\xi}_k})(dy_k) \right].$$

Suppose that at least one of the i_k is different from the other i_j , $j \neq k$. Without loss of generality, we assume that this is the case for $k = p$. We then observe that

$$\begin{aligned} & \mathbb{E} \left[\int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(\mu)(\mathbf{y}) \bigotimes_{k=1}^p (\delta_{\xi_{i_k}} - \delta_{\hat{\xi}_k})(dy_k) \right] \\ &= \mathbb{E} \left[\int_{\mathbb{R}^{(p-1)d}} \frac{\delta^p U}{\delta m^p}(\mu)(y_1, \dots, y_{p-1}, \xi_{i_p}) \bigotimes_{k=1}^{p-1} (\delta_{\xi_{i_k}} - \delta_{\hat{\xi}_k})(dy_k) \right] \\ & \quad - \mathbb{E} \left[\int_{\mathbb{R}^{(p-1)d}} \frac{\delta^p U}{\delta m^p}(\mu)(y_1, \dots, y_{p-1}, \hat{\xi}^p) \bigotimes_{k=1}^{p-1} (\delta_{\xi_{i_k}} - \delta_{\hat{\xi}_k})(dy_k) \right] = 0, \end{aligned}$$

by conditioning on $\xi_{i_1}, \dots, \xi_{i_{p-1}}, \hat{\xi}^1, \dots, \hat{\xi}^{p-1}$. Therefore, when $i_1 = \dots = i_p$,

$$\mathbb{E} \left[\int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(\mu)(\mathbf{y}) (\mu_N - \mu)^{\otimes p}(d\mathbf{y}) \right] = \frac{1}{N^{p-1}} \mathbb{E} \left[\int_{\mathbb{R}^{pd}} \frac{\delta^p U}{\delta m^p}(\mu)(\mathbf{y}) \bigotimes_{k=1}^p (\delta_{\xi} - \delta_{\hat{\xi}_k})(dy_k) \right].$$

It remains to study the remainder term R above. We rewrite

$$R(q, N, t) = \frac{1}{N^q} \sum_{1 \leq i_1, \dots, i_q \leq N} \mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q}(m_t^N)(\mathbf{y}) \bigotimes_{p=1}^q (\delta_{\xi_{i_p}} - \delta_{\hat{\xi}_p})(dy_p) \right].$$

Let \mathcal{L} be a subset of $\omega = \{1, \dots, q\}$. We denote $\mathcal{L}^c := \{1, \dots, q\} \setminus \mathcal{L}$ and introduce

$$\begin{aligned} \mathcal{I}^{\mathcal{L}} := \{ \mathbf{i} = (i_1, \dots, i_q) \in \{1, \dots, N\}^q \mid & \forall \ell, \ell' \in \mathcal{L}, i_\ell = i_{\ell'}, \forall k, k' \in \mathcal{L}^c \text{ s.t. } k \neq k', i_k \neq i_{k'} \\ & \text{and } \forall (\ell, k) \in \mathcal{L} \times \mathcal{L}^c, i_\ell \neq i_k \}. \end{aligned}$$

Then

$$R(q, N, t) = \frac{1}{N^q} \sum_{j=1}^q \sum_{\mathcal{L}, |\mathcal{L}|=j} \sum_{\mathbf{i} \in \mathcal{I}^{\mathcal{L}}} \mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q}(m_t^N)(\mathbf{y}) \bigotimes_{p=1}^q (\delta_{\xi_{i_p}} - \delta_{\hat{\xi}_p})(dy_p) \right].$$

For $j = q$, we simply observe that

$$\frac{1}{N^q} \sum_{\mathbf{i} \in \mathcal{I}^\omega} \mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q} (m_t^N)(\mathbf{y}) \bigotimes_{p=1}^q (\delta_{\xi_{i_p}} - \delta_{\hat{\xi}_p})(dy_p) \right] = O\left(\frac{1}{N^{q-1}}\right). \quad (4.2.16)$$

For $1 \leq j < q$, we consider $\mathcal{I}^\mathcal{L}$ defined above and work with the special choice $\mathcal{L} = \{1, \dots, j\}$, which implies, by exchangeability, that

$$\begin{aligned} & \sum_{\mathbf{i} \in \mathcal{I}^\mathcal{L}} \mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q} (m_t^N)(\mathbf{y}) \bigotimes_{p=1}^q (\delta_{\xi_{i_p}} - \delta_{\hat{\xi}_p})(dy_p) \right] \\ &= N(N-1) \dots (N-(q-j)) \mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q} (m_t^N)(\mathbf{y}) \bigotimes_{p=1}^j (\delta_{\xi_1} - \delta_{\hat{\xi}_p})(dy_p) \bigotimes_{p=j+1}^q (\delta_{\xi_p} - \delta_{\hat{\xi}_p})(dy_p) \right]. \end{aligned} \quad (4.2.17)$$

For later use, we denote

$$\Delta(d\mathbf{y}) := \bigotimes_{p=1}^j (\delta_{\xi_1} - \delta_{\hat{\xi}_p})(dy_p) \bigotimes_{p=j+1}^q (\delta_{\xi_p} - \delta_{\hat{\xi}_p})(dy_p).$$

We will now work iteratively from $j+1$ to q .

Firstly, we introduce

$$\tilde{m}_t^N := m_t^N + \frac{t}{N} (\delta_{\tilde{\xi}_{j+1}} - \delta_{\xi_{j+1}}) \quad \text{and} \quad m_{t, s_{j+1}}^N := \tilde{m}_t^N + s_{j+1} (m_t^N - \tilde{m}_t^N),$$

where we define independent random variables $\{\tilde{\xi}_u\}_{j+1 \leq u \leq q}$ that are also independent of $(\xi_i)_{1 \leq i \leq q}$ and $(\hat{\xi}^i)_{1 \leq i \leq q}$, but with the same law. We then compute that

$$\mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q} (m_t^N)(\mathbf{y}) \Delta(d\mathbf{y}) \right] = \mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q} (\tilde{m}_t^N)(\mathbf{y}) \Delta(d\mathbf{y}) \right] \quad (4.2.18)$$

$$+ \frac{t}{N} \int_0^1 \mathbb{E} \left[\int_{\mathbb{R}^{(q+1)d}} \frac{\delta^{q+1} U}{\delta m^{q+1}} (m_{t, s_{j+1}}^N)(\mathbf{y}, y_{q+1}) \Delta(d\mathbf{y}) (\delta_{\tilde{\xi}_{j+1}} - \delta_{\xi_{j+1}})(dy_{q+1}) \right] ds_{j+1}. \quad (4.2.19)$$

As before,

$$\begin{aligned} & \mathbb{E} \left[\int_{\mathbb{R}^{(q-1)d}} \frac{\delta^q U}{\delta m^q} (\tilde{m}_t^N)(y_1, \dots, y_j, \xi_{j+1}, y_{j+2}, \dots, y_q) \bigotimes_{p=1}^j (\delta_{\xi_1} - \delta_{\hat{\xi}_p})(dy_p) \bigotimes_{p=j+2}^q (\delta_{\xi_p} - \delta_{\hat{\xi}_p})(dy_p) \right] \\ &= \mathbb{E} \left[\int_{\mathbb{R}^{(q-1)d}} \frac{\delta^q U}{\delta m^q} (\tilde{m}_t^N)(y_1, \dots, y_j, \hat{\xi}^{j+1}, y_{j+2}, \dots, y_q) \bigotimes_{p=1}^j (\delta_{\xi_1} - \delta_{\hat{\xi}_p})(dy_p) \bigotimes_{p=j+2}^q (\delta_{\xi_p} - \delta_{\hat{\xi}_p})(dy_p) \right], \end{aligned}$$

so the term on the right hand side of (4.2.18) is equal to zero. Next, for $u \in \{j+1, \dots, q-1\}$, we define inductively

$$\begin{cases} \tilde{m}_{t, s_{j+1}, \dots, s_u}^N := m_{t, s_{j+1}, \dots, s_u}^N + \frac{t}{N} (\delta_{\tilde{\xi}_{u+1}} - \delta_{\xi_{u+1}}), \\ m_{t, s_{j+1}, \dots, s_{u+1}}^N := \tilde{m}_{t, s_{j+1}, \dots, s_u}^N + s_{u+1} (\tilde{m}_{t, s_{j+1}, \dots, s_u}^N - m_{t, s_{j+1}, \dots, s_u}^N). \end{cases}$$

This procedure is then iterated from $j+2$ to q on the remainder term in (4.2.19). We thus have

$$\mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q} (m_t^N)(\mathbf{y}) \Delta(d\mathbf{y}) \right]$$

$$\begin{aligned}
&= \left(\frac{t}{N}\right)^{q-j} \int_0^1 \cdots \int_0^1 \mathbb{E} \left[\int_{\mathbb{R}^{(2q-j)d}} \frac{\delta^{2q-j} U}{\delta m^{2q-j}} (m_{t, s_{j+1}, \dots, s_q}^N)(\mathbf{y}, y_{q+1}, \dots, y_{2q-j}) \right. \\
&\quad \left. \Delta(d\mathbf{y}) \bigotimes_{k=j+1}^q (\delta_{\tilde{\xi}_k} - \delta_{\xi_k})(dy_{q-j+k}) \right] ds_{j+1} \cdots ds_q. \tag{4.2.20}
\end{aligned}$$

Next, by (4.2.10), we estimate the integral by

$$\begin{aligned}
&\left| \mathbb{E} \left[\int_{\mathbb{R}^{(2q-j)d}} \frac{\delta^{2q-j} U}{\delta m^{2q-j}} (m_{t, s_{j+1}, \dots, s_q}^N)(\mathbf{y}, y_{q+1}, \dots, y_{2q-j}) \Delta(d\mathbf{y}) \bigotimes_{k=j+1}^q (\delta_{\tilde{\xi}_k} - \delta_{\xi_k})(dy_{q-j+k}) \right] \right| \\
&\leq \mathbb{E} \left[\sum_{y_1 \in \{\xi_1, \tilde{\xi}^1\}} \cdots \sum_{y_j \in \{\xi_1, \tilde{\xi}^j\}} \sum_{y_{j+1} \in \{\xi_{j+1}, \tilde{\xi}^{j+1}\}} \cdots \sum_{y_q \in \{\xi_q, \tilde{\xi}^q\}} \sum_{y_{q+1} \in \{\tilde{\xi}_{j+1}, \tilde{\xi}^{j+1}\}} \cdots \sum_{y_{2q-j} \in \{\tilde{\xi}_q, \tilde{\xi}^q\}} \right. \\
&\quad \left. \left| \frac{\delta^{2q-j} U}{\delta m^{2q-j}} (m_{t, s_{j+1}, \dots, s_q}^N)(y_1, \dots, y_{2q-j}) \right| \right] \\
&\leq C 2^{4q-2j} L_{(U, m)}, \tag{4.2.21}
\end{aligned}$$

where we used assumption (p-LFD). Combining with (4.2.20) and (4.2.21) gives

$$\mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q} (m_t^N)(\mathbf{y}) \Delta(d\mathbf{y}) \right] = O\left(\frac{1}{N^{q-j}}\right).$$

Finally, combining with (4.2.17) yields

$$\frac{1}{N^q} \sum_{j=1}^q \sum_{\mathcal{L}, |\mathcal{L}|=j} \sum_{\mathbf{i} \in \mathcal{I}^{\mathcal{L}}} \mathbb{E} \left[\int_{\mathbb{R}^{qd}} \frac{\delta^q U}{\delta m^q} (m_t^N)(\mathbf{y}) \bigotimes_{p=1}^q (\delta_{\xi_{i_p}} - \delta_{\tilde{\xi}_p})(dy_p) \right] = O\left(\frac{1}{N^{q-1}}\right).$$

□

4.3 Full expansion in terms of regularity of the drift and diffusion functions

In this subsection, we explore a sufficient condition for the expansion of an arbitrary order purely in terms of regularity of the drift and diffusion functions. It turns out that proving regularity conditions for higher order expansions for class \mathcal{D} is highly non-trivial and therefore we work with the class \mathcal{M}_k defined in Definition 3.3.5. Since the expansion involves simplex coordinates in time, we extend the definition of \mathcal{M}_k to cover this case.

Definition 4.3.1. A function $\mathcal{V} : \Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ is said to be in $\mathcal{M}_k(\Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d))$, if

1. • $m = 1$: $s \mapsto \mathcal{V}(s, \mu)$ is continuously differentiable on $[0, T]$.
- $m > 1$: for all $(\tau_1, \dots, \tau_{m-1}) \in \Delta_T^{m-1}$ with $\tau_{m-1} > 0$ and for all $\mu \in \mathcal{P}_2(\mathbb{R}^d)$, the function

$$[0, \tau_{m-1}] \ni s \mapsto \mathcal{V}((\tau_1, \dots, \tau_{m-1}, s), \mu) \in \mathbb{R}$$

is continuously differentiable on $[0, \tau_{m-1}]$.

2. $\mathcal{V}(\mathbf{t}, \cdot) \in \mathcal{M}_k(\mathcal{P}_2(\mathbb{R}^d))$, for each $\mathbf{t} \in \Delta_T^m$, where the constant C in (3.3.3) and (3.3.4) is uniform in \mathbf{t} .
3. All L-derivatives (including the zeroth order derivative) of $\mathcal{V}(\cdot, \cdot)$ up to the k th order are jointly continuous in time and measure.

We now state the key result, which certifies that the expansion along the dynamics is licit.

Theorem 4.3.2. Assume (UB). Suppose that b and σ belong to the class $\mathcal{M}_{2k}(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$. Moreover, suppose that $\Phi : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ also belongs to the class $\mathcal{M}_{2k}(\mathcal{P}_2(\mathbb{R}^d))$. Then Definition 4.2.3 is well-posed for $m \in \{1, \dots, k\}$.

Proof. We prove by induction on $m \in \{1, \dots, k\}$ and prove that for each $m \in \{1, \dots, k\}$, $\mathcal{V}^{(m)} \in \mathcal{M}_{2k-2m+2}(\Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d)) \subseteq \mathcal{M}_2(\Delta_T^m \times \mathcal{P}_2(\mathbb{R}^d))$ and therefore $\mathcal{V}^{(m)} \in \mathcal{D}(\Delta_T^m)$, which establishes the claim.

For simplicity of notations, we present this proof in the case of dimension one. We commence the proof by noting that $\Phi \in \mathcal{M}_{2k}$ and $b, \sigma \in \mathcal{M}_{2k}$, therefore it follows from Theorem 3.5.2 that $\mathcal{V}^{(1)} \in \mathcal{M}_{2k}$.

Suppose that for $m \in \{1, \dots, k-1\}$, $\mathcal{V}^{(m)} \in \mathcal{M}_{2k-2m+2}$. We recall the definition of $\Phi^{(m)} : \Delta_T^m \times \mathcal{P}_2(\mathbb{R}) \rightarrow \mathbb{R}$ as

$$\Phi^{(m)}(\mathbf{t}, \mu) = \int_{\mathbb{R}} \partial_{\mu}^2 \mathcal{V}^{(m)}(\mathbf{t}, \mu)(x, x) (\sigma(x, \mu))^2 \mu(dx).$$

Fix $\mathbf{t} \in \Delta_T^m$. We shall first establish the smoothness of $\Phi^{(m)}(\mathbf{t}, \cdot)$. Let $p : \mathbb{R} \times \mathcal{P}_2(\mathbb{R}) \rightarrow \mathbb{R}$ be a continuous function defined by

$$p(x, \mu) := \partial_{\mu}^2 \mathcal{V}^{(m)}(\mathbf{t}, \mu)(x, x) (\sigma(x, \mu))^2.$$

Since $\mathcal{V}^{(m)} \in \mathcal{M}_{2k-2m+2}$, by Theorem 3.2.3, we know that for each $x \in \mathbb{R}$, $p(x, \cdot)$ is also differentiable in measure with its derivative given by

$$\partial_{\mu} p(x, \mu)(y) = \partial_{\mu}^3 \mathcal{V}^{(m)}(\mathbf{t}, \mu)(x, x, y) (\sigma(x, \mu))^2 + 2 \partial_{\mu}^2 \mathcal{V}^{(m)}(\mathbf{t}, \mu)(x, x) (\sigma(x, \mu)) \partial_{\mu} \sigma(x, \mu)(y). \quad (4.3.1)$$

We observe that $\partial_{\mu} p(x, \mu)(y)$ and $\partial_x p(x, \mu)$ are both continuous and uniformly bounded in space and measure. Therefore, by Theorem 3.2.4, $\Phi^{(m)}(\mathbf{t}, \cdot)$ is differentiable in measure with its derivative given by

$$\partial_{\mu} \Phi^{(m)}(\mathbf{t}, \mu)(y) = \partial_x p(y, \mu) + \int_{\mathbb{R}} \partial_{\mu} p(x, \mu)(y) \mu(dx),$$

where $\partial_x p(y, \mu)$ is given by

$$\begin{aligned} \partial_x p(y, \mu) &= \left[\partial_{v_1} \partial_{\mu}^2 \mathcal{V}^{(m)}(\mathbf{t}, \mu)(y, y) + \partial_{v_2} \partial_{\mu}^2 \mathcal{V}^{(m)}(\mathbf{t}, \mu)(y, y) \right] (\sigma(y, \mu))^2 \\ &\quad + 2 \partial_{\mu}^2 \mathcal{V}^{(m)}(\mathbf{t}, \mu)(y, y) \sigma(y, \mu) \partial_y \sigma(y, \mu). \end{aligned} \quad (4.3.2)$$

Formulae (4.3.1) and (4.3.2) tell us that $\partial_{\mu} \Phi^{(m)}(\mathbf{t}, \mu)(y)$ is uniformly bounded in measure and space. Furthermore, each of $\partial_x p(y, \mu)$ and $\partial_{\mu} p(x, \mu)(y)$ is a finite sum of products of uniformly bounded Lipschitz functions in measure and space, and is hence Lipschitz continuous as well. Finally, by the duality formula for the Kantorovich-Rubinstein distance (Proposition 2.1.1), we note that there exist constants $C_1, C_2, C_3 > 0$ such that for every $\mu_1, \mu_2 \in \mathcal{P}_2(\mathbb{R})$ and $y_1, y_2 \in \mathbb{R}$,

$$\begin{aligned} & \left| \partial_{\mu} \Phi^{(m)}(\mathbf{t}, \mu_1)(y_1) - \partial_{\mu} \Phi^{(m)}(\mathbf{t}, \mu_2)(y_2) \right| \\ & \leq C_1 \left(|y_1 - y_2| + W_2(\mu_1, \mu_2) + \left| \int_{\mathbb{R}} \partial_{\mu} p(x, \mu)(y_1) \mu_1(dx) - \int_{\mathbb{R}} \partial_{\mu} p(x, \mu)(y_2) \mu_1(dx) \right| \right. \\ & \quad \left. + \left| \int_{\mathbb{R}} \partial_{\mu} p(x, \mu)(y_2) \mu_1(dx) - \int_{\mathbb{R}} \partial_{\mu} p(x, \mu)(y_2) \mu_2(dx) \right| \right) \\ & \leq C_2 \left(|y_1 - y_2| + W_2(\mu_1, \mu_2) + \left| \int_{\mathbb{R}} \partial_{\mu} p(x, \mu)(y_2) \mu_1(dx) - \int_{\mathbb{R}} \partial_{\mu} p(x, \mu)(y_2) \mu_2(dx) \right| \right) \\ & \leq C_2 \left(|y_1 - y_2| + W_2(\mu_1, \mu_2) + \|\partial_{\mu} p\|_{\text{Lip}} W_1(\mu_1, \mu_2) \right) \\ & \leq C_3 \left(|y_1 - y_2| + W_2(\mu_1, \mu_2) \right), \end{aligned}$$

where W_1 denotes the 1-Wasserstein metric.

Subsequently, we can repeat the same procedure to prove existence and regularity properties of higher order derivatives of $\Phi^{(m)}(\mathbf{t}, \cdot)$. In particular, we can show that $\partial_{\mu}^2 \Phi^{(m)}(\mathbf{t}, \mu, v_1, v_2)$ and

$\partial_{v_1} \partial_\mu \Phi^{(m)}(\mathbf{t}, \mu, v_1)$ exist, by expressing them in terms of derivatives of $\mathcal{V}^{(m)}$ up to the fourth order, and derivatives of σ up to the second order, which also allows us to show that they are uniformly bounded and Lipschitz continuous. In general, for any multi-index (n, β) such that $|(n, \beta)| \leq 2k - 2m$, we can show that $D^{(n, \beta)} \Phi^{(m)}(\mathbf{t}, \mu, v_1, \dots, v_n)$ exists, by expressing it in terms of derivatives of $\mathcal{V}^{(m)}$ up to the $(2k - 2m + 2)$ th order, and derivatives of σ up to the $(2k - 2m)$ th order, which again allows us to show that it is uniformly bounded and Lipschitz continuous. Thus, $\Phi^{(m)}(\mathbf{t}, \cdot) \in \mathcal{M}_{2k-2m}$.

Next, we note that since $\mathcal{V}^{(m)} \in \mathcal{M}_{2k-2m+2}(\Delta_T^m \times \mathcal{P}_2(\mathbb{R}))$, $\mathcal{V}^{(m)}$ is continuously differentiable in the last component of time, for each $\mathbf{t} \in \Delta_T^m$ such that $t_{m-1} > 0$, and so is $\Phi^{(m)}$. Moreover, as mentioned above, each derivative $D^{(n, \beta)} \Phi^{(m)}(\mathbf{t}, \mu, v_1, \dots, v_n)$ up to the $(2k - 2m)$ th order can be expressed in terms of derivatives of $\mathcal{V}^{(m)}$ up to the $(2k - 2m + 2)$ th order and derivatives of σ up to the $(2k - 2m)$ th order, which implies that each derivative $D^{(n, \beta)} \Phi^{(m)}(\mathbf{t}, \mu, v_1, \dots, v_n)$ is jointly continuous in time, measure and space, since $\mathcal{V}^{(m)} \in \mathcal{M}_{2k-2m+2}(\Delta_T^m \times \mathcal{P}_2(\mathbb{R}))$. Therefore, by Definition 3.3.5, $\Phi^{(m)} \in \mathcal{M}_{2k-2m}(\Delta_T^m \times \mathcal{P}_2(\mathbb{R}))$.

We now recall the definition of $\mathcal{V}^{(m+1)} : \Delta_T^{m+1} \times \mathcal{P}_2(\mathbb{R}) \rightarrow \mathbb{R}$, given by

$$\mathcal{V}^{(m+1)}((\tau, t), \mu) = \Phi^{(m)}(\tau, \mathcal{L}(X_{\tau_m}^{t, \mu})), \quad \tau \in \Delta_T^m.$$

For fixed $\tau \in \Delta_T^m$ with $\tau_m > 0$, it follows from Theorem 3.5.2 that $\mathcal{V}^{(m+1)}((\tau, \cdot), \cdot)$ is continuously differentiable in time and that $\mathcal{V}^{(m+1)}((\tau, t), \cdot) \in \mathcal{M}_{2k-2m}$, for each $t \in [0, \tau_m]$. Note that for $\tau \in \Delta_T^m$ with $\tau_m = 0$,

$$\mathcal{V}^{(m+1)}((\tau_1, \dots, \tau_{m-1}, 0, 0), \mu) = \Phi^{(m)}((\tau_1, \dots, \tau_{m-1}, 0), \mu).$$

Finally, all derivatives in measure of $\mathcal{V}^{(m+1)}$ up to the $(2k - 2m)$ th order are jointly continuous in time and measure, since $\Phi^{(m)} \in \mathcal{M}_{2k-2m}$. This implies that $\mathcal{V}^{(m+1)} \in \mathcal{M}_{2k-2m}$, which concludes the proof by the principle of induction. \square

The following theorem is the main result of this chapter and is a direct consequence of Theorem 4.2.6, Theorem 4.2.10, Theorem 4.3.2 and Remark 4.2.8(i).

Theorem 4.3.3 (Main result on regularity: Full expansion). *Assume (UB). Suppose that b and σ belong to the class $\mathcal{M}_{2k+1}(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$. Moreover, suppose that $\Phi : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ also belongs to the class $\mathcal{M}_{2k+1}(\mathcal{P}_2(\mathbb{R}^d))$. Finally, suppose that the initial condition satisfies $\mathbb{E}[|\xi_1|^{2k+1}] < +\infty$. Then*

$$\mathbb{E}[\Phi(\mu_T^{Y, N})] - \Phi(\mathcal{L}(X_T^{0, \xi})) = \sum_{j=1}^{k-1} \frac{C_j}{N^j} + O\left(\frac{1}{N^k}\right),$$

where C_1, \dots, C_{k-1} are constants that do not depend on N .

Proof. We commence the proof by noting that Φ , b and σ all belong to \mathcal{M}_{2k+1} , therefore it follows from Theorem 3.5.2 that $\mathcal{V}^{(1)} \in \mathcal{M}_{2k+1}$. As in the proof of Theorem 4.3.2, we prove by induction on $m \in \{1, \dots, k\}$ in order to establish that for each $m \in \{1, \dots, k\}$, $\mathcal{V}^{(m)} \in \mathcal{M}_{2k-2m+3}$. By Theorem 4.3.2, Definition 4.2.3 is well-posed for $m \in \{1, \dots, k\}$. Therefore, by Theorem 4.2.6, we have

$$\mathbb{E}[\Phi(\mu_T^{Y, N})] - \Phi(\mathcal{L}(X_T^{0, \xi})) = \sum_{j=0}^{k-1} \frac{1}{N^j} (C_j + \mathcal{I}_{j+1}^N) + O\left(\frac{1}{N^k}\right), \quad (4.3.3)$$

for some constants $C_0 = 0, C_1, \dots, C_{k-1} > 0$, where

$$\begin{cases} \mathcal{I}_1^N := \mathbb{E}[\mathcal{V}(0, \mu_0^{Y, N}) - \mathcal{V}(0, \mathcal{L}(\xi))] , \\ \mathcal{I}_{j+1}^N := \int_{\Delta_T^j} \left(\mathbb{E}[\mathcal{V}^{(j+1)}((\tau, 0), \mu_0^{Y, N})] - \mathcal{V}^{(j+1)}((\tau, 0), \mathcal{L}(\xi)) \right) d\tau, \quad \text{for } j \in \{1, \dots, k-1\}. \end{cases}$$

Recall that $\mathcal{V}^{(1)} \in \mathcal{M}_{2(k+1)-1}$. By Remark 4.2.8(i) and Theorem 4.2.10,

$$\mathcal{I}_1^N = \mathbb{E}\left[\mathcal{V}(0, \mu_0^{Y,N}) - \mathcal{V}(0, \mathcal{L}(\xi))\right] = \sum_{\ell=1}^{k-1} \frac{C_\ell^{(1)}}{N^\ell} + O\left(\frac{1}{N^k}\right), \quad (4.3.4)$$

for some constants $C_1^{(1)}, \dots, C_{k-1}^{(1)} > 0$. Similarly, for every $j \in \{1, \dots, k-1\}$, since $\mathcal{V}^{(j+1)} \in \mathcal{M}_{2(k-j+1)-1}$, it also follows by Remark 4.2.8(i) and Theorem 4.2.10³ that

$$\mathcal{I}_{j+1}^N = \sum_{\ell=1}^{k-j-1} \frac{C_\ell^{(j)}}{N^\ell} + O\left(\frac{1}{N^{k-j}}\right), \quad (4.3.5)$$

for some constants $C_1^{(j)}, \dots, C_{k-j-1}^{(j)} > 0$. The result follows by combining (4.3.3), (4.3.4) and (4.3.5). \square

³Note that for $U \in \mathcal{M}_{2(k-j+1)-1}(\Delta_T^{j+1} \times \mathcal{P}_2(\mathbb{R}^d))$, the constant C in Lemma 3.3.7 is uniform in $\mathbf{t} \in \Delta_T^{j+1}$. Therefore, the constant C in the same inequality (4.2.10) in Theorem 4.2.10 is also uniform in $\mathbf{t} \in \Delta_T^{j+1}$. The fact that the constants $C_1^{(j)}, \dots, C_{k-j-1}^{(j)}$ are well-defined follows from a similar argument as the first part of the proof of Theorem 4.2.6.

Chapter 5

Antithetic Multi-level Monte Carlo approximation

The content of this chapter is extracted from [62].

5.1 Comparison of computational complexity of different algorithms

We begin by recalling the conclusion from Section 4.1. In this section, we consider b and σ of the forms (4.1.1) and (4.1.2) respectively. As before, we aim to find an estimator $\mathcal{E}(\epsilon)$ of $\Phi(\mu_T^X)$ that achieves a mean-square error of $O(\epsilon^2)$, i.e.

$$\mathbb{E}[(\mathcal{E}(\epsilon) - \Phi(\mu_T^X))^2] \leq C\epsilon^2, \quad \text{for every } \epsilon > 0, \quad \text{for some constant } C > 0.$$

To achieve a mean-square error of $O(\epsilon^2)$ in the approximation, by standard Monte-Carlo, the order of interactions is $O(\epsilon^{-2(p+1)})$. By introducing ensembles of particles (see (4.1.6)), the order of interactions is $O(\epsilon^{-2-p})$. Then, by introducing Romberg extrapolation to the ensembles of particles (see (4.1.4)), the order of interactions can be reduced to $O(\epsilon^{-2-p/k})$. However, this requires the conditions in Theorem 4.3.3 to hold, which are very strong assumptions on the smoothness. Therefore, in principle, as the number k in the assumption of Theorem 4.3.3 gets sufficiently large, the order of interactions is very close to $O(\epsilon^{-2})$. In this chapter, we shall show that the Antithetic Multi-level Monte-Carlo (MLMC) algorithm allows us to nearly achieve this order, whilst assuming weaker conditions on b and σ , if $p = 1$.

How does the algorithm work? The first core idea of the algorithm is to obtain better complexity of simulation using the Multilevel Monte Carlo approach of Giles and Heinrich [29, 36, 43] (see also 2-level Monte-Carlo of Kebaier [43]). The method of MLMC breaks down the simulation into a sequence of approximations G_0, G_1, \dots, G_L with increasing accuracy, but also with increasing cost. If the variance between successive approximations $G_\ell - G_{\ell-1}$ converges to zero as the level increases, then MLMC reduces the computational cost of simulation by carefully combining many simulations on low levels with low accuracy (at a corresponding low cost); with relatively few simulations on high levels with low accuracy (and at a high cost).

The second core idea of the algorithm is the combination of the notion of antithetic estimation with MLMC. At each level ℓ , instead of simulating $G_\ell - G_{\ell-1}$ based on standard Monte-Carlo, the random variable $G_{\ell-1}$ is simulated using the same noise as the simulation of G_ℓ . More precisely, $G_{\ell-1}$ is the arithmetic average of two sub-particle systems, each of which is generated using a mutually disjoint subset of the Brownian motions that are used to generate G_ℓ . This idea of antithetic MLMC is not new. It was done in [30] with Milstein discretisation and was applied specifically to the simulation of McKean-Vlasov SDEs in [32].

By using the algorithm of Antithetic MLMC, Theorem 5.3.2 proves that the order of interactions can be reduced to $O(\epsilon^{-1-p}(\log \epsilon)^{(p+1)\max\{2-p, 0\}})$. The following table summarises the order of interactions for each estimator, along with the corresponding regularity assumptions

on $\mathcal{I}_{1,i}$ (i.e. on b), $\mathcal{I}_{2,i,j}$ (i.e. on σ) and the test function Φ .

Table 5.1: Comparison of the order of interactions for different estimators

Estimator	Order of interactions	Regularity assumption of		
		$\mathcal{I}_{1,i}$	$\mathcal{I}_{2,i,j}$	Φ
Ensembles of particles (4.1.6)	$O(\epsilon^{-2-p})$	$C_{b,\text{Lip}}^3((\mathbb{R}^d)^{p+1})$	$C_{b,\text{Lip}}^3((\mathbb{R}^d)^{p+1})$ and uniformly bounded	\mathcal{M}_3
Romberg extrapolation (4.1.4)	$O(\epsilon^{-2-p/k})$	$C_{b,\text{Lip}}^{2k+1}((\mathbb{R}^d)^{p+1})$	$C_{b,\text{Lip}}^{2k+1}((\mathbb{R}^d)^{p+1})$ and uniformly bounded	\mathcal{M}_{2k+1}
Antithetic MLMC in Section 5.3	$O(\epsilon^{-2}(\log \epsilon)^2)$, for $p = 1$, $O(\epsilon^{-1-p})$, for $p > 1$.	$C_{b,\text{Lip}}^4((\mathbb{R}^d)^{p+1})$	$C_{b,\text{Lip}}^4((\mathbb{R}^d)^{p+1})$	\mathcal{M}_4

For practical purposes, time discretisation is generally needed to simulate SDEs. We consider the time discretisation of (2.1.5), as in seminal papers by Bossy and Talay [7, 8], by working with an Euler scheme. Take partition $\{t_k\}_k$ of $[0, T]$, with $t_k - t_{k-1} = h$ and define $\eta(t) := t_k$ if $t \in [t_k, t_{k+1})$. The continuous Euler scheme reads

$$Z_t^{i,N,h} = Z_{t_k}^{i,N,h} + b(Z_{\eta(t)}^{i,N,h}, \mu_{\eta(t)}^{Z,N,h})(t - t_k) + \sigma(Z_{\eta(t)}^{i,N,h}, \mu_{\eta(t)}^{Z,N,h})(W_t^i - W_{t_k}^i),$$

or its integral form, as

$$\begin{cases} Z_t^{i,N,h} = \xi_i + \int_0^t b(Z_{\eta(r)}^{i,N,h}, \mu_{\eta(r)}^{Z,N,h}) dr + \int_0^t \sigma(Z_{\eta(r)}^{i,N,h}, \mu_{\eta(r)}^{Z,N,h}) dW_r^i, \\ \mu_s^{Z,N,h} := \frac{1}{N} \sum_{i=1}^N \delta_{Z_s^{i,N,h}}. \end{cases} \quad (5.1.1)$$

To compute $\Phi(\mu_T^X)$, for some test function $\Phi : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, we are interested in the computational complexity of achieving a mean-square-error of $O(\epsilon^2)$ via the Monte-Carlo estimator corresponding to ensembles of particles with time discretisation:

$$Q_{M,N,h} := \frac{1}{M} \sum_{\theta=1}^M \Phi(\mu_T^{Z,N,h,(\theta)}), \quad (5.1.2)$$

where $\mu_T^{Z,N,h,(\theta)}$ denotes the empirical measure obtained for each i.i.d. sample $\theta \in \{1, \dots, M\}$. We decompose the mean-square error as follows.

$$\begin{aligned} \text{Mean-square error} &= \mathbb{E} \left[(Q_{M,N,h} - \Phi(\mu_T^X))^2 \right] \\ &= \mathbb{E} \left[(Q_{M,N,h} - \mathbb{E}Q_{M,N,h})^2 \right] + (\mathbb{E}Q_{M,N,h} - \Phi(\mu_T^X))^2 \\ &= \text{Var}(Q_{M,N,h}) + (\mathbb{E}Q_{M,N,h} - \Phi(\mu_T^X))^2. \end{aligned} \quad (5.1.3)$$

It will be shown in Theorem 5.4.1 that the weak error between $\mu_T^{Z,N,h}$ and μ_T^X is bounded by

$$|\mathbb{E}\Phi(\mu_T^{Z,N,h}) - \Phi(\mu_T^X)| \leq C\left(\frac{1}{N} + h\right), \quad (5.1.4)$$

which is an extension of Theorem 4.3.3 to include time discretisation. Next, by the proof of Theorem 5.4.1, namely (5.4.5) and the strong error analogue of (5.4.4) (which follows from Lemma 5.2.2), we observe that

$$\mathbb{E}|\Phi(\mu_T^{Z,N,h}) - \Phi(\mu_T^X)|^2 \leq C\left(\frac{1}{N} + h\right). \quad (5.1.5)$$

Therefore, by (5.1.4) and (5.1.5), we have

$$(\mathbb{E}Q_{M,N,h} - \Phi(\mu_T^X))^2 = (\mathbb{E}\Phi(\mu_T^{Z,N,h}) - \Phi(\mu_T^X))^2 \leq C\left(\frac{1}{N} + h\right)^2$$

and

$$\begin{aligned} \text{Var}(Q_{M,N,h}) &= \frac{1}{M} \text{Var}[\Phi(\mu_T^{Z,N,h})] = \frac{1}{M} \text{Var}[\Phi(\mu_T^{Z,N,h}) - \Phi(\mu_T^X)] \leq \frac{1}{M} \mathbb{E}|\Phi(\mu_T^{Z,N,h}) - \Phi(\mu_T^X)|^2 \\ &\leq \frac{C}{M} \left(\frac{1}{N} + h\right). \end{aligned}$$

Therefore, by setting $N = M = \epsilon^{-1}$ and $h = \epsilon$, we obtain that

$$\text{Mean-square error} \leq C\epsilon^2.$$

By Definition 4.1.1, since there are M clouds, the total complexity is given by

$$\text{Complexity} \leq C(N^{p+1}M)h^{-1} = C\epsilon^{-3-p}.$$

As before, this analysis with time discretisation can be done with Romberg extrapolation, for which the computational complexity becomes $O(\epsilon^{-3-p/k})$. The computation follows the same principles as previous calculations and is omitted. Finally, Theorem 5.4.4 in Section 5.4 proves that, by using an Euler time-discretisation, the computational complexity upon applying antithetic MLMC is $O(\epsilon^{-2-p})$. The following table provides a summary.

Table 5.2: Comparison of the complexity for different algorithms

Algorithm	Complexity	Regularity assumption of		
		$\mathcal{I}_{1,i}$	$\mathcal{I}_{2,i,j}$	Φ
Ensembles of particles (5.1.2)	$O(\epsilon^{-3-p})$	$C_{b,\text{Lip}}^3((\mathbb{R}^d)^{p+1})$	$C_{b,\text{Lip}}^3((\mathbb{R}^d)^{p+1})$ and uniformly bounded	\mathcal{M}_3
Romberg extrapolation with time discretisation	$O(\epsilon^{-3-p/k})$	$C_{b,\text{Lip}}^{2k+1}((\mathbb{R}^d)^{p+1})$	$C_{b,\text{Lip}}^{2k+1}((\mathbb{R}^d)^{p+1})$ and uniformly bounded	\mathcal{M}_{2k+1}
Antithetic MLMC with time discretisation in Section 5.4	$O(\epsilon^{-2-p})$	$C_{b,\text{Lip}}^4((\mathbb{R}^d)^{p+1})$	constant	\mathcal{M}_4

Tables 5.1 and 5.2 manifest the superiority of the antithetic MLMC algorithm for the case of first-degree interaction (i.e. for the case when $p = 1$). The goal of this chapter is indeed to show the respective order of interactions and complexity under the antithetic MLMC algorithm. To prove this, we need a dimension-independent rate of uniform strong propagation of chaos for sufficiently smooth drift and diffusion functions (Theorem 5.2.5) and an L^2 estimate of the antithetic difference for i.i.d. random variables, under general smooth functionals in measures (Theorem 5.2.6), which are results that might be of independent interest. This is the goal of the next section.

5.2 Dimension-independent rate of uniform strong propagation of chaos and L^2 estimate of antithetic difference for i.i.d. random variables

We begin this section with the following lemma on the W_2 metric.

Lemma 5.2.1. *Let $\eta \in \mathbb{R}^d$ and $m \in \mathcal{P}_2(\mathbb{R}^d)$. Then*

$$W_2\left(\frac{1}{N}\delta_\eta + \frac{N-1}{N}m, m\right)^2 \leq \frac{2}{N} \left(|\eta|^2 + \int_{\mathbb{R}^d} |x|^2 m(dx)\right).$$

Proof. Let Y be a random variable with law m and let $\Omega' \in \mathcal{F}$ be a measurable event that is independent of $\sigma(Y)$, with probability $\frac{N-1}{N}$. Let X be a random variable defined by

$$X(\omega) := \begin{cases} Y(\omega), & \omega \in \Omega', \\ \eta, & \omega \notin \Omega'. \end{cases}$$

Then the law of X is $\frac{1}{N}\delta_\eta + \frac{N-1}{N}m$. Therefore, by the definition of the 2-Wasserstein metric,

$$\begin{aligned} W_2\left(\frac{1}{N}\delta_\eta + \frac{N-1}{N}m, m\right)^2 &\leq \mathbb{E}[|X - Y|^2] \\ &= \mathbb{E}[|X - Y|^2|\Omega']\mathbb{P}(\Omega') + \mathbb{E}[|X - Y|^2|(\Omega')^c]\mathbb{P}((\Omega')^c) \\ &= \frac{1}{N}\mathbb{E}[|\eta - Y|^2] \\ &\leq \frac{2}{N}(|\eta|^2 + \mathbb{E}[|Y|^2]). \end{aligned}$$

□

For any functional from $\mathcal{P}_2(\mathbb{R}^d)$ to \mathbb{R} , the following lemma gives a bound on the error between the value of empirical measures under the functional and its limiting law under the functional. It relies on the regularity conditions stipulated in Theorem 3.3.7. The proof of the following lemma is similar to Lemma 5.10 in [21]. However, the following result is slightly more general, as the first and second order linear functional derivatives are only of linear and quadratic growth respectively (Theorem 3.3.7), whereas they are assumed to be uniformly bounded and W_1 -Lipschitz continuous in Lemma 5.10 of [21]. The following result is stated in a way with a constant that does not depend on the functional of measure, nor on the limiting law, so that it is useful with the relevant conditioning argument in the proof of Proposition 5.2.4. The technique of the following proof is also adopted in the proof of Theorem 5.2.6.

Lemma 5.2.2. *Let $U \in \mathcal{M}_3(\mathcal{P}_2(\mathbb{R}^d))$. Let $m_0 \in \mathcal{P}_{12}(\mathbb{R}^d)$ and $m^N = \frac{1}{N}\sum_{i=1}^N \delta_{\zeta_i}$, where ζ_1, \dots, ζ_N are i.i.d samples with law m_0 . Then there exists a constant $C > 0$ (which does not depend on $U, \zeta_1, \dots, \zeta_N$ and m_0) such that*

$$\mathbb{E}[|U(m^N) - U(m_0)|^4] \leq \frac{C}{N^2} \prod_{i=1}^3 \left(1 + \|\partial_\mu^i U\|_\infty^4\right) \left(1 + \int_{\mathbb{R}^d} |x|^{12} m_0(dx)\right).$$

Proof. In this proof, C denotes an absolute constant that does not depend on $U, \zeta_1, \dots, \zeta_N$ and m_0 , whose value may vary from line to line. By the definition of linear functional derivatives, we have

$$\begin{aligned} U(m^N) - U(m_0) &= \int_0^1 \int_{\mathbb{R}^d} \frac{\delta U}{\delta m}(\lambda m^N + (1-\lambda)m_0, v) (m^N - m_0)(dv) d\lambda \\ &= \frac{1}{N} \sum_{i=1}^N \int_0^1 \varphi_\lambda^i d\lambda, \end{aligned}$$

where, for $i \in \{1, \dots, N\}$ and $\lambda \in [0, 1]$,

$$\varphi_\lambda^i = \frac{\delta U}{\delta m}(\lambda m^N + (1-\lambda)m_0, \zeta_i) - \tilde{\mathbb{E}}\left[\frac{\delta U}{\delta m}(\lambda m^N + (1-\lambda)m_0, \tilde{\zeta})\right]. \quad (5.2.1)$$

By the bound on $\frac{\delta U}{\delta m}$ in Theorem 3.3.7, we know that for distinct $i, j \in \{1, \dots, N\}$,

$$\mathbb{E}[(\varphi_\lambda^i)^4 + (\varphi_\lambda^i)^2(\varphi_\lambda^j)^2 + \varphi_\lambda^i(\varphi_\lambda^j)^3] \leq C\|\partial_\mu U\|_\infty^4 \mathbb{E}[|\zeta_1|^4]. \quad (5.2.2)$$

We have the estimate

$$\begin{aligned}
\mathbb{E}[|U(m^N) - U(m_0)|^4] &\leq \frac{1}{N^4} \int_0^1 \mathbb{E} \left[\left(\sum_{i=1}^N \varphi_\lambda^i \right)^4 \right] d\lambda \\
&\leq C \left(\frac{1}{N^2} \|\partial_\mu U\|_\infty^4 \mathbb{E}[|\zeta_1|^4] \right. \\
&\quad \left. + \frac{1}{N^4} \int_0^1 \mathbb{E} \left[\sum_{i_1, i_2, i_3 \text{ distinct}} \varphi_\lambda^{i_1} \varphi_\lambda^{i_2} (\varphi_\lambda^{i_3})^2 + \sum_{i_1, i_2, i_3, i_4 \text{ distinct}} \varphi_\lambda^{i_1} \varphi_\lambda^{i_2} \varphi_\lambda^{i_3} \varphi_\lambda^{i_4} \right] d\lambda \right). \tag{5.2.3}
\end{aligned}$$

For any distinct i_1, i_2, i_3 , we define $m^{N, -(i_1, i_2, i_3)} := \frac{1}{N-3} \sum_{\ell \neq i_1, i_2, i_3} \delta_{\zeta_\ell}$, which implies that

$$m^N - m^{N, -(i_1, i_2, i_3)} = \frac{1}{N} (\delta_{\zeta_{i_1}} + \delta_{\zeta_{i_2}} + \delta_{\zeta_{i_3}}) - \frac{3}{N(N-3)} \sum_{\ell \neq i_1, i_2, i_3} \delta_{\zeta_\ell}.$$

By the definition of second-order linear functional derivatives, we observe that

$$\begin{aligned}
&\frac{\delta U}{\delta m}(\lambda m^N + (1-\lambda)m_0, \zeta_i) - \frac{\delta U}{\delta m}(\lambda m^{N, -(i_1, i_2, i_3)} + (1-\lambda)m_0, \zeta_i) \\
&= \int_0^1 \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2} \left(s\lambda m^N + (1-s)\lambda m^{N, -(i_1, i_2, i_3)} + (1-\lambda)m_0, \zeta_i, v \right) (m^N - m^{N, -(i_1, i_2, i_3)})(dv) ds \\
&= \int_0^1 \frac{1}{N} \left[\sum_{\ell=i_1, i_2, i_3} \frac{\delta^2 U}{\delta m^2} \left(s\lambda m^N + (1-s)\lambda m^{N, -(i_1, i_2, i_3)} + (1-\lambda)m_0, \zeta_i, \zeta_\ell \right) \right. \\
&\quad \left. - \frac{3}{N-3} \sum_{\ell \neq i_1, i_2, i_3} \frac{\delta^2 U}{\delta m^2} \left(s\lambda m^N + (1-s)\lambda m^{N, -(i_1, i_2, i_3)} + (1-\lambda)m_0, \zeta_i, \zeta_\ell \right) \right] ds. \tag{5.2.4}
\end{aligned}$$

By the bound on $\frac{\delta^2 U}{\delta m^2}$ in Theorem 3.3.7,

$$\mathbb{E} \left| \frac{\delta U}{\delta m}(\lambda m^N + (1-\lambda)m_0, \zeta_i) - \frac{\delta U}{\delta m}(\lambda m^{N, -(i_1, i_2, i_3)} + (1-\lambda)m_0, \zeta_i) \right|^4 \leq \frac{C}{N^4} \|\partial_\mu^2 U\|_\infty^4 \mathbb{E}[|\zeta_1|^8].$$

Similarly, by applying the same argument to the second term in (5.2.1), we obtain that

$$\begin{aligned}
&\mathbb{E} \left| \mathbb{E} \left[\frac{\delta U}{\delta m}(\lambda m^N + (1-\lambda)m_0, \tilde{\zeta}) \right] - \mathbb{E} \left[\frac{\delta U}{\delta m}(\lambda m^{N, -(i_1, i_2, i_3)} + (1-\lambda)m_0, \tilde{\zeta}) \right] \right|^4 \\
&\leq \frac{C}{N^4} \|\partial_\mu^2 U\|_\infty^4 \mathbb{E}[|\zeta_1|^8],
\end{aligned}$$

which implies that

$$\mathbb{E} |\varphi_\lambda^i - \varphi_\lambda^{i, -(i_1, i_2, i_3)}|^4 \leq \frac{C}{N^4} \|\partial_\mu^2 U\|_\infty^4 \mathbb{E}[|\zeta_1|^8], \tag{5.2.5}$$

where

$$\varphi_\lambda^{i, -(i_1, i_2, i_3)} = \frac{\delta U}{\delta m}(\lambda m^{N, -(i_1, i_2, i_3)} + (1-\lambda)m_0, \zeta_i) - \mathbb{E} \left[\frac{\delta U}{\delta m}(\lambda m^{N, -(i_1, i_2, i_3)} + (1-\lambda)m_0, \tilde{\zeta}) \right]. \tag{5.2.6}$$

Finally, by writing $\varphi_\lambda^i = (\varphi_\lambda^i - \varphi_\lambda^{i, -(i_1, i_2, i_3)}) + \varphi_\lambda^{i, -(i_1, i_2, i_3)}$ and applying the generalised Hölder's inequality to (5.2.2) and (5.2.5),

$$\begin{aligned}
&\sum_{i_1, i_2, i_3 \text{ distinct}} \mathbb{E} \left[\varphi_\lambda^{i_1} \varphi_\lambda^{i_2} (\varphi_\lambda^{i_3})^2 \right] \\
&\leq \sum_{i_1, i_2, i_3 \text{ distinct}} \left[\frac{C}{N} (1 + \|\partial_\mu U\|_\infty^4) (1 + \|\partial_\mu^2 U\|_\infty^4) \mathbb{E}[|\zeta_1|^8] \right]
\end{aligned}$$

$$\begin{aligned}
& + \mathbb{E} \left[\varphi_\lambda^{i_1, -(i_1, i_2, i_3)} \varphi_\lambda^{i_2, -(i_1, i_2, i_3)} (\varphi_\lambda^{i_3, -(i_1, i_2, i_3)})^2 \right] \\
& \leq CN^2 (1 + \|\partial_\mu U\|_\infty^4) (1 + \|\partial_\mu^2 U\|_\infty^4) \mathbb{E} [|\zeta_1|^8] \\
& \quad + \sum_{\substack{i_1, i_2, i_3 \\ \text{distinct}}} \mathbb{E} \left[\varphi_\lambda^{i_1, -(i_1, i_2, i_3)} \varphi_\lambda^{i_2, -(i_1, i_2, i_3)} (\varphi_\lambda^{i_3, -(i_1, i_2, i_3)})^2 \right]. \tag{5.2.7}
\end{aligned}$$

Let \mathcal{F}^{-i} be the σ -algebra generated by ζ_1, \dots, ζ_N except ζ_i . Since ζ_1, \dots, ζ_N are independent, for any distinct i_1, i_2, i_3 ,

$$\begin{aligned}
& \mathbb{E} \left[\varphi_\lambda^{i_1, -(i_1, i_2, i_3)} \varphi_\lambda^{i_2, -(i_1, i_2, i_3)} (\varphi_\lambda^{i_3, -(i_1, i_2, i_3)})^2 \right] \\
& = \mathbb{E} \left[\varphi_\lambda^{i_2, -(i_1, i_2, i_3)} (\varphi_\lambda^{i_3, -(i_1, i_2, i_3)})^2 \mathbb{E} \left[\varphi_\lambda^{i_1, -(i_1, i_2, i_3)} | \mathcal{F}^{-i_1} \right] \right] = 0, \tag{5.2.8}
\end{aligned}$$

which implies that

$$\sum_{i_1, i_2, i_3 \text{ distinct}} \mathbb{E} \left[\varphi_\lambda^{i_1} \varphi_\lambda^{i_2} (\varphi_\lambda^{i_3})^2 \right] \leq CN^2 (1 + \|\partial_\mu U\|_\infty^4) (1 + \|\partial_\mu^2 U\|_\infty^4) \mathbb{E} [|\zeta_1|^8]. \tag{5.2.9}$$

Next, we define analogously the notation $\varphi^{i, -(i_1, i_2, i_3, i_4)}$ as (5.2.6). As above, by applying the generalised Hölder's inequality to (5.2.2) and (5.2.5), followed by a similar reasoning as (5.2.8), we have

$$\begin{aligned}
& \sum_{\substack{i_1, i_2, i_3, i_4 \\ \text{distinct}}} \mathbb{E} \left[\varphi_\lambda^{i_1} \varphi_\lambda^{i_2} \varphi_\lambda^{i_3} \varphi_\lambda^{i_4} \right] \\
& \leq \sum_{\substack{i_1, i_2, i_3, i_4 \\ \text{distinct}}} \left[\frac{C}{N^2} (1 + \|\partial_\mu U\|_\infty^4) (1 + \|\partial_\mu^2 U\|_\infty^4) \mathbb{E} [|\zeta_1|^8] \right. \\
& \quad \left. + \mathbb{E} \left[\sum_{j=1}^4 (\varphi_\lambda^{i_j} - \varphi_\lambda^{i_j, -(i_1, i_2, i_3, i_4)}) \prod_{\substack{k=1 \\ k \neq j}}^4 \varphi_\lambda^{i_k, -(i_1, i_2, i_3, i_4)} \right] \right. \\
& \quad \left. + \mathbb{E} \left[\varphi_\lambda^{i_1, -(i_1, i_2, i_3, i_4)} \varphi_\lambda^{i_2, -(i_1, i_2, i_3, i_4)} \varphi_\lambda^{i_3, -(i_1, i_2, i_3, i_4)} \varphi_\lambda^{i_4, -(i_1, i_2, i_3, i_4)} \right] \right] \\
& \leq CN^2 (1 + \|\partial_\mu U\|_\infty^4) (1 + \|\partial_\mu^2 U\|_\infty^4) \mathbb{E} [|\zeta_1|^8] \\
& \quad + \sum_{\substack{i_1, i_2, i_3, i_4 \\ \text{distinct}}} \mathbb{E} \left[\sum_{j=1}^4 (\varphi_\lambda^{i_j} - \varphi_\lambda^{i_j, -(i_1, i_2, i_3, i_4)}) \prod_{\substack{k=1 \\ k \neq j}}^4 \varphi_\lambda^{i_k, -(i_1, i_2, i_3, i_4)} \right]. \tag{5.2.10}
\end{aligned}$$

Note that (5.2.5) only gives a growth in the order of $O(N^3)$ for the final term in (5.2.10), therefore it is insufficient.

By (5.2.4) followed by an application of the definition of third order linear functional derivatives, we have

$$\begin{aligned}
& \frac{\delta U}{\delta m} (\lambda m^N + (1 - \lambda) m_0, \zeta_i) - \frac{\delta U}{\delta m} (\lambda m^{N, -(i_1, i_2, i_3, i_4)} + (1 - \lambda) m_0, \zeta_i) \\
& = \frac{1}{N} \left[\sum_{\ell=i_1, i_2, i_3, i_4} \frac{\delta^2 U}{\delta m^2} (\lambda m^{N, -(i_1, i_2, i_3, i_4)} + (1 - \lambda) m_0, \zeta_i, \zeta_\ell) \right. \\
& \quad \left. - \frac{4}{N-4} \sum_{\ell \neq i_1, i_2, i_3, i_4} \frac{\delta^2 U}{\delta m^2} (\lambda m^{N, -(i_1, i_2, i_3, i_4)} + (1 - \lambda) m_0, \zeta_i, \zeta_\ell) \right] + \varepsilon_N^{i, -(i_1, i_2, i_3, i_4)}, \tag{5.2.11}
\end{aligned}$$

where

$$\varepsilon_N^{i, -(i_1, i_2, i_3, i_4)}$$

$$\begin{aligned}
&= \int_0^1 \frac{s\lambda}{N^2} \left[\sum_{\ell=i_1, i_2, i_3, i_4} \int_0^1 \left[\sum_{\ell'=i_1, i_2, i_3, i_4} \frac{\delta^3 U}{\delta m^3} (ts\lambda m^N + (1-ts)\lambda m^{N, -(i_1, i_2, i_3, i_4)} + (1-\lambda)m_0, \right. \right. \\
&\quad \zeta_i, \zeta_\ell, \zeta_{\ell'}) - \frac{4}{N-4} \sum_{\ell' \neq i_1, i_2, i_3, i_4} \frac{\delta^3 U}{\delta m^3} (ts\lambda m^N + (1-ts)\lambda m^{N, -(i_1, i_2, i_3, i_4)} \\
&\quad \left. \left. + (1-\lambda)m_0, \zeta_i, \zeta_\ell, \zeta_{\ell'}) \right] dt \right. \\
&\quad \left. - \frac{4}{N-4} \sum_{\ell \neq i_1, i_2, i_3, i_4} \int_0^1 \left[\sum_{\ell'=i_1, i_2, i_3, i_4} \frac{\delta^3 U}{\delta m^3} (ts\lambda m^N + (1-ts)\lambda m^{N, -(i_1, i_2, i_3, i_4)} + (1-\lambda)m_0, \right. \right. \\
&\quad \zeta_i, \zeta_\ell, \zeta_{\ell'}) - \frac{4}{N-4} \sum_{\ell' \neq i_1, i_2, i_3, i_4} \frac{\delta^3 U}{\delta m^3} (ts\lambda m^N + (1-ts)\lambda m^{N, -(i_1, i_2, i_3, i_4)} \\
&\quad \left. \left. + (1-\lambda)m_0, \zeta_i, \zeta_\ell, \zeta_{\ell'}) \right] dt \right] ds,
\end{aligned}$$

which implies that

$$\mathbb{E}|\varepsilon_N^{i, -(i_1, i_2, i_3, i_4)}|^4 \leq \frac{C}{N^8} \|\partial_\mu^3 U\|_\infty^4 \mathbb{E}[|\zeta_1|^{12}],$$

by the bound on $\frac{\delta^3 U}{\delta m^3}$ in Theorem 3.3.7. Repeating the same argument to the other term in (5.2.1) gives

$$\begin{aligned}
&\varphi_\lambda^i - \varphi_\lambda^{i, -(i_1, i_2, i_3, i_4)} \\
&= \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2} (\lambda m^{N, -(i_1, i_2, i_3, i_4)} + (1-\lambda)m_0, \zeta_i, v) (m^N - m^{N, -(i_1, i_2, i_3, i_4)})(dv) \\
&\quad - \tilde{\mathbb{E}} \left[\int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2} (\lambda m^{N, -(i_1, i_2, i_3, i_4)} + (1-\lambda)m_0, \tilde{\zeta}, v) (m^N - m^{N, -(i_1, i_2, i_3, i_4)})(dv) \right] \\
&\quad + \tilde{\varepsilon}_N^{i, -(i_1, i_2, i_3, i_4)},
\end{aligned}$$

where

$$\mathbb{E}|\tilde{\varepsilon}_N^{i, -(i_1, i_2, i_3, i_4)}|^4 \leq \frac{C}{N^8} \|\partial_\mu^3 U\|_\infty^4 \mathbb{E}[|\zeta_1|^{12}]. \quad (5.2.12)$$

Note that we can write the difference $\varphi_\lambda^{i_1} - \varphi_\lambda^{i_1, -(i_1, i_2, i_3, i_4)} - \tilde{\varepsilon}_N^{i_1, -(i_1, i_2, i_3, i_4)}$ as

$$\varphi_\lambda^{i_1} - \varphi_\lambda^{i_1, -(i_1, i_2, i_3, i_4)} - \tilde{\varepsilon}_N^{i_1, -(i_1, i_2, i_3, i_4)} = \sum_{j=2}^4 F_j((\zeta_r)_{r \neq i_1, \dots, i_4}, \zeta_{i_1}, \zeta_{i_j}),$$

for some measurable functions $F_2, F_3, F_4 : (\mathbb{R}^d)^{N-2} \rightarrow \mathbb{R}$. Therefore,

$$\begin{aligned}
&\mathbb{E} \left[\left(\varphi_\lambda^{i_1} - \varphi_\lambda^{i_1, -(i_1, i_2, i_3, i_4)} - \tilde{\varepsilon}_N^{i_1, -(i_1, i_2, i_3, i_4)} \right) \varphi_\lambda^{i_2, -(i_1, i_2, i_3, i_4)} \varphi_\lambda^{i_3, -(i_1, i_2, i_3, i_4)} \varphi_\lambda^{i_4, -(i_1, i_2, i_3, i_4)} \right] \\
&= \mathbb{E} \left[\left(\sum_{j \in \{3, 4\}} F_j((\zeta_r)_{r \neq i_1, \dots, i_4}, \zeta_{i_1}, \zeta_{i_j}) \right) \varphi_\lambda^{i_3, -(i_1, i_2, i_3, i_4)} \varphi_\lambda^{i_4, -(i_1, i_2, i_3, i_4)} \mathbb{E} \left[\varphi_\lambda^{i_2, -(i_1, i_2, i_3, i_4)} \middle| \mathcal{F}^{-i_2} \right] \right] \\
&\quad + \mathbb{E} \left[F_2((\zeta_r)_{r \neq i_1, \dots, i_4}, \zeta_{i_1}, \zeta_{i_2}) \varphi_\lambda^{i_2, -(i_1, i_2, i_3, i_4)} \varphi_\lambda^{i_4, -(i_1, i_2, i_3, i_4)} \mathbb{E} \left[\varphi_\lambda^{i_3, -(i_1, i_2, i_3, i_4)} \middle| \mathcal{F}^{-i_3} \right] \right] = 0.
\end{aligned}$$

Applying the generalised Hölder's inequality to (5.2.12) and (5.2.2) gives

$$\begin{aligned}
&\mathbb{E} \left[\left(\varphi_\lambda^{i_1} - \varphi_\lambda^{i_1, -(i_1, i_2, i_3, i_4)} \right) \varphi_\lambda^{i_2, -(i_1, i_2, i_3, i_4)} \varphi_\lambda^{i_3, -(i_1, i_2, i_3, i_4)} \varphi_\lambda^{i_4, -(i_1, i_2, i_3, i_4)} \right] \\
&\leq \frac{C}{N^2} \|\partial_\mu^3 U\|_\infty (\mathbb{E}[|\zeta_1|^{12}])^{1/4} \|\partial_\mu U\|_\infty^3 (\mathbb{E}[|\zeta_1|^4])^{3/4}
\end{aligned}$$

$$\leq \frac{C}{N^2} \left(1 + \|\partial_\mu U\|_\infty^4\right) \left(1 + \|\partial_\mu^3 U\|_\infty^4\right) \left(1 + \mathbb{E}[|\zeta_1|^{12}]\right).$$

By the same reasoning, we can show that

$$\begin{aligned} & \sum_{\substack{i_1, i_2, i_3, i_4 \\ \text{distinct}}} \mathbb{E} \left[\sum_{j=1}^4 \left(\varphi_\lambda^{i_j} - \varphi_\lambda^{i_j, -(i_1, i_2, i_3, i_4)} \right) \prod_{\substack{k=1 \\ k \neq j}}^4 \varphi_\lambda^{i_k, -(i_1, i_2, i_3, i_4)} \right] \\ & \leq CN^2 \left(1 + \|\partial_\mu U\|_\infty^4\right) \left(1 + \|\partial_\mu^3 U\|_\infty^4\right) \left(1 + \mathbb{E}[|\zeta_1|^{12}]\right). \end{aligned} \quad (5.2.13)$$

We conclude the result by combining (5.2.3), (5.2.9), (5.2.10) and (5.2.13). \square

Due to Lemma 5.2.2, in many of the subsequent theorems, we assume that the initial law ν satisfies the following assumption.

Assumption 5.2.3.

$$\int_{\mathbb{R}^d} |x|^{12} \nu(dx) < +\infty. \quad (\text{Int})$$

The following proposition is essential to the proofs of Theorem 5.2.5 and Theorem 5.3.1. We define

$$\mu_t^{X, N} := \frac{1}{N} \sum_{j=1}^N \delta_{X_t^j}.$$

Proposition 5.2.4. Assume (Lip) and (Int). Suppose that $\varphi \in \mathcal{M}_3(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$. Then

$$\frac{1}{N} \sum_{i=1}^N \sup_{t \in [0, T]} \mathbb{E} \left| \varphi(X_t^i, \mu_t^{X, N}) - \varphi(X_t^i, \mu_t^X) \right|^4 \leq \frac{C}{N^2},$$

for some constant $C > 0$.

Proof.

$$\begin{aligned} & \frac{1}{N} \sum_{i=1}^N \sup_{t \in [0, T]} \mathbb{E} \left[\left| \varphi\left(X_t^i, \frac{1}{N} \sum_{j=1}^N \delta_{X_t^j}\right) - \varphi(X_t^i, \mu_t^X) \right|^4 \right] \\ & = \frac{1}{N} \sum_{i=1}^N \sup_{t \in [0, T]} \mathbb{E} \left[\left[\mathbb{E} \left[\left| \varphi\left(\eta, \frac{1}{N} \delta_\eta + \frac{N-1}{N} \cdot \frac{1}{N-1} \sum_{\substack{1 \leq j \leq N \\ j \neq i}} \delta_{X_t^j}\right) - \varphi(\eta, \mu_t^X) \right|^4 \right] \Big|_{\eta=X_t^i} \right] \right] \\ & \leq \frac{8}{N} \sum_{i=1}^N \sup_{t \in [0, T]} \mathbb{E} \left[\left[\mathbb{E} \left[\left| \varphi\left(\eta, \frac{1}{N} \delta_\eta + \frac{N-1}{N} \cdot \frac{1}{N-1} \sum_{\substack{1 \leq j \leq N \\ j \neq i}} \delta_{X_t^j}\right) \right. \right. \right. \right. \\ & \quad \left. \left. \left. - \varphi\left(\eta, \frac{1}{N-1} \sum_{\substack{1 \leq j \leq N \\ j \neq i}} \delta_{X_t^j}\right) \right|^4 \right] \Big|_{\eta=X_t^i} \right] \right] \\ & \quad + \frac{8}{N} \sum_{i=1}^N \sup_{t \in [0, T]} \mathbb{E} \left[\left[\mathbb{E} \left[\left| \varphi\left(\eta, \frac{1}{N-1} \sum_{\substack{1 \leq j \leq N \\ j \neq i}} \delta_{X_t^j}\right) - \varphi(\eta, \mu_t^X) \right|^4 \right] \Big|_{\eta=X_t^i} \right] \right] \\ & =: \Pi_1 + \Pi_2. \end{aligned}$$

By Lemma 5.2.1,

$$\Pi_1 \leq \frac{8}{N} \sum_{i=1}^N \sup_{t \in [0, T]} \mathbb{E} \left[\frac{4}{N^2} \left(|X_t^i|^2 + \frac{1}{N-1} \sum_{\substack{1 \leq j \leq N \\ j \neq i}} |X_t^j|^2 \right)^2 \right] \lesssim \frac{1}{N^2}. \quad (5.2.14)$$

By the assumption on φ , we observe that for any $\eta \in \mathbb{R}^d$, the uniform bounds on $\partial_\mu \varphi(\eta, \cdot)$, $\partial_\mu^2 \varphi(\eta, \cdot)$ and $\partial_\mu^3 \varphi(\eta, \cdot)$ do not depend on η . Finally, since b and σ are Lipschitz and $\mathbb{E}[|\xi|^{12}] < +\infty$, we have $\sup_{t \in [0, T]} \mathbb{E}[|X_t|^{12}] < +\infty$. Therefore, Lemma 5.2.2 implies that

$$\Pi_2 \lesssim \frac{1}{(N-1)^2} \prod_{i=1}^3 \left(1 + \sup_{\eta \in \mathbb{R}^d} \|\partial_\mu^i \varphi(\eta, \cdot)\|_\infty^4 \right) \left(1 + \sup_{t \in [0, T]} \int_{\mathbb{R}^d} |y|^{12} \mu_t^X(dy) \right). \quad (5.2.15)$$

A combination of (5.2.14) and (5.2.15) yields the result. \square

Recall that Theorem 2.2.6 (from [61]) gives a strong error between the particle system (2.2.4) and its coupling (2.2.5). However, it requires a particular structure (First order) and the proof does not hold for arbitrary integrating kernels b and σ . Nonetheless, we can still conclude something by resorting to the Wasserstein metric. Assuming (Lip) and (Int), Theorem 10.2.7 in [58] gives us a rate of convergence of

$$\mathbb{E} \left[\sup_{t \in [0, T]} W_2(\mu_t^X, \mu_t^{X, N})^2 \right] \leq \frac{C}{N^{2/(d+8)}}. \quad (5.2.16)$$

There are results in the literature that give a slightly better rate of convergence of the W_2 norm of empirical measures of i.i.d. random variables. However, they are not for i.i.d. processes and are still dimensionally dependent. Moreover, the rates of convergence (in the L^2 norm) in those results are all substantially slower than $O(N^{-1/2})$.

Proposition 5.2.4 allows us to completely bypass the consideration of the Wasserstein distance between empirical measures and their limiting law. The following result gives a uniform rate of strong propagation of chaos between the particle system (2.2.4) and its coupled mean-field limit (2.2.5), under the assumption that b and σ are sufficiently smooth.

Theorem 5.2.5 (Uniform strong propagation of chaos). *Assume (Int). Suppose that $b, \sigma \in \mathcal{M}_3(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$. Then*

$$\mathbb{E} \left[W_{C_T, 2}(\mu^{Y, N}, \mu^{X, N})^4 \right] \leq \mathbb{E} \left[\frac{1}{N} \sum_{i=1}^N \left(\sup_{t \in [0, T]} |X_t^i - Y_t^{i, N}|^4 \right) \right] \leq \frac{C}{N^2},$$

for some constant $C > 0$.

Proof. By the Hölder and Buckholder-Davis-Gundy inequalities, estimating the L^4 difference between (2.2.4) and (2.2.5) gives

$$\begin{aligned} \mathbb{E} \left[\sup_{s \in [0, t]} |X_s^i - Y_s^{i, N}|^4 \right] &\leq C \left(\int_0^t \mathbb{E} |b(X_s^i, \mu_s^X) - b(Y_s^{i, N}, \mu_s^{Y, N})|^4 ds \right. \\ &\quad \left. + \int_0^t \mathbb{E} |\sigma(X_s^i, \mu_s^X) - \sigma(Y_s^{i, N}, \mu_s^{Y, N})|^4 ds \right), \end{aligned} \quad (5.2.17)$$

for every $t \in [0, T]$. By Lipschitz continuity of b and σ ,

$$\begin{aligned} \mathbb{E} \left[\sup_{s \in [0, t]} |X_s^i - Y_s^{i, N}|^4 \right] &\leq C \left(\int_0^t \mathbb{E} \left[\sup_{u \in [0, s]} |X_u^i - Y_u^{i, N}|^4 \right] ds + \int_0^t \mathbb{E} |b(X_s^i, \mu_s^X) - b(X_s^i, \mu_s^{Y, N})|^4 ds \right. \\ &\quad \left. + \int_0^t \mathbb{E} |\sigma(X_s^i, \mu_s^X) - \sigma(X_s^i, \mu_s^{Y, N})|^4 ds \right), \end{aligned}$$

for every $t \in [0, T]$, which gives, upon taking average over i ,

$$\begin{aligned} \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\sup_{s \in [0, t]} |X_s^i - Y_s^{i, N}|^4 \right] &\leq C \left(\int_0^t \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\sup_{u \in [0, s]} |X_u^i - Y_u^{i, N}|^4 \right] ds \right. \\ &\quad \left. + \int_0^t \frac{1}{N} \sum_{i=1}^N \mathbb{E} |b(X_s^i, \mu_s^X) - b(X_s^i, \mu_s^{Y, N})|^4 ds \right) \end{aligned}$$

$$+ \int_0^t \frac{1}{N} \sum_{i=1}^N \mathbb{E} |\sigma(X_s^i, \mu_s^X) - \sigma(X_s^i, \mu_s^{Y,N})|^4 ds \Big). \quad (5.2.18)$$

Also, the empirical measure of the particles can be replaced by the empirical measure of the coupled system by the bound

$$\mathbb{E}[W_2(\mu_s^{X,N}, \mu_s^{Y,N})^4] \leq \left[\left(\frac{1}{N} \sum_{i=1}^N \mathbb{E} |Y_s^{i,N} - X_s^i|^2 \right)^2 \right] \leq \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\sup_{u \in [0,s]} |X_u^i - Y_u^{i,N}|^4 \right]. \quad (5.2.19)$$

A combination of (5.2.18) and (5.2.19) gives

$$\begin{aligned} \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\sup_{s \in [0,t]} |X_s^i - Y_s^{i,N}|^4 \right] &\leq C \left(\int_0^t \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\sup_{u \in [0,s]} |X_u^i - Y_u^{i,N}|^4 \right] ds \right. \\ &\quad + \int_0^t \frac{1}{N} \sum_{i=1}^N \sup_{u \in [0,s]} \mathbb{E} |b(X_u^i, \mu_u^X) - b(X_u^i, \mu_u^{X,N})|^4 ds \\ &\quad \left. + \int_0^t \frac{1}{N} \sum_{i=1}^N \sup_{u \in [0,s]} \mathbb{E} |\sigma(X_u^i, \mu_u^X) - \sigma(X_u^i, \mu_u^{X,N})|^4 ds \right). \end{aligned}$$

Therefore, by Proposition 5.2.4 and Gronwall's inequality, we have

$$\frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\sup_{s \in [0,T]} |X_s^i - Y_s^{i,N}|^4 \right] \leq \frac{C}{N^2},$$

for every $t \in [0, T]$. □

We now recall, from Section 9 in [29], that the the second moment of the antithetic difference (see (5.3.1) for the definition of $\mu^{Y,2N,(1)}$ and $\mu^{Y,2N,(2)}$) given by

$$U(\mu_0^{Y,2N}) - \frac{1}{2} (U(\mu_0^{Y,2N,(1)}) + U(\mu_0^{Y,2N,(2)}))$$

converges to 0 in the rate $O(1/N^2)$, for functions $U : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ of the form

$$U(\mu) := F \left(\int_{\mathbb{R}^d} G(x) \mu(dx) \right), \quad (5.2.20)$$

where $G : \mathbb{R}^d \rightarrow \mathbb{R}$ is an integrable function and $F : \mathbb{R} \rightarrow \mathbb{R}$ is a twice-differentiable function with bounded derivatives. The following theorem gives a similar result for functions U with a more general form (at the price of requiring extra regularity assumptions).

Theorem 5.2.6 (Antithetic error on the initial conditions). *Suppose that $\nu \in \mathcal{P}_8(\mathbb{R}^d)$ and $U \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$. Then there exists a constant $C > 0$ such that*

$$\mathbb{E} \left| U(\mu_0^{Y,2N}) - \frac{1}{2} (U(\mu_0^{Y,2N,(1)}) + U(\mu_0^{Y,2N,(2)})) \right|^2 \leq \frac{C}{N^2}.$$

Proof. For simplicity of notations, let

$$\mu_{2N} := \mu_0^{Y,2N}, \quad \mu_{2N,(1)} := \mu_0^{Y,2N,(1)}, \quad \mu_{2N,(2)} := \mu_0^{Y,2N,(2)}.$$

For every $t \in [0, 1]$, let

$$m_t^{2N} := (1-t)\nu + t\mu_{2N}, \quad m_t^{2N,(1)} := (1-t)\nu + t\mu_{2N,(1)}, \quad m_t^{2N,(2)} := (1-t)\nu + t\mu_{2N,(2)}.$$

We define

$$[0, 1] \ni t \mapsto f(t) = U((1-t)\nu + t\mu_{2N}) = U(\nu + t(\mu_{2N} - \nu)) \in \mathbb{R}$$

and apply Taylor-Lagrange formula to f up to order 2, namely

$$f(1) - f(0) = f'(0) + \int_0^1 (1-t)f^{(2)}(t) dt.$$

This yields

$$U(\mu_{2N}) - U(\nu) = \int_{\mathbb{R}^d} \frac{\delta U}{\delta m}(\nu)(\mathbf{y}) (\mu_{2N} - \nu)(d\mathbf{y}) + \int_0^1 (1-t) \left[\int_{\mathbb{R}^{2d}} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(\mathbf{y}) (\mu_{2N} - \nu)^{\otimes 2}(d\mathbf{y}) \right] dt. \quad (5.2.21)$$

Similarly,

$$\begin{aligned} U(\mu_{2N,(1)}) - U(\nu) &= \int_{\mathbb{R}^d} \frac{\delta U}{\delta m}(\nu)(\mathbf{y}) (\mu_{2N,(1)} - \nu)(d\mathbf{y}) \\ &+ \int_0^1 (1-t) \left[\int_{\mathbb{R}^{2d}} \frac{\delta^2 U}{\delta m^2}(m_t^{2N,(1)})(\mathbf{y}) (\mu_{2N,(1)} - \nu)^{\otimes 2}(d\mathbf{y}) \right] dt \end{aligned} \quad (5.2.22)$$

and

$$\begin{aligned} U(\mu_{2N,(2)}) - U(\nu) &= \int_{\mathbb{R}^d} \frac{\delta U}{\delta m}(\nu)(\mathbf{y}) (\mu_{2N,(2)} - \nu)(d\mathbf{y}) \\ &+ \int_0^1 (1-t) \left[\int_{\mathbb{R}^{2d}} \frac{\delta^2 U}{\delta m^2}(m_t^{2N,(2)})(\mathbf{y}) (\mu_{2N,(2)} - \nu)^{\otimes 2}(d\mathbf{y}) \right] dt. \end{aligned} \quad (5.2.23)$$

Computing the difference of (5.2.21) with the arithmetic average of (5.2.22) and (5.2.23) gives

$$\begin{aligned} &U(\mu_{2N}) - \frac{1}{2}(U(\mu_{2N,(1)}) + U(\mu_{2N,(2)})) \\ &= \int_0^1 (1-t) \left[\int_{\mathbb{R}^{2d}} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(\mathbf{y}) (\mu_{2N} - \nu)^{\otimes 2}(d\mathbf{y}) \right] dt \\ &\quad - \frac{1}{2} \int_0^1 (1-t) \left[\int_{\mathbb{R}^{2d}} \frac{\delta^2 U}{\delta m^2}(m_t^{2N,(1)})(\mathbf{y}) (\mu_{2N,(1)} - \nu)^{\otimes 2}(d\mathbf{y}) \right] dt \\ &\quad - \frac{1}{2} \int_0^1 (1-t) \left[\int_{\mathbb{R}^{2d}} \frac{\delta^2 U}{\delta m^2}(m_t^{2N,(2)})(\mathbf{y}) (\mu_{2N,(2)} - \nu)^{\otimes 2}(d\mathbf{y}) \right] dt. \end{aligned} \quad (5.2.24)$$

The rest of the proof is very similar to the proof of Lemma 5.2.2. It suffices to consider only the first term in (5.2.24). The other two terms can be handled in a similar way. We rewrite

$$\begin{aligned} &\int_{\mathbb{R}^{2d}} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(\mathbf{y}) (\mu_{2N} - \nu)^{\otimes 2}(d\mathbf{y}) \\ &= \int_{\mathbb{R}^d} \left[\frac{1}{2N} \sum_{i=1}^{2N} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(\xi_i, y_2) - \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(z, y_2) \nu(dz) \right] (\mu_{2N} - \nu)(dy_2) \\ &= \frac{1}{(2N)^2} \sum_{i,j=1}^{2N} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(\xi_i, \xi_j) - \frac{1}{2N} \sum_{j=1}^{2N} \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(z, \xi_j) \nu(dz) \\ &\quad - \frac{1}{2N} \sum_{i=1}^{2N} \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(\xi_i, z) \nu(dz) + \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(z, z') \nu(dz) \nu(dz') \end{aligned}$$

$$= \frac{1}{(2N)^2} \sum_{i,j=1}^{2N} \varphi_t^{(i,j)}, \quad (5.2.25)$$

where

$$\begin{aligned} \varphi_t^{(i,j)} &:= \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(\xi_i, \xi_j) - \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(z, \xi_j) \nu(dz) \\ &\quad - \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(\xi_i, z) \nu(dz) + \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(z, z') \nu(dz) \nu(dz'). \end{aligned}$$

Next, we observe that

$$\begin{aligned} &\mathbb{E} \left| \frac{1}{(2N)^2} \sum_{i,j=1}^{2N} \varphi_t^{(i,j)} \right|^2 \\ &\lesssim \frac{1}{N^2} + \frac{1}{N^4} \left[\sum_{\substack{i_1, j_1, i_2, j_2 \in \{1, \dots, 2N\} \\ \text{exactly two of } i_1, j_1, i_2, j_2 \text{ are identical}}} \mathbb{E} \left[\varphi_t^{(i_1, j_1)} \varphi_t^{(i_2, j_2)} \right] \right. \\ &\quad \left. + \sum_{\substack{i_1, j_1, i_2, j_2 \in \{1, \dots, 2N\} \\ i_1, j_1, i_2, j_2 \text{ are distinct}}} \mathbb{E} \left[\varphi_t^{(i_1, j_1)} \varphi_t^{(i_2, j_2)} \right] \right]. \end{aligned} \quad (5.2.26)$$

We first consider the case where exactly two of i_1, i_2, j_1, j_2 are identical. Without loss of generality, suppose that $i_1 = i_2$. As in the proof of Lemma 5.2.2, we define

$$\begin{aligned} &\varphi_t^{(i,j), -(i_1, j_1, j_2)} \\ &:= \frac{\delta^2 U}{\delta m^2}(m_t^{2N, -(i_1, j_1, j_2)})(\xi_i, \xi_j) - \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N, -(i_1, j_1, j_2)})(z, \xi_j) \nu(dz) \\ &\quad - \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N, -(i_1, j_1, j_2)})(\xi_i, z) \nu(dz) + \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \frac{\delta^2 U}{\delta m^2}(m_t^{2N, -(i_1, j_1, j_2)})(z, z') \nu(dz) \nu(dz'), \end{aligned} \quad (5.2.27)$$

where

$$m_t^{2N, -(i_1, j_1, j_2)} := (1-t)\nu + t \left[\frac{1}{2N-3} \sum_{\substack{1 \leq \ell \leq 2N \\ \ell \notin \{i_1, j_1, j_2\}}} \delta_{\xi_\ell} \right].$$

By the same argument as in the proof of Lemma 5.2.2, along with the bound on $\frac{\delta^3 U}{\delta m^3}$ in Theorem 3.3.7 (see (5.2.4) for details), we have

$$\mathbb{E} |\varphi_t^{(i,j)} - \varphi_t^{(i,j), -(i_1, j_1, j_2)}|^2 \lesssim \frac{1}{N^2}.$$

Then, we write

$$\begin{aligned} \mathbb{E} \left[\varphi_t^{(i_1, j_1)} \varphi_t^{(i_1, j_2)} \right] &= \mathbb{E} \left[(\varphi_t^{(i_1, j_1)} - \varphi_t^{(i_1, j_1), -(i_1, j_1, j_2)}) (\varphi_t^{(i_1, j_2)} - \varphi_t^{(i_1, j_2), -(i_1, j_1, j_2)}) \right] \\ &\quad + \mathbb{E} \left[(\varphi_t^{(i_1, j_1)} - \varphi_t^{(i_1, j_1), -(i_1, j_1, j_2)}) \varphi_t^{(i_1, j_2), -(i_1, j_1, j_2)} \right] \\ &\quad + \mathbb{E} \left[\varphi_t^{(i_1, j_1), -(i_1, j_1, j_2)} (\varphi_t^{(i_1, j_2)} - \varphi_t^{(i_1, j_2), -(i_1, j_1, j_2)}) \right] \\ &\quad + \mathbb{E} \left[\varphi_t^{(i_1, j_1), -(i_1, j_1, j_2)} \varphi_t^{(i_1, j_2), -(i_1, j_1, j_2)} \right]. \end{aligned}$$

By the Cauchy-Schwarz inequality and the bound on $\frac{\delta^2 U}{\delta m^2}$ in Theorem 3.3.7, the first three terms converge to 0 in the order $O(1/N)$. Let \mathcal{F}^{-i} be the σ -algebra generated by ξ_1, \dots, ξ_N except

ξ_i . Then

$$\mathbb{E}\left[\varphi_t^{(i_1, j_1), -(i_1, j_1, j_2)} \varphi_t^{(i_1, j_2), -(i_1, j_1, j_2)}\right] = \mathbb{E}\left[\varphi_t^{(i_1, j_1), -(i_1, j_1, j_2)} \mathbb{E}\left[\varphi_t^{(i_1, j_2), -(i_1, j_1, j_2)} \middle| \mathcal{F}^{-j_2}\right]\right] = 0.$$

Therefore,

$$\frac{1}{N^4} \sum_{\substack{i_1, j_1, i_2, j_2 \in \{1, \dots, 2N\} \\ \text{exactly two of } i_1, j_1, i_2, j_2 \text{ are identical}}} \mathbb{E}\left[\varphi_t^{(i_1, j_1)} \varphi_t^{(i_2, j_2)}\right] \lesssim \frac{1}{N^2}. \quad (5.2.28)$$

Finally, we consider the case where i_1, j_1, i_2, j_2 are mutually distinct. We define $\varphi_t^{(i, j), -(i_1, j_1, i_2, j_2)}$ analogously, as the definition of $\varphi_t^{(i, j), -(i_1, j_1, j_2)}$ in (5.2.27). As above, we write

$$\begin{aligned} \mathbb{E}\left[\varphi_t^{(i_1, j_1)} \varphi_t^{(i_2, j_2)}\right] &= \mathbb{E}\left[\left(\varphi_t^{(i_1, j_1)} - \varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)}\right) \left(\varphi_t^{(i_2, j_2)} - \varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)}\right)\right] \\ &\quad + \mathbb{E}\left[\left(\varphi_t^{(i_1, j_1)} - \varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)}\right) \varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)}\right] \\ &\quad + \mathbb{E}\left[\varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)} \left(\varphi_t^{(i_2, j_2)} - \varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)}\right)\right] \\ &\quad + \mathbb{E}\left[\varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)} \varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)}\right]. \end{aligned}$$

As before, we have

$$\mathbb{E}|\varphi_t^{(i, j)} - \varphi_t^{(i, j), -(i_1, j_1, i_2, j_2)}|^2 \lesssim \frac{1}{N^2}$$

and hence

$$\mathbb{E}\left|\left(\varphi_t^{(i_1, j_1)} - \varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)}\right) \left(\varphi_t^{(i_2, j_2)} - \varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)}\right)\right| \lesssim \frac{1}{N^2}, \quad (5.2.29)$$

by the Cauchy-Schwarz inequality. By the same argument as in the proof of Lemma 5.2.2 through considering the fourth order linear functional derivative of U , along with the bound on $\frac{\delta^4 U}{\delta m^4}$ in Theorem 3.3.7 (see (5.2.11) and (5.2.12) for details), we obtain that

$$\begin{aligned} &\varphi_t^{(i_1, j_1)} - \varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)} \\ &= F_1((\xi_r)_{r \neq i_1, j_1, i_2, j_2}, \xi_{i_1}, \xi_{j_1}, \xi_{i_2}) + F_2((\xi_r)_{r \neq i_1, j_1, i_2, j_2}, \xi_{i_1}, \xi_{j_1}, \xi_{j_2}) + \tilde{\varepsilon}_N^{(i_1, j_1), -(i_1, j_1, i_2, j_2)}, \end{aligned}$$

for some measurable functions $F_1, F_2 : (\mathbb{R}^d)^{2N-1} \rightarrow \mathbb{R}$, where

$$\mathbb{E}\left|\tilde{\varepsilon}_N^{(i_1, j_1), -(i_1, j_1, i_2, j_2)}\right|^2 \lesssim \frac{1}{N^4}.$$

By a similar conditioning argument as the proof of Lemma 5.2.2,

$$\begin{aligned} &\mathbb{E}\left[\left(\varphi_t^{(i_1, j_1)} - \varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)} - \tilde{\varepsilon}_N^{(i_1, j_1), -(i_1, j_1, i_2, j_2)}\right) \varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)}\right] \\ &= \mathbb{E}\left[F_1((\xi_r)_{r \neq i_1, j_1, i_2, j_2}, \xi_{i_1}, \xi_{j_1}, \xi_{i_2}) \mathbb{E}\left[\varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)} \middle| \mathcal{F}^{-j_2}\right]\right] \\ &\quad + \mathbb{E}\left[F_2((\xi_r)_{r \neq i_1, j_1, i_2, j_2}, \xi_{i_1}, \xi_{j_1}, \xi_{j_2}) \mathbb{E}\left[\varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)} \middle| \mathcal{F}^{-i_2}\right]\right] = 0, \end{aligned}$$

which implies, by the Cauchy-Schwarz inequality and the bound on $\frac{\delta^2 U}{\delta m^2}$ in Theorem 3.3.7, that

$$\mathbb{E}\left|\left(\varphi_t^{(i_1, j_1)} - \varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)}\right) \varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)}\right| \lesssim \frac{1}{N^2}. \quad (5.2.30)$$

Similarly,

$$\mathbb{E}\left|\varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)} \left(\varphi_t^{(i_2, j_2)} - \varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)}\right)\right| \lesssim \frac{1}{N^2}. \quad (5.2.31)$$

By the same conditioning argument,

$$\mathbb{E}\left[\varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)} \varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)}\right] = \mathbb{E}\left[\varphi_t^{(i_1, j_1), -(i_1, j_1, i_2, j_2)} \mathbb{E}\left[\varphi_t^{(i_2, j_2), -(i_1, j_1, i_2, j_2)} \middle| \mathcal{F}^{-i_2}\right]\right] = 0. \quad (5.2.32)$$

A combination of (5.2.29), (5.2.30), (5.2.31) and (5.2.32) implies that

$$\frac{1}{N^4} \sum_{\substack{i_1, j_1, i_2, j_2 \in \{1, \dots, 2N\} \\ i_1, j_1, i_2, j_2 \text{ are distinct}}} \mathbb{E}\left[\varphi_t^{(i_1, j_1)} \varphi_t^{(i_2, j_2)}\right] \lesssim \frac{1}{N^2}. \quad (5.2.33)$$

Finally, a combination of (5.2.25), (5.2.26), (5.2.28) and (5.2.33) implies that

$$\mathbb{E}\left|\int_{\mathbb{R}^{2d}} \frac{\delta^2 U}{\delta m^2}(m_t^{2N})(\mathbf{y}) (\mu_{2N} - \nu)^{\otimes 2}(d\mathbf{y})\right|^2 \lesssim \frac{1}{N^2}.$$

□

5.3 Antithetic MLMC without time discretisation

We begin this section by elaborating on the idea of multilevel Monte-Carlo simulation that is discussed in Section 5.1. As outlined in the introduction, we want to estimate the quantity $\Phi(\mu_T^X)$. In contrast to direct Monte-Carlo simulations, we sample not just from one approximation $\mathbb{E}[\Phi(\mu_T^{Y, N})]$, but from different approximations $\mathbb{E}[\Phi(\mu_T^{Y, N_\ell})]$, over levels $\ell \in \{0, \dots, L\}$. By the linearity of expectation,

$$\mathbb{E}[\Phi(\mu_T^{Y, N_L})] = \mathbb{E}[\Phi(\mu_T^{Y, N_0})] + \sum_{\ell=1}^L (\mathbb{E}[\Phi(\mu_T^{Y, N_\ell})] - \mathbb{E}[\Phi(\mu_T^{Y, N_{\ell-1}})]).$$

Hence, the expectation on the finest level is equal to the expectation on the coarsest level, plus a sum of corrections adding the difference in expectation between simulations on consecutive levels. The idea is to independently estimate each of these expectations such that the overall variance is minimised for a fixed computational cost.

For each level ℓ , we approximate $\mathbb{E}[\Phi(\mu_T^{Y, N_\ell})]$ by a standard Monte-Carlo estimator. Subsequently, we combine this approximation with the antithetic trick, which involves estimating the second random variables of the differences in the telescopic sum by the arithmetic average of two sub-particle systems. For simplicity, we set

$$N_\ell := 2^\ell, \quad \ell \in \{0, \dots, L\}.$$

We also set the two sub-particle systems to have the same number of particles. More precisely, we define the pair of sub-particle systems to $\{Y^{i, 2N}\}_{i=1}^{2N}$ as

$$\begin{aligned} Y_t^{i, 2N, (1)} &= \xi_i + \int_0^t b\left(Y_r^{i, 2N, (1)}, \mu_r^{Y, 2N, (1)}\right) dr + \int_0^t \sigma\left(Y_r^{i, 2N, (1)}, \mu_r^{Y, 2N, (1)}\right) dW_r^i, \quad 1 \leq i \leq N, \\ Y_t^{i, 2N, (2)} &= \xi_i + \int_0^t b\left(Y_r^{i, 2N, (2)}, \mu_r^{Y, 2N, (2)}\right) dr + \int_0^t \sigma\left(Y_r^{i, 2N, (2)}, \mu_r^{Y, 2N, (2)}\right) dW_r^i, \quad N+1 \leq i \leq 2N, \end{aligned}$$

where

$$\mu_r^{Y, 2N, (1)} := \frac{1}{N} \sum_{i=1}^N \delta_{Y_r^{i, 2N, (1)}} \quad \text{and} \quad \mu_r^{Y, 2N, (2)} := \frac{1}{N} \sum_{i=N+1}^{2N} \delta_{Y_r^{i, 2N, (2)}}. \quad (5.3.1)$$

Therefore, we define the theoretical MLMC estimator (without time discretisation) as

$$\mathcal{A}^{\text{Theo.}} := \frac{1}{M_0} \sum_{\theta=1}^{M_0} \Phi(\mu_T^{Y, N_0, (\theta), (0)})$$

$$+ \sum_{\ell=1}^L \left[\frac{1}{M_\ell} \sum_{\theta=1}^{M_\ell} \left[\Phi(\mu_T^{Y, N_\ell, (\theta), (\ell)}) - \frac{1}{2} \left(\Phi(\mu_T^{Y, N_\ell, (1), (\theta), (\ell)}) + \Phi(\mu_T^{Y, N_\ell, (2), (\theta), (\ell)}) \right) \right] \right], \quad (5.3.2)$$

where $\mu_T^{Y, N_\ell, (\theta), (\ell)}$, $\mu_T^{Y, N_\ell, (1), (\theta), (\ell)}$ and $\mu_T^{Y, N_\ell, (2), (\theta), (\ell)}$ are defined similarly as μ_T^{Y, N_ℓ} , $\mu_T^{Y, N_\ell, (1)}$ and $\mu_T^{Y, N_\ell, (2)}$ respectively, but correspond to the $\sum_{\ell=0}^L M_\ell$ independent clouds of particles indexed by $\ell \in \{0, \dots, L\}$ and $\theta \in \{1, \dots, M_\ell\}$. Each cloud (indexed by ℓ, θ) has particles with initial conditions $\xi_{i, \ell, \theta}$, $i \in \{1, \dots, N_\ell\}$, driven by Brownian motions $W^{i, \ell, \theta}$, $i \in \{1, \dots, N_\ell\}$, where $\{\xi_{i, \ell, \theta}\}$ and $\{W^{i, \ell, \theta}\}$ are independent over i, ℓ and θ .

The following theorem states that the variance of the antithetic difference in (5.3.2) converges in N in the rate $O(1/N^2)$. In the proof, Proposition 5.2.4 and Theorem 5.2.5 provide us with the necessary estimates when we revert to the mean-field limit.

Theorem 5.3.1 (Variance of antithetic difference). *Assume (Int). Suppose that $b, \sigma \in \mathcal{M}_4(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$. Then*

$$\begin{aligned} & \text{Var} \left[\Phi(\mu_T^{Y, 2N}) - \frac{1}{2} \left(\Phi(\mu_T^{Y, 2N, (1)}) + \Phi(\mu_T^{Y, 2N, (2)}) \right) \right] \\ & \leq \mathbb{E} \left| \Phi(\mu_T^{Y, 2N}) - \frac{1}{2} \left(\Phi(\mu_T^{Y, 2N, (1)}) + \Phi(\mu_T^{Y, 2N, (2)}) \right) \right|^2 \leq \frac{C}{N^2}, \end{aligned}$$

where C is a constant that depends on Φ, b, σ and T , but does not depend on N .

Proof. Let \mathcal{V} be defined by (3.5.1), where t is set to be T . By Lemma 4.2.5, we have

$$\begin{aligned} \Phi(\mu_T^{Y, N}) - \Phi(\mu_T^X) &= (\mathcal{V}(T, \mu_T^{Y, N}) - \mathcal{V}(0, \mu_0^{Y, N})) + (\mathcal{V}(0, \mu_0^{Y, N}) - \mathcal{V}(0, \nu)) \\ &= (\mathcal{V}(0, \mu_0^{Y, N}) - \mathcal{V}(0, \nu)) \\ &\quad + \int_0^T \frac{1}{2} \left[\frac{1}{N^2} \sum_{i=1}^N \text{Tr} \left(a(Y_s^{i, N}, \mu_s^{Y, N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y, N})(Y_s^{i, N}, Y_s^{i, N}) \right) \right] ds \\ &\quad + \frac{1}{N} \sum_{i=1}^N \int_0^T \sigma(Y_s^{i, N}, \mu_s^{Y, N})^T \partial_\mu \mathcal{V}(s, \mu_s^{Y, N})(Y_s^{i, N}) \cdot dW_s^i. \end{aligned} \quad (5.3.3)$$

Hence,

$$\Phi(\mu_T^{Y, 2N}) - \frac{1}{2} \left(\Phi(\mu_T^{Y, 2N, (1)}) + \Phi(\mu_T^{Y, 2N, (2)}) \right) = \mathcal{A} + \mathcal{D} + \mathcal{S},$$

where

$$\mathcal{A} := \mathcal{V}(0, \mu_0^{Y, 2N}) - \frac{1}{2} \left(\mathcal{V}(0, \mu_0^{Y, 2N, (1)}) + \mathcal{V}(0, \mu_0^{Y, 2N, (2)}) \right),$$

$$\begin{aligned} \mathcal{D} &:= \int_0^T \frac{1}{2} \left[\frac{1}{(2N)^2} \sum_{i=1}^{2N} \text{Tr} \left(a(Y_s^{i, 2N}, \mu_s^{Y, 2N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y, 2N})(Y_s^{i, 2N}, Y_s^{i, 2N}) \right) \right] \\ &\quad - \frac{1}{2N^2} \left[\sum_{i=1}^N \text{Tr} \left(a(Y_s^{i, 2N, (1)}, \mu_s^{Y, 2N, (1)}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y, 2N, (1)})(Y_s^{i, 2N, (1)}, Y_s^{i, 2N, (1)}) \right) \right] \\ &\quad + \sum_{i=N+1}^{2N} \text{Tr} \left(a(Y_s^{i, 2N, (2)}, \mu_s^{Y, 2N, (2)}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y, 2N, (2)})(Y_s^{i, 2N, (2)}, Y_s^{i, 2N, (2)}) \right) \right] ds \end{aligned}$$

and

$$\mathcal{S} := \sum_{i=1}^{2N} \int_0^T \frac{1}{2N} \partial_\mu \mathcal{V}(s, \mu_s^{Y, 2N})(Y_s^{i, 2N})^T \sigma(Y_s^{i, 2N}, \mu_s^{Y, 2N}) dW_s^i$$

$$\begin{aligned}
& -\frac{1}{2N} \left(\sum_{i=1}^N \int_0^T \partial_\mu \mathcal{V}(\mu_s^{Y_s^{i,2N},(1)}) (Y_s^{i,2N,(1)})^T \sigma(Y_s^{i,2N,(1)}, \mu_s^{Y_s^{i,2N},(1)}) dW_s^i \right. \\
& \left. + \sum_{i=N+1}^{2N} \int_0^T \partial_\mu \mathcal{V}(s, \mu_s^{Y_s^{i,2N},(2)}) (Y_s^{i,2N,(2)})^T \sigma(Y_s^{i,2N,(2)}, \mu_s^{Y_s^{i,2N},(2)}) dW_s^i \right).
\end{aligned}$$

By the assumptions on b , σ and Φ , it follows from Theorem 3.5.2 that $\mathcal{V} \in \mathcal{M}_4([0, T] \times \mathcal{P}_2(\mathbb{R}^d))$. We can therefore see that

$$\mathbb{E}[\mathcal{D}^2] \lesssim 1/N^2.$$

In particular, $\mathcal{V}(0, \cdot) \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$. Therefore, by Theorem 5.2.6, we obtain that

$$\mathbb{E}[\mathcal{A}^2] \lesssim 1/N^2.$$

Hence, it remains to show that $\mathbb{E}[\mathcal{S}^2] \lesssim 1/N^2$. Define $\Sigma(t, x, \mu) := \partial_\mu \mathcal{V}(t, \mu)(x)^T \sigma(x, \mu)$. By the independence of the Brownian motions, we first rewrite $\mathbb{E}[\mathcal{S}^2]$ as

$$\begin{aligned}
\mathbb{E}[\mathcal{S}^2] &= \mathbb{E} \left[\left(\frac{1}{2N} \sum_{i=1}^N \int_0^T \Sigma(s, Y_s^{i,2N}, \mu_s^{Y_s^{i,2N}}) - \Sigma(s, Y_s^{i,2N,(1)}, \mu_s^{Y_s^{i,2N,(1)}}) dW_s^i \right)^2 \right] \\
&+ \mathbb{E} \left[\left(\frac{1}{2N} \sum_{i=N+1}^{2N} \int_0^T \Sigma(s, Y_s^{i,2N}, \mu_s^{Y_s^{i,2N}}) - \Sigma(s, Y_s^{i,2N,(2)}, \mu_s^{Y_s^{i,2N,(2)}}) dW_s^i \right)^2 \right].
\end{aligned}$$

Using the independence of the Brownian motions and Itô's isometry,

$$\begin{aligned}
& \mathbb{E} \left[\left(\frac{1}{2N} \sum_{i=1}^N \int_0^T \Sigma(s, Y_s^{i,2N}, \mu_s^{Y_s^{i,2N}}) - \Sigma(s, Y_s^{i,2N,(1)}, \mu_s^{Y_s^{i,2N,(1)}}) dW_s^i \right)^2 \right] \\
&= \frac{1}{4N^2} \sum_{i=1}^N \mathbb{E} \left[\left(\int_0^T \Sigma(s, Y_s^{i,2N}, \mu_s^{Y_s^{i,2N}}) - \Sigma(s, Y_s^{i,2N,(1)}, \mu_s^{Y_s^{i,2N,(1)}}) dW_s^i \right)^2 \right] \\
&= \frac{1}{4N^2} \sum_{i=1}^N \int_0^T \mathbb{E} \left[\left| \Sigma(s, Y_s^{i,2N}, \mu_s^{Y_s^{i,2N}}) - \Sigma(s, Y_s^{i,2N,(1)}, \mu_s^{Y_s^{i,2N,(1)}}) \right|^2 \right] ds.
\end{aligned}$$

Note that $\mathcal{V} \in \mathcal{M}_4([0, T] \times \mathcal{P}_2(\mathbb{R}^d))$. Therefore, $\partial_\mu \mathcal{V}$ is Lipschitz continuous and uniformly bounded. Also, note that σ is Lipschitz continuous. By Theorem 5.2.5,

$$\begin{aligned}
& \sup_{t \in [0, T]} \mathbb{E} \left[\left| \Sigma(t, Y_t^{i,2N}, \mu_t^{Y_t^{i,2N}}) - \Sigma(t, X_t^i, \mu_t^{X_t^{i,2N}}) \right|^2 \right] \\
&= \sup_{t \in [0, T]} \mathbb{E} \left[\left| \partial_\mu \mathcal{V}(t, \mu_t^{Y_t^{i,2N}}) (Y_t^{i,2N})^T \sigma(Y_t^{i,2N}, \mu_t^{Y_t^{i,2N}}) - \partial_\mu \mathcal{V}(t, \mu_t^{X_t^{i,2N}}) (X_t^i)^T \sigma(X_t^i, \mu_t^{X_t^{i,2N}}) \right|^2 \right] \\
&\lesssim \sup_{t \in [0, T]} \mathbb{E} \left[\left| \partial_\mu \mathcal{V}(t, \mu_t^{Y_t^{i,2N}}) (Y_t^{i,2N})^T (\sigma(Y_t^{i,2N}, \mu_t^{Y_t^{i,2N}}) - \sigma(X_t^i, \mu_t^{X_t^{i,2N}})) \right|^2 \right] \\
&+ \sup_{t \in [0, T]} \mathbb{E} \left[\left| (\partial_\mu \mathcal{V}(t, \mu_t^{Y_t^{i,2N}}) (Y_t^{i,2N})^T - \partial_\mu \mathcal{V}(t, \mu_t^{X_t^{i,2N}}) (X_t^i)^T) \sigma(X_t^i, \mu_t^{X_t^{i,2N}}) \right|^2 \right] \\
&\lesssim \sup_{t \in [0, T]} \mathbb{E} \left[\left| \partial_\mu \mathcal{V}(t, \mu_t^{Y_t^{i,2N}}) (Y_t^{i,2N})^T (\sigma(Y_t^{i,2N}, \mu_t^{Y_t^{i,2N}}) - \sigma(X_t^i, \mu_t^{X_t^{i,2N}})) \right|^2 \right] \\
&+ \sup_{t \in [0, T]} \left(\mathbb{E} \left[\left| (\partial_\mu \mathcal{V}(t, \mu_t^{Y_t^{i,2N}}) (Y_t^{i,2N}) - \partial_\mu \mathcal{V}(t, \mu_t^{X_t^{i,2N}}) (X_t^i)) \right|^4 \right] \right)^{1/2} \left(\mathbb{E} \left[\left| \sigma(X_t^i, \mu_t^{X_t^{i,2N}}) \right|^4 \right] \right)^{1/2} \\
&\lesssim \sup_{t \in [0, T]} \mathbb{E} \left[\left| Y_t^{i,2N} - X_t^i \right|^2 \right] + \frac{1}{2N} \sum_{j=1}^{2N} \sup_{t \in [0, T]} \mathbb{E} \left[\left| Y_t^{j,2N} - X_t^j \right|^2 \right] \\
&+ \left(\sup_{t \in [0, T]} \mathbb{E} \left[\left| Y_t^{i,2N} - X_t^i \right|^4 \right] \right)^{1/2} + \left(\frac{1}{2N} \sum_{j=1}^{2N} \sup_{t \in [0, T]} \mathbb{E} \left[\left| Y_t^{j,2N} - X_t^j \right|^4 \right] \right)^{1/2} \lesssim \frac{1}{N}. \quad (5.3.4)
\end{aligned}$$

Similarly, we can show that

$$\sup_{t \in [0, T]} \mathbb{E} \left[\left| \Sigma(t, Y_t^{i, 2N, (1)}, \mu_t^{Y, 2N, (1)}) - \Sigma(t, X_t^i, \mu_t^{X, N}) \right|^2 \right] \lesssim \frac{1}{N}. \quad (5.3.5)$$

Next, we apply Proposition 5.2.4 to σ and $\partial_\mu \mathcal{V}(t, \cdot)(\cdot)$. (Note that the constant C in Proposition 5.2.4 corresponding to $\varphi = \partial_\mu \mathcal{V}(t, \cdot)(\cdot)$ does not depend on time, since the first, second and third order derivatives in measure of this function are uniformly bounded in time.) By a similar calculation as (5.3.4), we obtain that

$$\begin{aligned} & \sup_{t \in [0, T]} \mathbb{E} \left[\left| \Sigma(t, X_t^i, \mu_t^{X, 2N}) - \Sigma(t, X_t^i, \mu_t^X) \right|^2 \right] \\ \lesssim & \sup_{t \in [0, T]} \mathbb{E} \left[\left| \partial_\mu \mathcal{V}(t, \mu_t^{X, 2N})(X_t^i)^T (\sigma(X_t^i, \mu_t^{X, 2N}) - \sigma(X_t^i, \mu_t^X)) \right|^2 \right] \\ & + \sup_{t \in [0, T]} \left(\mathbb{E} \left[\left| (\partial_\mu \mathcal{V}(t, \mu_t^{X, 2N})(X_t^i) - \partial_\mu \mathcal{V}(t, \mu_t^X)(X_t^i)) \right|^4 \right] \right)^{1/2} \left(\mathbb{E} \left[\left| \sigma(X_t^i, \mu_t^X) \right|^4 \right] \right)^{1/2} \lesssim \frac{1}{N}. \end{aligned} \quad (5.3.6)$$

Similarly,

$$\sup_{t \in [0, T]} \mathbb{E} \left[\left| \Sigma(t, X_t^i, \mu_t^{X, N}) - \Sigma(t, X_t^i, \mu_t^X) \right|^2 \right] \lesssim \frac{1}{N}. \quad (5.3.7)$$

A combination of (5.3.4), (5.3.5), (5.3.6) and (5.3.7) gives

$$\mathbb{E} \left[\left(\frac{1}{2N} \sum_{i=1}^N \int_0^T \Sigma(s, Y_s^{i, 2N}, \mu_s^{Y, 2N}) - \Sigma(s, Y_s^{i, 2N, (1)}, \mu_s^{Y, 2N, (1)}) dW_s^i \right)^2 \right] \lesssim \frac{1}{N^2}.$$

Similarly,

$$\mathbb{E} \left[\left(\frac{1}{2N} \sum_{i=N+1}^{2N} \int_0^T \Sigma(s, Y_s^{i, 2N}, \mu_s^{Y, 2N}) - \Sigma(s, Y_s^{i, 2N, (2)}, \mu_s^{Y, 2N, (2)}) dW_s^i \right)^2 \right] \lesssim \frac{1}{N^2}.$$

Consequently, $\mathbb{E}[\mathcal{L}^2] \lesssim \frac{1}{N^2}$. \square

We now perform an analysis on the order of interactions of this algorithm by assuming that b and σ are of the forms (4.1.1) and (4.1.2) respectively. Recall that, by Theorem 4.3.3,

$$|\mathbb{E}[\Phi(\mu_T^{Y, N_\ell})] - \Phi(\mu_T^X)| \leq \frac{C}{N_\ell}. \quad (i)$$

Moreover, by Theorem 5.3.1, we have

$$\text{Var} \left[\Phi(\mu_T^{Y, N_\ell, (\theta), (\ell)}) - \frac{1}{2} \left(\Phi(\mu_T^{Y, N_\ell, (1), (\theta), (\ell)}) + \Phi(\mu_T^{Y, N_\ell, (2), (\theta), (\ell)}) \right) \right] \leq \frac{C}{N_\ell^2}. \quad (ii)$$

By Definition 4.1.1, the order of interactions of the antithetic difference is bounded by

$$\text{Order of interactions} \left[\Phi(\mu_T^{Y, N_\ell, (\theta), (\ell)}) - \frac{1}{2} \left(\Phi(\mu_T^{Y, N_\ell, (1), (\theta), (\ell)}) + \Phi(\mu_T^{Y, N_\ell, (2), (\theta), (\ell)}) \right) \right] \leq CN_\ell^{p+1}. \quad (iii)$$

Properties (i) to (iii) allow us to conclude the order of interactions of the theoretical antithetic MLMC estimator.

Theorem 5.3.2 (Order of interactions of theoretical antithetic MLMC). *Assume (Int). Suppose that b and σ are of the forms (4.1.1) and (4.1.2) respectively. Furthermore, suppose that $b, \sigma \in \mathcal{M}_4(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$. Then there exist constants $C_1, C_2 > 0$ such that for any $\epsilon < e^{-1}$, there exist a value L and a sequence $\{M_\ell\}_{\ell=0}^L$ such that the mean-square error of*

$\mathcal{A}^{Theo.}$ is bounded by

$$\mathbb{E}[(\mathcal{A}^{Theo.} - \Phi(\mu_T^X))^2] \leq C_1 \epsilon^2$$

and the order of interactions of $\mathcal{A}^{Theo.}$ is bounded by

$$\text{Order of interactions } (\mathcal{A}^{Theo.}) \leq \begin{cases} C_2 \epsilon^{-2} (\log \epsilon)^2, & p = 1, \\ C_2 \epsilon^{-1-p}, & p > 1. \end{cases}$$

Proof. The proof of this theorem is almost identical to the proof of Theorem 1 in [18] and is therefore omitted. Nonetheless, the proof for the complexity of the antithetic MLMC estimator with time discretisation (Theorem 5.4.4) will be presented in detail for completeness. \square

5.4 Antithetic MLMC with Euler time discretisation

In this section, we construct an MLMC estimator in the same way as the previous section, but with time discretisation. We set

$$N_\ell := 2^\ell, \quad h_\ell := \frac{T}{N_\ell}, \quad \ell \in \{0, \dots, L\}.$$

We also set the two sub-particle systems to have the same number of particles. We define the pair of sub-particle systems to $\{Z^{i,2N,h}\}_{i=1}^{2N}$ as

$$\begin{aligned} Z_t^{i,2N,(1),h} &= \xi_i + \int_0^t b\left(Z_{\eta(r)}^{i,2N,(1),h}, \mu_{\eta(r)}^{Z,2N,(1),h}\right) dr + \int_0^t \sigma\left(Z_{\eta(r)}^{i,2N,(1),h}, \mu_{\eta(r)}^{Z,2N,(1),h}\right) dW_r^i, \\ & \qquad \qquad \qquad 1 \leq i \leq N, \\ Z_t^{i,2N,(2),h} &= \xi_i + \int_0^t b\left(Z_{\eta(r)}^{i,2N,(2),h}, \mu_{\eta(r)}^{Z,2N,(2),h}\right) dr + \int_0^t \sigma\left(Z_{\eta(r)}^{i,2N,(2),h}, \mu_{\eta(r)}^{Z,2N,(2),h}\right) dW_r^i, \\ & \qquad \qquad \qquad N+1 \leq i \leq 2N, \end{aligned}$$

where

$$\mu_r^{Z,2N,(1),h} := \frac{1}{N} \sum_{i=1}^N \delta_{Z_r^{i,2N,(1),h}} \quad \text{and} \quad \mu_r^{Z,2N,(2),h} := \frac{1}{N} \sum_{i=N+1}^{2N} \delta_{Z_r^{i,2N,(2),h}}.$$

Therefore, we define the MLMC estimator with time discretisation as

$$\begin{aligned} \mathcal{A} &:= \frac{1}{M_0} \sum_{\theta=1}^{M_0} \Phi(\mu_T^{Z, N_0, h_0, (\theta), (0)}) \\ &+ \sum_{\ell=1}^L \left[\frac{1}{M_\ell} \sum_{\theta=1}^{M_\ell} \left[\Phi(\mu_T^{Z, N_\ell, h_\ell, (\theta), (\ell)}) - \frac{1}{2} \left(\Phi(\mu_T^{Z, N_\ell, (1), 2h_\ell, (\theta), (\ell)}) + \Phi(\mu_T^{Z, N_\ell, (2), 2h_\ell, (\theta), (\ell)}) \right) \right] \right], \end{aligned} \tag{5.4.1}$$

where $\mu_T^{Z, N_\ell, h_\ell, (\theta), (\ell)}$, $\mu_T^{Z, N_\ell, (1), 2h_\ell, (\theta), (\ell)}$ and $\mu_T^{Z, N_\ell, (2), 2h_\ell, (\theta), (\ell)}$ are defined similarly as $\mu_T^{Z, N_\ell, h_\ell}$, $\mu_T^{Z, N_\ell, (1), 2h_\ell}$ and $\mu_T^{Z, N_\ell, (2), 2h_\ell}$ respectively, but correspond to the $\sum_{\ell=0}^L M_\ell$ independent clouds of particles indexed by $\ell \in \{0, \dots, L\}$ and $\theta \in \{1, \dots, M_\ell\}$. Each cloud (indexed by ℓ, θ) has particles with initial conditions $\xi_{i,\ell,\theta}$, $i \in \{1, \dots, N_\ell\}$, driven by Brownian motions $W^{i,\ell,\theta}$, $i \in \{1, \dots, N_\ell\}$, where $\{\xi_{i,\ell,\theta}\}$ and $\{W^{i,\ell,\theta}\}$ are independent over i, ℓ and θ .

First, we prove the analogue of (i) under time discretisation. Note that, under (Lip), it follows by a standard Gronwall-type argument that

$$\sup_{N \in \mathbb{N}} \sup_{u \in [0, T]} \mathbb{E} \left[\frac{1}{N} \sum_{i=1}^N |Y_u^{i,N}|^2 \right] < +\infty, \quad \sup_{N \in \mathbb{N}} \sup_{u \in [0, T]} \mathbb{E} \left[\frac{1}{N} \sum_{i=1}^N |Z_{\eta(u)}^{i,N,h}|^2 \right] < +\infty, \tag{5.4.2}$$

for some $C > 0$.

Theorem 5.4.1. *Suppose that $b, \sigma \in \mathcal{M}_2(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and $\Phi \in \mathcal{M}_2(\mathcal{P}_2(\mathbb{R}^d))$. Then the weak error in the particle approximation with Euler scheme satisfies*

$$\left| \mathbb{E}[\Phi(\mu_T^{Z,N,h})] - \Phi(\mu_T^X) \right| \leq C \left(\frac{1}{N} + h \right), \quad (5.4.3)$$

where C is a constant that depends on Φ, b, σ and T , but does not depend on N or h .

Proof. Let \mathcal{V} be defined by (3.5.1), where t is set to be T . Let $\mathbf{Z}^{N,h} := (Z^{1,N,h}, \dots, Z^{N,N,h})$. As before, by Theorem 4.2.9 and Remark 4.2.8,

$$\left| \mathbb{E}(\mathcal{V}(0, \mu_0^{Z,N,h}) - \mathcal{V}(0, \nu)) \right| \leq \frac{C}{N}. \quad (5.4.4)$$

Next, by the time-discretised analogue of Lemma 4.2.5, we observe that

$$\begin{aligned} & (\Phi(\mu_T^{Z,N,h}) - \Phi(\mu_T^X)) - (\mathcal{V}(0, \mu_0^{Z,N,h}) - \mathcal{V}(0, \nu)) \\ &= \mathcal{V}(T, \mu_T^{Z,N,h}) - \mathcal{V}(0, \mu_0^{Z,N,h}) \\ &= \int_0^T \sum_{i=1}^N \left[\frac{1}{N} \partial_\mu \mathcal{V}(s, \mu_s^{Z,N,h})(Z_s^{i,N,h}) (b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - b(Z_s^{i,N,h}, \mu_s^{Z,N,h})) \right. \\ & \quad \left. + \frac{1}{2} \text{Tr} \left((a(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - a(Z_s^{i,N,h}, \mu_s^{Z,N,h})) \frac{1}{N} \partial_v \partial_\mu \mathcal{V}(s, \mu_s^{Z,N,h})(Z_s^{i,N,h}) \right) \right. \\ & \quad \left. + \frac{1}{2} \text{Tr} \left(a(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) \frac{1}{N^2} \partial_\mu^2 \mathcal{V}(s, \mu_s^{Z,N,h})(Z_s^{i,N,h}, Z_s^{i,N,h}) \right) \right] ds \\ & \quad + \int_0^T \sum_{i=1}^N \frac{1}{N} \partial_\mu \mathcal{V}(s, \mu_s^{Z,N,h})(Z_s^{i,N,h})^T \sigma(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) dW_s^i \\ &= \int_0^T \sum_{i=1}^N \left[\frac{1}{N} \partial_\mu \mathcal{V}(s, \mu_{\eta(s)}^{Z,N,h})(Z_{\eta(s)}^{i,N,h}) (b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - b(Z_s^{i,N,h}, \mu_s^{Z,N,h})) \right. \\ & \quad \left. + \frac{1}{2} \text{Tr} \left((a(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - a(Z_s^{i,N,h}, \mu_s^{Z,N,h})) \frac{1}{N} \partial_v \partial_\mu \mathcal{V}(s, \mu_{\eta(s)}^{Z,N,h})(Z_{\eta(s)}^{i,N,h}) \right) \right. \\ & \quad \left. + \frac{1}{N} \left[(\partial_\mu \mathcal{V}(s, \mu_s^{Z,N,h})(Z_s^{i,N,h}) - \partial_\mu \mathcal{V}(s, \mu_{\eta(s)}^{Z,N,h})(Z_{\eta(s)}^{i,N,h})) \right. \right. \\ & \quad \left. \left. \times (b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - b(Z_s^{i,N,h}, \mu_s^{Z,N,h})) \right] \right. \\ & \quad \left. + \frac{1}{2} \text{Tr} \left((a(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - a(Z_s^{i,N,h}, \mu_s^{Z,N,h})) \frac{1}{N} \left(\partial_v \partial_\mu \mathcal{V}(s, \mu_s^{Z,N,h})(Z_s^{i,N,h}) \right. \right. \right. \\ & \quad \left. \left. \left. - \partial_v \partial_\mu \mathcal{V}(s, \mu_{\eta(s)}^{Z,N,h})(Z_{\eta(s)}^{i,N,h}) \right) \right) \right. \\ & \quad \left. + \frac{1}{2} \text{Tr} \left(a(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) \frac{1}{N^2} \partial_\mu^2 \mathcal{V}(s, \mu_s^{Z,N,h})(Z_s^{i,N,h}, Z_s^{i,N,h}) \right) \right] ds \\ & \quad + \int_0^T \sum_{i=1}^N \frac{1}{N} \partial_\mu \mathcal{V}(s, \mu_s^{Z,N,h})(Z_s^{i,N,h})^T \sigma(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) dW_s^i. \end{aligned} \quad (5.4.5)$$

Let $\{\mathcal{F}_t\}_{t \in [0, T]}$ be the filtration generated by W^1, \dots, W^N . Then, by the Itô's formula, for each $k \in \{1, \dots, d\}$,

$$\begin{aligned} & \mathbb{E} \left[b_k(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - b_k(Z_s^{i,N,h}, \mu_s^{Z,N,h}) \middle| \mathcal{F}_{\eta(s)} \right] \\ &= -\mathbb{E} \left[\int_{\eta(s)}^s \left(\partial_x b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h}) + \frac{1}{N} \partial_\mu b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{i,N,h}) \right) \cdot dZ_r^{i,N,h} \right] \end{aligned}$$

$$\begin{aligned}
& + \sum_{j \neq i} \int_{\eta(s)}^s \frac{1}{N} \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}) \cdot dZ_r^{j,N,h} \\
& + \int_{\eta(s)}^s \text{Tr} \left(\left(\partial_x^2 b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h}) + \frac{2}{N} \partial_x \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{i,N,h}) \right. \right. \\
& + \left. \left. \frac{1}{N} \partial_v \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{i,N,h}) + \frac{1}{N^2} \partial_{\mu}^2 b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{i,N,h}, Z_r^{i,N,h}) \right) d \langle Z^{i,N,h} \rangle_r \right) \\
& + \sum_{j \neq i} \int_{\eta(s)}^s \text{Tr} \left(\left(\frac{1}{N} \partial_v \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}) \right. \right. \\
& + \left. \left. \frac{1}{N^2} \partial_{\mu}^2 b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}, Z_r^{j,N,h}) \right) d \langle Z^{j,N,h} \rangle_r \right) \Big| \mathcal{F}_{\eta(s)} \Big] \\
= & - \mathbb{E} \left[\int_{\eta(s)}^s \sum_{j=1}^N \frac{1}{N} \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}) b(Z_{\eta(r)}^{j,N,h}, \mu_{\eta(r)}^{Z,N,h}) dr \right. \\
& + \int_{\eta(s)}^s \partial_x b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h}) b(Z_{\eta(r)}^{i,N,h}, \mu_{\eta(r)}^{Z,N,h}) dr \\
& + \sum_{j=1}^N \int_{\eta(s)}^s \frac{1}{N} \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h})^T \sigma(Z_{\eta(r)}^{j,N,h}, \mu_{\eta(r)}^{Z,N,h}) dW_r^j \\
& + \frac{1}{N} \int_{\eta(s)}^s \partial_x b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})^T \sigma(Z_{\eta(r)}^{i,N,h}, \mu_{\eta(r)}^{Z,N,h}) dW_r^i \\
& + \sum_{j=1}^N \int_{\eta(s)}^s \text{Tr} \left(\left(\frac{1}{N} \partial_v \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}) \right. \right. \\
& + \left. \left. \frac{1}{N^2} \partial_{\mu}^2 b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}, Z_r^{j,N,h}) \right) a(Z_{\eta(r)}^{j,N,h}, \mu_{\eta(r)}^{Z,N,h}) \right) dr \\
& + \int_{\eta(s)}^s \text{Tr} \left(\left(\partial_x^2 b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h}) + \frac{2}{N} \partial_x \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{i,N,h}) \right) \right. \\
& \left. \times a(Z_{\eta(r)}^{i,N,h}, \mu_{\eta(r)}^{Z,N,h}) \right) dr \Big| \mathcal{F}_{\eta(s)} \Big] \\
= & - \int_{\eta(s)}^s \mathbb{E} \left[\sum_{j=1}^N \frac{1}{N} \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}) b(Z_{\eta(r)}^{j,N,h}, \mu_{\eta(r)}^{Z,N,h}) \right. \\
& + \partial_x b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h}) b(Z_{\eta(r)}^{i,N,h}, \mu_{\eta(r)}^{Z,N,h}) \\
& + \sum_{j=1}^N \text{Tr} \left(\left(\frac{1}{N} \partial_v \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}) \right. \right. \\
& + \left. \left. \frac{1}{N^2} \partial_{\mu}^2 b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}, Z_r^{j,N,h}) \right) a(Z_{\eta(r)}^{j,N,h}, \mu_{\eta(r)}^{Z,N,h}) \right) \\
& + \text{Tr} \left(\left(\partial_x^2 b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h}) + \frac{2}{N} \partial_x \partial_{\mu} b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{i,N,h}) \right) a(Z_{\eta(r)}^{i,N,h}, \mu_{\eta(r)}^{Z,N,h}) \right) \Big| \mathcal{F}_{\eta(s)} \Big] dr. \tag{5.4.6}
\end{aligned}$$

Hence, upon taking expectation, by (5.4.6), the first term of (5.4.5) can be rewritten as

$$\begin{aligned}
& \int_0^T \sum_{i=1}^N \mathbb{E} \left[\frac{1}{N} \partial_{\mu} \mathcal{V}(s, \mu_{\eta(s)}^{Z,N,h})(Z_{\eta(s)}^{i,N,h}) (b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - b(Z_s^{i,N,h}, \mu_s^{Z,N,h})) \right] ds \\
= & \int_0^T \frac{1}{N} \sum_{i=1}^N \sum_{k=1}^d \mathbb{E} \left[\left(\partial_{\mu} \mathcal{V}(s, \mu_{\eta(s)}^{Z,N,h})(Z_{\eta(s)}^{i,N,h}) \right)_k \right]
\end{aligned}$$

$$\begin{aligned}
& \times \mathbb{E} \left[\left(b_k(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - b_k(Z_s^{i,N,h}, \mu_s^{Z,N,h}) \right) \Big| \mathcal{F}_{\eta(s)} \right] ds \\
= & - \int_0^T \int_{\eta(s)}^s \frac{1}{N} \sum_{i=1}^N \sum_{k=1}^d \mathbb{E} \left[\left(\partial_\mu \mathcal{V}(s, \mu_{\eta(s)}^{Z,N,h})(Z_{\eta(s)}^{i,N,h}) \right)_k \times \right. \\
& \left[\sum_{j=1}^N \frac{1}{N} \partial_\mu b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}) b(Z_{\eta(r)}^{j,N,h}, \mu_{\eta(r)}^{Z,N,h}) + \partial_x b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h}) b(Z_{\eta(r)}^{i,N,h}, \mu_{\eta(r)}^{Z,N,h}) \right. \\
& + \sum_{j=1}^N \text{Tr} \left(\left(\frac{1}{N} \partial_v \partial_\mu b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}) \right. \right. \\
& \left. \left. + \frac{1}{N^2} \partial_\mu^2 b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{j,N,h}, Z_r^{j,N,h}) \right) a(Z_{\eta(r)}^{j,N,h}, \mu_{\eta(r)}^{Z,N,h}) \right) \\
& \left. \left. + \text{Tr} \left(\left(\partial_x^2 b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h}) + \frac{2}{N} \partial_x \partial_\mu b_k(Z_r^{i,N,h}, \mu_r^{Z,N,h})(Z_r^{i,N,h}) \right) a(Z_{\eta(r)}^{i,N,h}, \mu_{\eta(r)}^{Z,N,h}) \right) \right] \right] dr ds.
\end{aligned}$$

Finally, by (5.4.2) and the fact that $\mathcal{V} \in \mathcal{M}_2([0, T] \times \mathcal{P}_2(\mathbb{R}^d))$, we have

$$\left| \int_0^T \sum_{i=1}^N \mathbb{E} \left[\frac{1}{N} \partial_\mu \mathcal{V}(s, \mu_{\eta(s)}^{Z,N,h})(Z_{\eta(s)}^{i,N,h}) (b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) - b(Z_s^{i,N,h}, \mu_s^{Z,N,h})) \right] ds \right| \leq Ch.$$

Similarly, upon taking expectation, the second term of (5.4.5) is bounded by Ch and the third and fourth terms of (5.4.5) are also bounded by Ch by the Cauchy-Schwarz inequality. This completes the proof. \square

To prove the analogue of Theorem 5.3.1 with time discretisation, we need the following lemma that provides a strong error bound between the particle system (2.2.4) and the Euler scheme (5.1.1). However, we require a higher-order approximation in time discretisation. Hence, we restrict ourselves to the case of constant diffusion, in order to avoid the complication of introducing the Milstein scheme of time discretisation.

Lemma 5.4.2. *Suppose that $b \in \mathcal{M}_2(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and σ is constant. Then*

$$\sup_{N \in \mathbb{N}} \sup_{s \in [0, T]} \mathbb{E}[W_2(\mu_s^{Y,N}, \mu_s^{Z,N,h})^2] \leq Ch^2,$$

for some constant C that does not depend on h .

Proof. The proof is presented in dimension one, for simplicity of notations. By Itô's formula,

$$(Y_t^{i,N} - Z_t^{i,N,h})^2 = 2 \int_0^t (Y_s^{i,N} - Z_s^{i,N,h}) (b(Y_s^{i,N}, \mu_s^{Y,N}) - b(Z_s^{i,N,h}, \mu_{\eta(s)}^{Z,N,h})) ds.$$

Take $0 \leq t' \leq t \leq T$. Then

$$\begin{aligned}
& \frac{1}{N} \sum_{i=1}^N \mathbb{E}(Y_{t'}^{i,N} - Z_{t'}^{i,N,h})^2 \\
= & \frac{2}{N} \sum_{i=1}^N \mathbb{E} \left[\int_0^{t'} (Y_s^{i,N} - Z_s^{i,N,h}) (b(Y_s^{i,N}, \mu_s^{Y,N}) - b(Z_s^{i,N,h}, \mu_s^{Z,N,h})) ds \right] \\
& + \frac{2}{N} \sum_{i=1}^N \mathbb{E} \left[\int_0^{t'} (Y_s^{i,N} - Z_s^{i,N,h}) (b(Z_s^{i,N,h}, \mu_s^{Z,N,h}) - b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h})) ds \right].
\end{aligned} \tag{5.4.7}$$

We first bound the first term of (5.4.7).

$$\begin{aligned}
& \frac{2}{N} \sum_{i=1}^N \mathbb{E} \left[\int_0^{t'} (Y_s^{i,N} - Z_s^{i,N,h}) (b(Y_s^{i,N}, \mu_s^{Y,N}) - b(Z_s^{i,N,h}, \mu_s^{Z,N,h})) ds \right] \\
& \leq C \mathbb{E} \left[\frac{1}{N} \sum_{i=1}^N \int_0^{t'} |Y_s^{i,N} - Z_s^{i,N,h}| \left(|Y_s^{i,N} - Z_s^{i,N,h}| + \left(\frac{1}{N} \sum_{j=1}^N |Y_s^{i,N} - Z_s^{i,N,h}|^2 \right)^{1/2} \right) ds \right] \\
& \leq \frac{C}{N} \sum_{i=1}^N \int_0^{t'} \mathbb{E} |Y_s^{i,N} - Z_s^{i,N,h}|^2 ds \leq C \int_0^t \sup_{u \in [0,s]} \left[\frac{1}{N} \sum_{i=1}^N \mathbb{E} |Y_u^{i,N} - Z_u^{i,N,h}|^2 \right] ds. \quad (5.4.8)
\end{aligned}$$

To bound the second term of (5.4.7), we proceed as in the proof of Theorem 5.4.1 by applying Itô's formula to the process

$$\left\{ (Y_s^{i,N} - Z_s^{i,N,h}) (b(Z_s^{i,N,h}, \mu_s^{Z,N,h}) - b(Z_{t_0}^{i,N,h}, \mu_{t_0}^{Z,N,h})) \right\}_{s \geq t_0},$$

which gives

$$\begin{aligned}
& (Y_s^{i,N} - Z_s^{i,N,h}) (b(Z_s^{i,N,h}, \mu_s^{Z,N,h}) - b(Z_{t_0}^{i,N,h}, \mu_{t_0}^{Z,N,h})) \\
& = \int_{t_0}^s (b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) - b(Z_{t_0}^{i,N,h}, \mu_{t_0}^{Z,N,h})) d(Y_u^{i,N} - Z_u^{i,N,h}) \\
& \quad + \sum_{j \neq i} \int_{t_0}^s (Y_u^{i,N} - Z_u^{i,N,h}) \left(\frac{1}{N} \partial_\mu b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{j,N,h}) \right) dZ_u^{j,N,h} \\
& \quad + \int_{t_0}^s (Y_u^{i,N} - Z_u^{i,N,h}) \left(\frac{1}{N} \partial_\mu b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{i,N,h}) + \partial_x b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) \right) dZ_u^{i,N,h} \\
& \quad + \frac{1}{2} \sum_{j \neq i} \int_{t_0}^s (Y_u^{i,N} - Z_u^{i,N,h}) \left(\frac{1}{N} \partial_v \partial_\mu b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{j,N,h}) \right) \\
& \quad + \frac{1}{N^2} \partial_\mu^2 b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{j,N,h}, Z_u^{j,N,h}) d \langle Z^{j,N,h} \rangle_u \\
& \quad + \frac{1}{2} \int_{t_0}^s (Y_u^{i,N} - Z_u^{i,N,h}) \left(\frac{1}{N} \partial_v \partial_\mu b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{i,N,h}) \right) \\
& \quad + \frac{1}{N^2} \partial_\mu^2 b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{i,N,h}, Z_u^{i,N,h}) + \frac{2}{N} \partial_x \partial_\mu b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{i,N,h}) \\
& \quad + \partial_x^2 b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) d \langle Z^{i,N,h} \rangle_u.
\end{aligned}$$

Putting $t_0 = \eta(s)$, taking average of i from 1 to N , taking expectation and rewriting terms, we have

$$\frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[(Y_s^{i,N} - Z_s^{i,N,h}) (b(Z_s^{i,N,h}, \mu_s^{Z,N,h}) - b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h})) \right] = \mathcal{I}_1 + \mathcal{I}_2,$$

where

$$\mathcal{I}_1 := \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\int_{\eta(s)}^s (b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) - b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h})) (b(Y_u^{i,N}, \mu_u^{Y,N}) - b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h})) du \right]$$

and

$$\mathcal{I}_2 := \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\int_{\eta(s)}^s (Y_u^{i,N} - Z_u^{i,N,h}) \mathcal{D}_u^i du \right],$$

where

$$\mathcal{D}_u^i := \frac{1}{N} \sum_{j=1}^N \left(\partial_\mu b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{j,N,h}) b(Z_{\eta(u)}^{j,N,h}, \mu_{\eta(u)}^{Z,N,h}) \right)$$

$$\begin{aligned}
& +\partial_x b(Z_u^{i,N,h}, \mu_u^{Z,N,h})b(Z_{\eta(u)}^{i,N,h}, \mu_{\eta(u)}^{Z,N,h}) \\
& +\frac{1}{2}\sigma^2 \sum_{j=1}^N \left(\frac{1}{N^2} \partial_\mu^2 b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{j,N,h}, Z_u^{j,N,h}) + \frac{1}{N} \partial_v \partial_\mu b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{j,N,h}) \right) \\
& +\frac{1}{2}\sigma^2 \left(\frac{2}{N} \partial_x \partial_\mu b(Z_u^{i,N,h}, \mu_u^{Z,N,h})(Z_u^{i,N,h}) + \partial_x^2 b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) \right).
\end{aligned}$$

By the hypothesis on b , all derivatives of b are uniformly bounded. Moreover, by [\(Lip\)](#), b has linear growth in space and measure. Therefore,

$$\frac{1}{N} \sum_{i=1}^N \mathbb{E} |\mathcal{D}_u^i|^2 \leq C \left(1 + \frac{1}{N} \sum_{i=1}^N \mathbb{E} |Z_{\eta(u)}^{i,N,h}|^2 \right).$$

Then, by [\(5.4.2\)](#),

$$\sup_{u \in [0, T]} \left[\frac{1}{N} \sum_{i=1}^N \mathbb{E} |\mathcal{D}_u^i|^2 \right] \leq C.$$

By first applying the Cauchy-Schwarz inequality to the expectation operator and then to the sum,

$$\begin{aligned}
\mathcal{I}_2 & \leq \int_{\eta(s)}^s \left(\frac{1}{N} \sum_{i=1}^N \mathbb{E} |Y_u^{i,N} - Z_u^{i,N,h}|^2 \right)^{1/2} \left(\frac{1}{N} \sum_{i=1}^N \mathbb{E} |\mathcal{D}_u^i|^2 \right)^{1/2} du \\
& \leq C \left(\sup_{u \in [0, s]} \frac{1}{N} \sum_{i=1}^N \mathbb{E} |Y_u^{i,N} - Z_u^{i,N,h}|^2 \right)^{1/2} h \\
& \leq C \left(\frac{1}{2} \sup_{u \in [0, s]} \frac{1}{N} \sum_{i=1}^N \mathbb{E} |Y_u^{i,N} - Z_u^{i,N,h}|^2 + \frac{1}{2} h^2 \right). \tag{5.4.9}
\end{aligned}$$

Next, we rewrite \mathcal{I}_1 as

$$\begin{aligned}
\mathcal{I}_1 & = \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\int_{\eta(s)}^s (b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) - b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h})) (b(Y_u^{i,N}, \mu_u^{Y,N}) - b(Z_u^{i,N,h}, \mu_u^{Z,N,h})) du \right] \\
& + \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\int_{\eta(s)}^s (b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) - b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}))^2 du \right].
\end{aligned}$$

It is clear that

$$\frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\int_{\eta(s)}^s (b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) - b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}))^2 du \right] \leq Ch^2. \tag{5.4.10}$$

By the Cauchy-Schwarz inequality and [\(Lip\)](#), the first term of \mathcal{I}_1 is bounded by

$$\begin{aligned}
& \frac{1}{N} \sum_{i=1}^N \mathbb{E} \left[\int_{\eta(s)}^s (b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) - b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h})) (b(Y_u^{i,N}, \mu_u^{Y,N}) - b(Z_u^{i,N,h}, \mu_u^{Z,N,h})) du \right] \\
& \leq \frac{1}{N} \sum_{i=1}^N \int_{\eta(s)}^s \left(\mathbb{E} \left| b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) - b(Z_{\eta(s)}^{i,N,h}, \mu_{\eta(s)}^{Z,N,h}) \right|^2 \right)^{1/2} \\
& \quad \left(\mathbb{E} \left| b(Y_u^{i,N}, \mu_u^{Y,N}) - b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) \right|^2 \right)^{1/2} du \\
& \leq \frac{1}{N} \sum_{i=1}^N C\sqrt{h} \int_{\eta(s)}^s \left(\mathbb{E} \left| b(Y_u^{i,N}, \mu_u^{Y,N}) - b(Z_u^{i,N,h}, \mu_u^{Z,N,h}) \right|^2 \right)^{1/2} du
\end{aligned}$$

$$\begin{aligned}
&\leq \frac{1}{N} \sum_{i=1}^N C\sqrt{h} \int_{\eta(s)}^s \left(\mathbb{E}|Y_u^{i,N} - Z_u^{i,N,h}|^2 + \frac{1}{N} \sum_{j=1}^N \mathbb{E}|Y_u^{j,N} - Z_u^{j,N,h}|^2 \right)^{1/2} du \\
&\leq \frac{2}{N} \sum_{i=1}^N C\sqrt{h} \int_{\eta(s)}^s (\mathbb{E}|Y_u^{i,N} - Z_u^{i,N,h}|^2)^{1/2} du \\
&\leq 2Ch^{3/2} \left[\sup_{u \in [0,s]} \left(\frac{1}{N} \sum_{i=1}^N \mathbb{E}|Y_u^{i,N} - Z_u^{i,N,h}|^2 \right) \right]^{1/2} \\
&\leq C \left(h^3 + \sup_{u \in [0,s]} \left(\frac{1}{N} \sum_{i=1}^N \mathbb{E}|Y_u^{i,N} - Z_u^{i,N,h}|^2 \right) \right). \tag{5.4.11}
\end{aligned}$$

A combination of (5.4.7), (5.4.8), (5.4.9), (5.4.10) and (5.4.11) gives

$$\sup_{u \in [0,t]} \left[\frac{1}{N} \sum_{i=1}^N \mathbb{E}(Y_u^{i,N} - Z_u^{i,N,h})^2 \right] \leq C \left(\int_0^t \sup_{u \in [0,s]} \left[\frac{1}{N} \sum_{i=1}^N \mathbb{E}|Y_u^{i,N} - Z_u^{i,N,h}|^2 \right] ds + h^2 \right), \quad \forall t \in [0, T],$$

which implies by Gronwall's inequality that

$$\sup_{u \in [0,T]} \left[\frac{1}{N} \sum_{i=1}^N \mathbb{E}(Y_u^{i,N} - Z_u^{i,N,h})^2 \right] \leq Ch^2.$$

Since the constant C does not depend on N , we conclude that

$$\sup_{N \in \mathbb{N}} \sup_{s \in [0,T]} \mathbb{E}[W_2(\mu_s^{Y,N}, \mu_s^{Z,N,h})^2] \leq \sup_{N \in \mathbb{N}} \sup_{s \in [0,T]} \left[\frac{1}{N} \sum_{i=1}^N \mathbb{E}(Y_s^{i,N} - Z_s^{i,N,h})^2 \right] \leq Ch^2.$$

□

A combination of Lemma 5.4.2 and Theorem 5.3.1 immediately gives the following result.

Theorem 5.4.3 (Variance of antithetic difference). *Assume (Int). Suppose that $b \in \mathcal{M}_4(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$. Moreover, suppose that σ is constant. Then*

$$\begin{aligned}
&\text{Var} \left[\Phi(\mu_T^{Z,N,h}) - \frac{1}{2} (\Phi(\mu_T^{Z,N,(1),2h}) + \Phi(\mu_T^{Z,N,(2),2h})) \right] \\
&\leq \mathbb{E} \left| \Phi(\mu_T^{Z,N,h}) - \frac{1}{2} (\Phi(\mu_T^{Z,N,(1),2h}) + \Phi(\mu_T^{Z,N,(2),2h})) \right|^2 \leq C \left(\frac{1}{N^2} + h^2 \right),
\end{aligned}$$

where C is a constant that depends on Φ , b , σ and T , but does not depend on N or h .

As before, we perform an analysis on the complexity of this algorithm by assuming that b is of the form (4.1.1) and that σ is constant. By Theorem 5.4.1, since $h_\ell = \frac{T}{N_\ell}$,

$$|\mathbb{E}[\Phi(\mu_T^{Z,N_\ell,h_\ell})] - \Phi(\mu_T^X)| \leq \frac{C}{N_\ell}. \tag{I}$$

Moreover, by Theorem 5.4.3, we have

$$\text{Var} \left[\Phi(\mu_T^{Z,N_\ell,h_\ell,(\theta),(\ell)}) - \frac{1}{2} (\Phi(\mu_T^{Z,N_\ell,(1),2h_\ell,(\theta),(\ell)}) + \Phi(\mu_T^{Z,N_\ell,(2),2h_\ell,(\theta),(\ell)})) \right] \leq \frac{C}{N_\ell^2}. \tag{II}$$

Finally, by Definition 4.1.1, the complexity of the antithetic difference is bounded by

$$\text{Complexity} \left[\Phi(\mu_T^{Z,N_\ell,h_\ell,(\theta),(\ell)}) - \frac{1}{2} (\Phi(\mu_T^{Z,N_\ell,(1),2h_\ell,(\theta),(\ell)}) + \Phi(\mu_T^{Z,N_\ell,(2),2h_\ell,(\theta),(\ell)})) \right] \leq CN_\ell^{p+2}. \tag{III}$$

Theorem 5.4.4 (Complexity of antithetic MLMC with time discretisation). *Assume (Int). Suppose that b is of the form (4.1.1). Furthermore, suppose that $b \in \mathcal{M}_4(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$, $\Phi \in$*

$\mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$ and σ is constant. Then there exist constants $C_1, C_2 > 0$ such that for any $\epsilon < e^{-1}$, there exist a value L and a sequence $\{M_\ell\}_{\ell=0}^L$ such that the mean-square error of \mathcal{A} is bounded by

$$\mathbb{E}[(\mathcal{A} - \Phi(\mu_T^X))^2] \leq C_1 \epsilon^2$$

and the complexity of \mathcal{A} is bounded by

$$\text{Complexity}(\mathcal{A}) \leq C_2 \epsilon^{-2-p}.$$

Proof. As in Theorem 5.3.2, the proof of this theorem is also almost identical to the proof of Theorem 1 in [18]. Nonetheless, we present the proof with explicit expressions for L and $\{M_\ell\}_{\ell=0}^L$ so that practitioners can implement this algorithm easily. Set

$$L := \lceil \log_2(\sqrt{2}\epsilon^{-1}) \rceil, \quad M_\ell := \lceil 2\epsilon^{-2}2^{pL/2}(1 - 2^{-p/2})^{-1}2^{-(p+4)\ell/2} \rceil, \quad \ell \in \{0, \dots, L\}.$$

As in (5.1.3), we have

$$\text{Mean-square error} = \text{Var}(\mathcal{A}) + (\mathbb{E}(\mathcal{A}) - \Phi(\mu_T^X))^2.$$

By the choice of L , $2^{-L} \leq \frac{\epsilon}{\sqrt{2}}$. Therefore, by Property (I),

$$|\mathbb{E}(\mathcal{A}) - \Phi(\mu_T^X)|^2 = |\mathbb{E}[\Phi(\mu_T^{Z, N_L, h_L})] - \Phi(\mu_T^X)|^2 \leq \left(\frac{C}{N_L}\right)^2 = (C2^{-L})^2 \leq C^2 \left(\frac{\epsilon^2}{2}\right). \quad (5.4.12)$$

On the other hand, by Property (II) and the choice of $\{M_\ell\}_{\ell=0}^L$,

$$\begin{aligned} \text{Var}(\mathcal{A}) &\leq \sum_{\ell=0}^L \frac{1}{M_\ell^2} \left[\sum_{\theta=1}^{M_\ell} \frac{C}{N_\ell^2} \right] \leq \sum_{\ell=0}^L \frac{C}{M_\ell} 2^{-2\ell} \leq \sum_{\ell=0}^L C 2^{-2\ell} \left(2^{-1} \epsilon^2 2^{-pL/2} (1 - 2^{-p/2}) 2^{(p+4)\ell/2} \right) \\ &= C 2^{-1} \epsilon^2 2^{-pL/2} (1 - 2^{-p/2}) \sum_{\ell=0}^L 2^{p\ell/2} \\ &< \frac{1}{2} C \epsilon^2. \end{aligned}$$

This verifies that the mean-square error is bounded by $\frac{1}{2}(C^2 + C)\epsilon^2$. Next, we note that

$$M_\ell \leq 2\epsilon^{-2}2^{pL/2}(1 - 2^{-p/2})^{-1}2^{-(p+4)\ell/2} + 1$$

and hence, by Property (III),

$$\text{Complexity}(\mathcal{A}) \leq C \left(\sum_{\ell=0}^L 2\epsilon^{-2}2^{pL/2}(1 - 2^{-p/2})^{-1}2^{-(p+4)\ell/2}2^{(p+2)\ell} + \sum_{\ell=0}^L 2^{(p+2)\ell} \right). \quad (5.4.13)$$

Note that the choice of L implies that $2^L \leq 2\sqrt{2}\epsilon^{-1}$.

$$\begin{aligned} \sum_{\ell=0}^L 2\epsilon^{-2}2^{pL/2}(1 - 2^{-p/2})^{-1}2^{-(p+4)\ell/2}2^{(p+2)\ell} &= 2\epsilon^{-2}2^{pL/2}(1 - 2^{-p/2})^{-1} \sum_{\ell=0}^L 2^{p\ell/2} \\ &< 2\epsilon^{-2}2^{pL/2}(1 - 2^{-p/2})^{-1} \left(2^{pL/2}(1 - 2^{-p/2})^{-1} \right) \\ &= 2\epsilon^{-2}2^{pL}(1 - 2^{-p/2})^{-2} \\ &\leq 2(2\sqrt{2})^p (1 - 2^{-p/2})^{-2} \epsilon^{-2-p}. \end{aligned} \quad (5.4.14)$$

Similarly,

$$\sum_{\ell=0}^L 2^{(p+2)\ell} \leq \frac{2^{(p+2)L}}{1 - 2^{-(p+2)}} \leq \frac{(2\sqrt{2})^{p+2}}{1 - 2^{-(p+2)}} \epsilon^{-(p+2)}. \quad (5.4.15)$$

A combination of (5.4.13), (5.4.14) and (5.4.15) finally gives

$$\text{Complexity}(\mathcal{A}) \leq C \left(2(2\sqrt{2})^p (1 - 2^{-p/2})^{-2} + \frac{(2\sqrt{2})^{p+2}}{1 - 2^{-(p+2)}} \right) \epsilon^{-2-p}.$$

□

Chapter 6

Higher order approximation and fluctuation of the standard particle system

Until this point, the focus is on approximating McKean-Vlasov SDEs by various methods, such as Romberg extrapolation and multilevel methods. Nonetheless, standard particle systems arise naturally in many PDEs and in the theory of mean-field games. Recalling Example 2 in the introduction, an N -player PDE system is difficult to solve analytically and can be very expensive to approximate numerically if the dimension is large. On the other hand, it can be approximated by the master equation (a “limiting” PDE), which therefore allows us to approximate the Nash equilibrium of the players in the mean-field limit. (See [21] and [22].)

In this section, we focus on the approximation of standard particle systems. Instead of replacing the empirical measure between the law of the evolving process itself, we construct alternative theoretical approximations to the standard particle systems. We divide our discussion into two parts: higher order fluctuation and higher order strong error approximation. Since the constructions corresponding to these approximations are defined in terms of L-derivatives, they are far from being implementable from a practical perspective, but are interesting from a theoretical perspective.

6.1 Higher order fluctuation

In the literature, one often considers the fluctuation of the empirical measure with the limiting law, defined by $S^N := \sqrt{N}(\mu^{Y,N} - \mu^X)$, as N goes to infinity. For every N , S^N is a signed measure. The space of signed measures endowed with the weak convergence topology is a non-metrizable topological space and is therefore not ideal to apply classical tightness arguments to prove convergence. This problem has been addressed by a few papers in the literature. The technique is to show that the sequence of random measures $(S^N)_{N \geq 1}$ converges in law as random variables taking values in some Sobolev space. This is done via a classical tightness argument, which implies the existence of a weak limit (through a subsequence) by the Prokhorov’s theorem. The limit is shown to satisfy an Ornstein-Uhlenbeck process in an appropriate space. In [37], the Sobolev space being considered is $C([0, T], \Phi'_p)$, where Φ'_p is the dual of Φ_p , with Φ_p being the completion of the Schwarz space of rapidly decreasing infinitely differentiable functions under a suitable class of seminorms $\|\cdot\|_p$. This result was generalised in [53] to the Sobolev space $C([0, T], W_0^{-(2+2D), D})$, whereas the limiting Ornstein-Uhlenbeck process is in $C([0, T], W_0^{-(4+2D), D})$, where $D = 1 + \lfloor \frac{d}{2} \rfloor$. A similar result was proven in [21] to include mean-field equations with additive common noise.

We first consider the above fluctuation at time T , but for general functionals of measures (i.e. not necessarily of the form $\mu \mapsto \int_{\mathbb{R}^d} \phi(x) \mu(dx)$). This is an easy consequence in the framework of analysis developed in the previous two chapters.

Theorem 6.1.1. Assume that the initial law $\nu = \delta_c$, for some $c \in \mathbb{R}^d$. Suppose that $b, \sigma \in \mathcal{M}_4(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$. Then, for each $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$, the sequence of random variables

$$\left\{ \sqrt{N} \left(\Phi(\mu_T^{Y,N}) - \Phi(\mu_T^X) \right) \right\}_{N \in \mathbb{N}}$$

converges in law to a centered normal random variable.

Proof. Let \mathcal{V} be defined by (3.5.1), where t is set to be T . By (5.3.3), upon multiplication by \sqrt{N} on both sides, the expression becomes

$$\begin{aligned} \sqrt{N} \left[\Phi(\mu_T^{Y,N}) - \Phi(\mu_T^X) \right] &= \int_0^T \frac{1}{2} \left[\frac{1}{N^{3/2}} \sum_{i=1}^N \text{Tr} \left(a(Y_s^{i,N}, \mu_s^{Y,N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}, Y_s^{i,N}) \right) \right] ds \\ &\quad + \frac{1}{\sqrt{N}} \sum_{i=1}^N \int_0^T \sigma(Y_s^{i,N}, \mu_s^{Y,N})^T \partial_\mu \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}) \cdot dW_s^i \\ &= \int_0^T \frac{1}{2} \left[\frac{1}{N^{3/2}} \sum_{i=1}^N \text{Tr} \left(a(Y_s^{i,N}, \mu_s^{Y,N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}, Y_s^{i,N}) \right) \right] ds \\ &\quad + \left[\frac{1}{\sqrt{N}} \sum_{i=1}^N \int_0^T \sigma(Y_s^{i,N}, \mu_s^{Y,N})^T \partial_\mu \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}) \cdot dW_s^i \right. \\ &\quad \left. - \frac{1}{\sqrt{N}} \sum_{i=1}^N \int_0^T \sigma(X_s^i, \mu_s^X)^T \partial_\mu \mathcal{V}(s, \mu_s^X)(X_s^i) \cdot dW_s^i \right] \\ &\quad + \frac{1}{\sqrt{N}} \sum_{i=1}^N \int_0^T \sigma(X_s^i, \mu_s^X)^T \partial_\mu \mathcal{V}(s, \mu_s^X)(X_s^i) \cdot dW_s^i. \end{aligned} \quad (6.1.1)$$

Since $\mathcal{V} \in \mathcal{M}_2([0, T] \times \mathcal{P}_2(\mathbb{R}^d))$ and σ is Lipschitz continuous,

$$\left\| \int_0^T \frac{1}{2} \left[\frac{1}{N^{3/2}} \sum_{i=1}^N \text{Tr} \left(a(Y_s^{i,N}, \mu_s^{Y,N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}, Y_s^{i,N}) \right) \right] ds \right\|_{L^2} \xrightarrow{N \rightarrow \infty} 0.$$

By (5.3.5) and (5.3.7),

$$\left\| \frac{1}{\sqrt{N}} \sum_{i=1}^N \int_0^T \left[\sigma(Y_s^{i,N}, \mu_s^{Y,N})^T \partial_\mu \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}) - \sigma(X_s^i, \mu_s^X)^T \partial_\mu \mathcal{V}(s, \mu_s^X)(X_s^i) \right] \cdot dW_s^i \right\|_{L^2} \xrightarrow{N \rightarrow \infty} 0.$$

Finally, by the central limit theorem, the final term in (6.1.1) converges in law to $\mathcal{N}(0, R)$, where the variance R is given by

$$R := \int_0^T \mathbb{E} \left| \sigma(X_s^1, \mu_s^X)^T \partial_\mu \mathcal{V}(s, \mu_s^X)(X_s^1) \right|^2 ds.$$

An application of Slutsky's theorem (see, e.g., Theorem 7.34 in [25]) concludes that $\sqrt{N} [\Phi(\mu_T^{Y,N}) - \Phi(\mu_T^X)]$ also converges to $\mathcal{N}(0, R)$ in law. \square

6.1.1 Higher order fluctuation via a correction term

In terms of numerical simulations, at each time t , it is very difficult to simulate the limiting measure μ_t^X directly, as most McKean-Vlasov equations do not have explicit solutions. In order to be able to observe the fluctuation, one typically has to apply a Monte-Carlo procedure to

¹Without this assumption, one would have to deal with the term $\sqrt{N}(\mathcal{V}(0, \mu_0^{Y,N}) - \mathcal{V}(0, \nu))$. However, the convergence of this term in N is not clear, as the central limit theorem is in general not applicable to functions \mathcal{V} with a non-linear dependence on the measure component.

simulate $\Phi(\mu_t^X)$ by its coupling $\Phi(\mu_t^{X,N})$. The following theorem shows that, by adding an extra term that only depends on the path of $\mu^{X,N}$, the fluctuation of $\mu^{X,N}$ with $\mu^{Y,N}$ exhibits higher order behaviour.

Theorem 6.1.2. *Assume (Int). Suppose that $b, \sigma \in \mathcal{M}_4(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$ and $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$. Then there exists a (deterministic) continuous function $\mathcal{S} : [0, T] \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ (defined in (6.1.4)) such that the sequence of random variables*

$$\left\{ N \left(\Phi(\mu_T^{Y,N}) - \left(\Phi(\mu_T^{X,N}) - \int_0^T \mathcal{S}(s, \mu_s^{X,N}) ds \right) \right) \right\}_{N \in \mathbb{N}}$$

converges in law through a subsequence to a centered random variable.

Proof. Let \mathcal{V} be defined by (3.5.1), where t is set to be T . By (5.3.3), upon multiplication by N on both sides, we have

$$\begin{aligned} N \left[\Phi(\mu_T^{Y,N}) - \Phi(\mu_T^X) \right] &= N(\mathcal{V}(0, \mu_0^{Y,N}) - \mathcal{V}(0, \nu)) \\ &+ \int_0^T \frac{1}{2} \left[\frac{1}{N} \sum_{i=1}^N \text{Tr} \left(a(Y_s^{i,N}, \mu_s^{Y,N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}, Y_s^{i,N}) \right) \right] ds \\ &+ \sum_{i=1}^N \int_0^T \sigma(Y_s^{i,N}, \mu_s^{Y,N})^T \partial_\mu \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}) \cdot dW_s^i. \\ &= N \left(\mathcal{V} \left(0, \frac{1}{N} \sum_{i=1}^N \delta_{\xi_i} \right) - \mathcal{V}(0, \nu) \right) \\ &+ \frac{1}{2} \int_0^T \int_{\mathbb{R}^d} \text{Tr} \left(a(x, \mu_s^{Y,N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y,N})(x, x) \right) \mu_s^{Y,N}(dx) ds \\ &+ \sum_{i=1}^N \int_0^T \sigma(Y_s^{i,N}, \mu_s^{Y,N})^T \partial_\mu \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}) \cdot dW_s^i. \end{aligned} \quad (6.1.2)$$

Applying the same argument as (4.2.4), but to the coupled processes X^1, \dots, X^N instead of $Y^{1,N}, \dots, Y^{N,N}$, we have

$$\begin{aligned} &\Phi(\mu_T^{X,N}) - \Phi(\mu_T^X) \\ &= \mathcal{V} \left(0, \frac{1}{N} \sum_{i=1}^N \delta_{\xi_i} \right) - \mathcal{V}(0, \nu) + \int_0^T \partial_s \mathcal{V}(s, \mu_s^{X,N}) + \sum_{i=1}^N \left[\frac{1}{N} \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(X_s^i) b(X_s^i, \mu_s^X) \right. \\ &\quad \left. + \frac{1}{2} \text{Tr} \left(a(X_s^i, \mu_s^X) \left(\frac{1}{N} \partial_v \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(X_s^i) + \frac{1}{N^2} \partial_\mu^2 \mathcal{V}(s, \mu_s^{X,N})(X_s^i, X_s^i) \right) \right) \right] ds \\ &\quad + \frac{1}{N} \sum_{i=1}^N \int_0^T \sigma(X_s^i, \mu_s^X)^T \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(X_s^i) \cdot dW_s^i \\ &= \mathcal{V} \left(0, \frac{1}{N} \sum_{i=1}^N \delta_{\xi_i} \right) - \mathcal{V}(0, \nu) + \int_0^T \partial_s \mathcal{V}(s, \mu_s^{X,N}) + \sum_{i=1}^N \frac{1}{N} \left[\partial_\mu \mathcal{V}(s, \mu_s^{X,N})(X_s^i) b(X_s^i, \mu_s^{X,N}) \right. \\ &\quad \left. + \frac{1}{2} \text{Tr} \left(a(X_s^i, \mu_s^{X,N}) \partial_v \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(X_s^i) \right) \right] ds \\ &\quad + \frac{1}{2N^2} \sum_{i=1}^N \int_0^T \text{Tr} \left(a(X_s^i, \mu_s^X) \partial_\mu^2 \mathcal{V}(s, \mu_s^{X,N})(X_s^i, X_s^i) \right) ds \\ &\quad + \frac{1}{N} \sum_{i=1}^N \int_0^T \sigma(X_s^i, \mu_s^X)^T \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(X_s^i) \cdot dW_s^i \\ &\quad + \int_0^T \int_{\mathbb{R}^d} \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(y) \left(b(y, \mu_s^X) - b(y, \mu_s^{X,N}) \right) \mu_s^{X,N}(dy) ds \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{2} \int_0^T \int_{\mathbb{R}^d} \text{Tr} \left(\partial_v \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(y) \left(a(y, \mu_s^X) - a(y, \mu_s^{X,N}) \right) \right) \mu_s^{X,N}(dy) ds \\
= & \mathcal{V} \left(0, \frac{1}{N} \sum_{i=1}^N \delta_{\xi_i} \right) - \mathcal{V}(0, \nu) + \frac{1}{2N^2} \sum_{i=1}^N \int_0^T \text{Tr} \left(a(X_s^i, \mu_s^X) \partial_\mu^2 \mathcal{V}(s, \mu_s^{X,N})(X_s^i, X_s^i) \right) ds \\
& + \frac{1}{N} \sum_{i=1}^N \int_0^T \sigma(X_s^i, \mu_s^X)^T \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(X_s^i) \cdot dW_s^i \\
& + \int_0^T \int_{\mathbb{R}^d} \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(y) \left(b(y, \mu_s^X) - b(y, \mu_s^{X,N}) \right) \mu_s^{X,N}(dy) ds \\
& + \frac{1}{2} \int_0^T \int_{\mathbb{R}^d} \text{Tr} \left(\partial_v \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(y) \left(a(y, \mu_s^X) - a(y, \mu_s^{X,N}) \right) \right) \mu_s^{X,N}(dy) ds, \tag{6.1.3}
\end{aligned}$$

where PDE (3.4.3) is applied in the last equality. Now, we define a deterministic function $\mathcal{S} : [0, T] \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ by

$$\begin{aligned}
\mathcal{S}(s, \mu) & := \int_{\mathbb{R}^d} \partial_\mu \mathcal{V}(s, \mu)(y) \left(b(y, \mu_s^X) - b(y, \mu) \right) \mu(dy) \\
& \quad - \frac{1}{2} \int_{\mathbb{R}^d} \text{Tr} \left(\partial_v \partial_\mu \mathcal{V}(s, \mu)(y) \left(a(y, \mu_s^X) - a(y, \mu) \right) \right) \mu(dy). \tag{6.1.4}
\end{aligned}$$

Next, we subtract (6.1.2) by (6.1.3) multiplied by N , which gives

$$N \left(\Phi(\mu_T^{Y,N}) - \left(\Phi(\mu_T^{X,N}) - \int_0^T \mathcal{S}(s, \mu_s^{X,N}) ds \right) \right) = E_N^{(1)} + E_N^{(2)},$$

where

$$\begin{aligned}
E_N^{(1)} & = \frac{1}{2N} \sum_{i=1}^N \int_0^T \text{Tr} \left(a(Y_s^{i,N}, \mu_s^{Y,N}) \partial_\mu^2 \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}, Y_s^{i,N}) \right) ds \\
& \quad - \frac{1}{2N} \sum_{i=1}^N \int_0^T \text{Tr} \left(a(X_s^i, \mu_s^X) \partial_\mu^2 \mathcal{V}(s, \mu_s^{X,N})(X_s^i, X_s^i) \right) ds
\end{aligned}$$

and

$$\begin{aligned}
E_N^{(2)} & = \sum_{i=1}^N \int_0^T \left[\sigma(Y_s^{i,N}, \mu_s^{Y,N})^T \partial_\mu \mathcal{V}(s, \mu_s^{Y,N})(Y_s^{i,N}) \right. \\
& \quad \left. - \sigma(X_s^i, \mu_s^X)^T \partial_\mu \mathcal{V}(s, \mu_s^{X,N})(X_s^i) \right] \cdot dW_s^i.
\end{aligned}$$

It follows from the same argument in the proof of Theorem 5.3.1 to deduce that

$$\|E_N^{(1)}\|_{L^1} \xrightarrow{N \rightarrow \infty} 0 \quad \text{and} \quad \sup_{N \in \mathbb{N}} \mathbb{E}|E_N^{(2)}|^2 \leq C, \tag{6.1.5}$$

for some constant $C > 0$. For any $\varepsilon > 0$, by the Chebyshev's inequality,

$$\mathbb{P} \left(|E_N^{(2)}| > \sqrt{\frac{C}{\varepsilon}} \right) \leq \frac{1}{\left(\sqrt{\frac{C}{\varepsilon}} \right)^2} \mathbb{E}|E_N^{(2)}|^2 \leq \varepsilon,$$

for every $N \in \mathbb{N}$. This shows that the set of measures $\{m_N := \mathcal{L}(E_N^{(2)})\}_{N \in \mathbb{N}}$ is tight. By the Prokhorov's theorem, we conclude that $\{m_N\}_{N \in \mathbb{N}}$ converges (through some subsequence $\{N_k\}_{k \in \mathbb{N}}$) to a probability measure m on \mathbb{R}^d . By the Skorokhod's representation theorem (see [60]), there exist a probability space $(\tilde{\Omega}, \tilde{\mathcal{F}}, \tilde{\mathbb{P}})$ and a sequence of measurable random variables $\{\eta_{N_k}\}_{k \in \mathbb{N}}$ such that η_{N_k} converges to η almost surely as $k \rightarrow \infty$, where $\mathcal{L}(\eta_{N_k}) = m_{N_k}$ and

$\mathcal{L}(\eta) = m$. By the second inequality in (6.1.5), we observe that $\{\eta_{N_k}\}_{k \in \mathbb{N}}$ is uniformly bounded in L^2 . Hence, η_{N_k} converges to η in L^1 , which implies that

$$\tilde{\mathbb{E}}[\eta] = \lim_{k \rightarrow \infty} \tilde{\mathbb{E}}[\eta_{N_k}] = 0. \quad (6.1.6)$$

Since the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ is atomless, we can construct an \mathbb{R}^d -valued random variable M on $(\Omega, \mathcal{F}, \mathbb{P})$ with probability distribution m . Moreover, M is centered, by (6.1.6). An application of Slutsky's theorem concludes that $E_N^{(1)} + E_N^{(2)}$ also converges to M in law through a subsequence. \square

6.1.2 Higher order fluctuation via common noise

Inspired by the idea in [12] of introducing space-time white noise for interacting diffusion processes, we introduce an alternative coupled McKean-Vlasov equation (X^1, \dots, X^N, C^N) , given by

$$\begin{cases} X_t^i = \xi_i + \int_0^t b(X_s^i, \mu_s^X) ds + \int_0^t \sigma(X_s^i, \mu_s^X) dW_s^i, & t \in [0, T], \quad 1 \leq i \leq N, \\ C_t^N = \theta + \int_0^t b(C_s^N, \mu_s^{C,N}) ds + \int_0^t \sigma(C_s^N, \mu_s^{C,N}) dW_s + \frac{1}{\sqrt{N}} \int_0^t \int_{\mathbb{R}^d} \sigma(\xi, \mu_s^{C,N}) B(d\xi, ds), \\ \mu_t^{C,N} := \text{Law}(C_t^N | \mathcal{G}), \end{cases} \quad (6.1.7)$$

where $B(d\xi, ds)$ is a d -dimensional space-time white noise defined by

$$B(d\xi, ds) := \frac{1}{\sqrt{N}} \sum_{i=1}^N \left[\delta_{X_s^i}(d\xi) \otimes dW_s^i \right]$$

and \mathcal{G} is the σ -algebra generated by ξ_1, \dots, ξ_N and the space-time white noise B . The initial condition θ is defined as

$$\theta := \left(\frac{1}{N} \sum_{i=1}^N \xi_i \right) + \xi - \mathbb{E}[\xi]. \quad (6.1.8)$$

The idea is to capture the trajectories of all N couplings X^1, \dots, X^N by a single process C^N , both in the initial condition and the diffusion term. It turns out that the randomness coming from the diffusion term can be reduced in this way, thus leading to higher order fluctuation, provided that the test function and the drift are linear.

Theorem 6.1.3. *Assume (Int). Suppose that b takes the form*

$$b(x, \mu) = k_1 + k_2 x + k_3 \int_{\mathbb{R}^d} y \mu(dy), \quad (6.1.9)$$

for some $k_1 \in \mathbb{R}^d$ and $k_2, k_3 \in \mathbb{R}$. Suppose that $\sigma \in \mathcal{M}_3(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$. Then

$$\sup_{t \in [0, T]} \left\| \sqrt{N} \left(\frac{1}{N} \sum_{i=1}^N Y_t^{i,N} - \mathbb{E}[C_t^N | \mathcal{G}] \right) \right\|_{L^2} \leq \frac{C}{\sqrt{N}}.$$

Moreover, at any time $t \in [0, T]$, the sequence of random variables

$$\left\{ N \left(\frac{1}{N} \sum_{i=1}^N Y_t^{i,N} - \mathbb{E}[C_t^N | \mathcal{G}] \right) \right\}_{N \in \mathbb{N}}$$

converges in law through a subsequence to a centered random variable.

We first prove a lemma that controls the error between μ^X and $\mu^{C,N}$.

Lemma 6.1.4. Assume (Lip). Then

$$\sup_{t \in [0, T]} \mathbb{E}[W_2(\mu_t^X, \mu_t^{C, N})^2] \leq \frac{C}{N},$$

for some constant $C > 0$.

Proof. Take any $t \in [0, T]$. By Proposition 2.1.1,

$$\begin{aligned} \mathbb{E}[W_2(\mu_t^X, \mu_t^{C, N})^2] &= \mathbb{E} \left[\sup_{\substack{\phi_1, \phi_2 \text{ Lipschitz} \\ \phi_1(x) + \phi_2(y) \leq |x-y|^2}} \left(\mathbb{E}[\phi_1(X_t)] + \mathbb{E}[\phi_2(C_t^N) | \mathcal{G}] \right) \right] \\ &= \mathbb{E} \left[\sup_{\substack{\phi_1, \phi_2 \text{ Lipschitz} \\ \phi_1(x) + \phi_2(y) \leq |x-y|^2}} \mathbb{E}[\phi_1(X_t) + \phi_2(C_t^N) | \mathcal{G}] \right] \\ &\leq \mathbb{E}[|X_t - C_t^N|^2]. \end{aligned} \quad (6.1.10)$$

By (6.1.8) and (Lip), estimating the L^2 difference between (2.1.5) and (6.1.7) gives

$$\begin{aligned} \mathbb{E}[|X_{t'} - C_{t'}^N|^2] &\leq C \left(\mathbb{E} \left[\left| \frac{1}{N} \sum_{i=1}^N \xi_i - \mathbb{E}[\xi] \right|^2 \right] + \int_0^{t'} \mathbb{E}|X_s - C_s^N|^2 + \mathbb{E}[W_2(\mu_s^X, \mu_s^{C, N})^2] ds + \frac{1}{N} \right) \\ &\leq C \left(\int_0^t \sup_{u \in [0, s]} \mathbb{E}|X_u - C_u^N|^2 ds + \frac{1}{N} \right), \end{aligned}$$

for every $t' \leq t$. Hence,

$$\sup_{u \in [0, t]} \mathbb{E}[|X_u - C_u^N|^2] \leq C \left(\int_0^t \sup_{u \in [0, s]} \mathbb{E}|X_u - C_u^N|^2 ds + \frac{1}{N} \right),$$

which implies that

$$\sup_{u \in [0, t]} \mathbb{E}[|X_u - C_u^N|^2] \leq \frac{C}{N},$$

by Gronwall's inequality. This concludes the result by (6.1.10). \square

Proof of Theorem 6.1.3. By the definition of (2.2.4), we observe that

$$\frac{1}{N} \sum_{i=1}^N Y_t^{i, N} = \frac{1}{N} \sum_{i=1}^N \xi_i + k_1 + (k_2 + k_3) \int_0^t \frac{1}{N} \sum_{i=1}^N Y_s^{i, N} ds + \frac{1}{N} \sum_{i=1}^N \int_0^t \sigma(Y_s^{i, N}, \mu_s^{Y, N}) dW_s^i. \quad (6.1.11)$$

Since ξ is independent of \mathcal{G} from its construction, taking conditional expectation on (6.1.8) gives

$$\mathbb{E}[\theta | \mathcal{G}] = \frac{1}{N} \sum_{i=1}^N \xi_i.$$

Also, by taking conditional expectation on both sides of (6.1.7) with respect to \mathcal{G} , we have

$$\mathbb{E}[C_t^N | \mathcal{G}] = \frac{1}{N} \sum_{i=1}^N \xi_i + k_1 + (k_2 + k_3) \int_0^t \mathbb{E}[C_s^N | \mathcal{G}] ds + \frac{1}{N} \sum_{i=1}^N \int_0^t \sigma(X_s^i, \mu_s^{C, N}) dW_s^i. \quad (6.1.12)$$

Taking the difference between (6.1.11) and (6.1.12), followed by a multiplication by \sqrt{N} , we obtain that

$$\sqrt{N} \left[\frac{1}{N} \sum_{i=1}^N Y_t^{i, N} - \mathbb{E}[C_t^N | \mathcal{G}] \right] = (k_2 + k_3) \int_0^t \sqrt{N} \left[\frac{1}{N} \sum_{i=1}^N Y_s^{i, N} - \mathbb{E}[C_s^N | \mathcal{G}] \right] ds$$

$$+ \frac{1}{\sqrt{N}} \sum_{i=1}^N \int_0^t \left[\sigma(Y_s^{i,N}, \mu_s^{Y,N}) - \sigma(X_s^i, \mu_s^{C,N}) \right] dW_s^i. \quad (6.1.13)$$

By Lemma 6.1.4, Theorem 5.2.5 and the Lipschitz property of σ , we have

$$\begin{aligned} & \sup_{s \in [0, T]} \left[\frac{1}{N} \sum_{i=1}^N \mathbb{E} \left| \sigma(Y_s^{i,N}, \mu_s^{Y,N}) - \sigma(X_s^i, \mu_s^{C,N}) \right|^2 \right] \\ & \leq C \left(\frac{1}{N} \sum_{i=1}^N \sup_{s \in [0, T]} \mathbb{E} \left| \sigma(X_s^i, \mu_s^{X,N}) - \sigma(X_s^i, \mu_s^X) \right|^2 + \frac{1}{N} \right). \end{aligned} \quad (6.1.14)$$

Then, by Proposition 5.2.4,

$$\frac{1}{N} \sum_{i=1}^N \sup_{s \in [0, T]} \mathbb{E} \left| \sigma(X_s^i, \mu_s^{X,N}) - \sigma(X_s^i, \mu_s^X) \right|^2 \leq \frac{C}{N}. \quad (6.1.15)$$

Therefore, by combining estimates (6.1.14), (6.1.15) and using the fact that the Brownian motions are independent, we have

$$\mathbb{E} \left[\left| \frac{1}{\sqrt{N}} \sum_{i=1}^N \int_0^t \left[\sigma(Y_s^{i,N}, \mu_s^{Y,N}) - \sigma(X_s^i, \mu_s^{C,N}) \right] dW_s^i \right|^2 \right] \leq \frac{C}{N},$$

for every $t \in [0, T]$. Finally, an application of Gronwall's inequality to (6.1.13) gives

$$\sup_{t \in [0, T]} \mathbb{E} \left[\left(\sqrt{N} \left| \frac{1}{N} \sum_{i=1}^N Y_t^{i,N} - \mathbb{E}[C_t^N | \mathcal{G}] \right| \right)^2 \right] \leq \frac{C}{N},$$

i.e.

$$\sup_{t \in [0, T]} \left\| \sqrt{N} \left(\frac{1}{N} \sum_{i=1}^N Y_t^{i,N} - \mathbb{E}[C_t^N | \mathcal{G}] \right) \right\|_{L^2} \leq \frac{C}{\sqrt{N}}. \quad (6.1.16)$$

For the second statement, it follows an identical argument as the final part in the proof of Theorem 6.1.2 to deduce from (6.1.16) that the sequence of random variables

$$E_N := N \left(\frac{1}{N} \sum_{i=1}^N Y_{t^*}^{i,N} - \mathbb{E}[C_{t^*}^N | \mathcal{G}] \right)$$

converges in law through a subsequence to some random variable M , at any fixed $t^* \in [0, T]$. Taking expectation on both sides of (6.1.11) and (6.1.12) gives

$$\mathbb{E} \left[\frac{1}{N} \sum_{i=1}^N Y_t^{i,N} \right] = \mathbb{E} \left[\frac{1}{N} \sum_{i=1}^N \xi_i \right] + k_1 + (k_2 + k_3) \int_0^t \mathbb{E} \left[\frac{1}{N} \sum_{i=1}^N Y_s^{i,N} \right] ds$$

and

$$\mathbb{E} \left[\mathbb{E}[C_t^N | \mathcal{G}] \right] = \mathbb{E} \left[\frac{1}{N} \sum_{i=1}^N \xi_i \right] + k_1 + (k_2 + k_3) \int_0^t \mathbb{E} \left[\mathbb{E}[C_s^N | \mathcal{G}] \right] ds.$$

An application of Gronwall's inequality to the difference between these two equations gives

$$\sup_{t \in [0, T]} \left| \mathbb{E} \left[\frac{1}{N} \sum_{i=1}^N Y_t^{i,N} \right] - \mathbb{E} \left[\mathbb{E}[C_t^N | \mathcal{G}] \right] \right| = 0.$$

Therefore, $\mathbb{E}[E_N] = 0$, for each N and hence $\mathbb{E}[M] = 0$. \square

6.2 Higher order approximation of the strong error

Recall that, by Theorem 5.2.5 (and Theorem 2.2.6 for a special form of b and σ), the strong error between the standard particle system (2.2.4) and its limiting equation (2.1.5) is given by

$$\sup_{t \in [0, T]} \mathbb{E} |Y_t^{i, N} - X_t^i|^2 \leq \frac{C}{N},$$

for some constant $C > 0$ that does not depend on N . This gives a rate of convergence of $O(N^{-1/2})$ in the L^2 norm. In this section, we construct an alternative coupled McKean-Vlasov equation $(X, \mathcal{H}^{1, N}, \dots, \mathcal{H}^{N, N})$ that gives a rate of convergence of $O(N^{-1})$ in the L^2 norm.

We assume that for each $j, k \in \{1, \dots, d\}$,

$$b_j(x, \mu) = B_j(x) + \Phi_j^{(1)}(\mu), \quad \sigma_{j, k}(x, \mu) = \Sigma_{j, k}(x) + \Phi_{j, k}^{(2)}(\mu), \quad (\text{Structure})$$

where $B_j : \mathbb{R}^d \rightarrow \mathbb{R}$ and $\Sigma_{j, k} : \mathbb{R}^d \rightarrow \mathbb{R}$ satisfy the condition that

$$B_j, \Sigma_{j, k} \in C_{b, \text{Lip}}^4(\mathbb{R}^d), \quad \text{for each } j, k \in \{1, \dots, d\}; \quad (\text{Reg-}B \text{ and } \Sigma)$$

whereas $\Phi_j^{(1)} : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ and $\Phi_{j, k}^{(2)} : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ satisfy the condition that

$$\Phi_j^{(1)}, \Phi_{j, k}^{(2)} \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d)), \quad \text{for each } j, k \in \{1, \dots, d\}. \quad (\mathcal{M}_4\text{-}\Phi^{(1)} \text{ and } \Phi^{(2)})$$

Note that the assumptions (Structure), (Reg- B and Σ) and ($\mathcal{M}_4\text{-}\Phi^{(1)}$ and $\Phi^{(2)}$) together imply that $b, \sigma \in \mathcal{M}_4(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$. Recall from (4.2.1) that

$$\Delta_T^2 = \left\{ (t_1, t_2) \mid 0 \leq t_2 \leq t_1 \leq T \right\}. \quad (6.2.1)$$

For each $\Phi : \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$, we define $\mathcal{V}^\Phi : \Delta_T^2 \times \mathcal{P}_2(\mathbb{R}^d) \rightarrow \mathbb{R}$ by

$$\mathcal{V}^\Phi((t_1, t_2), \mu) = \Phi(\mathcal{L}(X_{t_1}^{t_2, \mu})). \quad (6.2.2)$$

We define a higher order limiting system $(X_t, \mathcal{H}_t^{1, N}, \dots, \mathcal{H}_t^{N, N})_{t \in [0, T]}$ by

$$\left\{ \begin{array}{l} X_{t, j} = \xi_j + \int_0^t b_j(X_s, \mu_s^X) ds + \sum_{k=1}^d \int_0^t \sigma_{j, k}(X_s, \mu_s^X) dW_s^k, \quad 1 \leq j \leq d, \\ \mathcal{H}_{t, j}^{i, N} = \xi_{i, j} + \int_0^t b_j(\mathcal{H}_s^{i, N}, \mu_s^X) ds + \sum_{k=1}^d \int_0^t \sigma_{j, k}(\mathcal{H}_s^{i, N}, \mu_s^X) dW_s^{i, k} \\ \quad - \int_0^t \left[\left(\mathcal{V}^{\Phi_j^{(1)}} \left((s, 0), \frac{1}{N} \sum_{\ell=1}^N \delta_{\xi_\ell} \right) - \mathcal{V}^{\Phi_j^{(1)}}((s, 0), \nu) \right) \right. \\ \quad \left. + \frac{1}{N} \sum_{\ell=1}^N \int_0^s \sigma(\mathcal{H}_u^{\ell, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^{\Phi_j^{(1)}}((s, u), \mu_u^X)(\mathcal{H}_u^{\ell, N}) \cdot dW_u^\ell \right] ds \\ \quad - \sum_{k=1}^d \int_0^t \left[\left(\mathcal{V}^{\Phi_{j, k}^{(2)}} \left((s, 0), \frac{1}{N} \sum_{\ell=1}^N \delta_{\xi_\ell} \right) - \mathcal{V}^{\Phi_{j, k}^{(2)}}((s, 0), \nu) \right) \right. \\ \quad \left. + \frac{1}{N} \sum_{\ell=1}^N \int_0^s \sigma(\mathcal{H}_u^{\ell, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^{\Phi_{j, k}^{(2)}}((s, u), \mu_u^X)(\mathcal{H}_u^{\ell, N}) \cdot dW_u^\ell \right] dW_s^{i, k}, \\ 1 \leq i \leq N, \quad 1 \leq j \leq d, \end{array} \right. \quad (6.2.3)$$

where, for each $t \in [0, T]$,

$$\mathcal{H}_t^{i,N} = (\mathcal{H}_{t,1}^{i,N}, \dots, \mathcal{H}_{t,d}^{i,N})^T, \quad \xi_i = (\xi_{i,1}, \dots, \xi_{i,d})^T, \quad X_t = (X_{t,1}, \dots, X_{t,d})^T, \quad W^i = (W^{i,1}, \dots, W^{i,d})^T,$$

denote the respective vectors of one-dimensional components.

The following proposition asserts that SDE (6.2.3) is well-defined and has a unique solution.

Proposition 6.2.1. *Assume (Int), (Structure), (Reg-B and Σ) and ($\mathcal{M}_4\text{-}\Phi^{(1)}$ and $\Phi^{(2)}$). Then (6.2.3) is well-defined and has a unique strong solution such that*

$$\sup_{t \in [0, T]} \left(\mathbb{E}[|X_t|^4] + \sum_{i=1}^N \mathbb{E}[|\mathcal{H}_t^{i,N}|^4] \right) < +\infty. \quad (6.2.4)$$

Proof. To begin the proof, we notice that the law of (2.1.1) is invariant under translation in time, i.e. for each $0 \leq u \leq s \leq T$, $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ and $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$,

$$\mathcal{V}^\Phi((s, u), \mu) = \Phi(\mathcal{L}(X_s^{u, \mu})) = \Phi(\mathcal{L}(X_T^{u+T-s, \mu})) = \mathcal{V}^\Phi((T, u+T-s), \mu). \quad (6.2.5)$$

This fact is established in the proof of Lemma 6.1 in [9]. By Theorem 3.5.2, we know that $\mathcal{V}^\Phi((T, \cdot), \cdot) \in \mathcal{M}_4(\mathbb{R}^d \times \mathcal{P}_2(\mathbb{R}^d))$. Therefore, the maps

$$s \mapsto \mathcal{V}^\Phi((s, u), \mu); \quad s \mapsto \partial_\mu \mathcal{V}^\Phi((s, u), \mu)(y)$$

are continuous. This shows that the time integrals in (6.2.3) are well-defined. Moreover, the stochastic integrals are well-defined, since for any $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$ and any sequence $(s_n)_n$ in $[0, T]$ converging to s ,

$$\begin{aligned} & \int_0^T \mathbf{1}_{(0, s_n]} \sigma(\mathcal{H}_u^{\ell, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^\Phi((s_n, u), \mu_u^X)(\mathcal{H}_u^{\ell, N}) \cdot dW_u^\ell \\ & \xrightarrow{n \rightarrow \infty, L^2} \int_0^s \sigma(\mathcal{H}_u^{\ell, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^\Phi((s, u), \mu_u^X)(\mathcal{H}_u^{\ell, N}) \cdot dW_u^\ell, \end{aligned}$$

by Itô's isometry and dominated convergence theorem, which shows that the map

$$s \mapsto \int_0^s \sigma(\mathcal{H}_u^{\ell, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^\Phi((s, u), \mu_u^X)(\mathcal{H}_u^{\ell, N}) \cdot dW_u^\ell$$

is continuous almost surely. To show that (6.2.3) has a unique solution, we rewrite (6.2.3) as

$$\left\{ \begin{array}{l} X_{t,j} = \xi_j + \int_0^t b_j(X_s, \mu_s^X) ds + \sum_{k=1}^d \int_0^t \sigma_{j,k}(X_s, \mu_s^X) dW_s^k, \quad 1 \leq j \leq d, \\ \mathcal{H}_{t,j}^{i,N} = \xi_{i,j} + \int_0^t \left[b_j(\mathcal{H}_s^{i,N}, \mu_s^X) - \left(\mathcal{V}^{\Phi_j^{(1)}} \left((s, 0), \frac{1}{N} \sum_{\ell=1}^N \delta_{\xi_s^\ell} \right) - \mathcal{V}^{\Phi_j^{(1)}} \left((s, 0), \nu \right) \right) - R_s^{(1,j)} \right] ds \\ \quad + \sum_{k=1}^d \int_0^t \left[\sigma_{j,k}(\mathcal{H}_s^{i,N}, \mu_s^X) - \left(\mathcal{V}^{\Phi_{j,k}^{(2)}} \left((s, 0), \frac{1}{N} \sum_{\ell=1}^N \delta_{\xi_s^\ell} \right) - \mathcal{V}^{\Phi_{j,k}^{(2)}} \left((s, 0), \nu \right) \right) \right. \\ \quad \quad \left. - R_s^{(2,j,k)} \right] dW_s^{i,k}, \quad 1 \leq i \leq N, \quad 1 \leq j \leq d, \\ R_t^{(1,j)} = \frac{1}{N} \sum_{\ell=1}^N \int_0^t \sigma(\mathcal{H}_u^{\ell, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^{\Phi_j^{(1)}}((t, u), \mu_u^X)(\mathcal{H}_u^{\ell, N}) \cdot dW_u^\ell, \quad 1 \leq j \leq d, \\ R_t^{(2,j,k)} = \frac{1}{N} \sum_{\ell=1}^N \int_0^t \sigma(\mathcal{H}_u^{\ell, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^{\Phi_{j,k}^{(2)}}((t, u), \mu_u^X)(\mathcal{H}_u^{\ell, N}) \cdot dW_u^\ell, \quad 1 \leq j \leq d, \quad 1 \leq k \leq d, \\ \xi_{t,j}^\ell = \xi_{\ell,j}, \quad 1 \leq \ell \leq N, \quad 1 \leq j \leq d, \end{array} \right.$$

(6.2.6)

where $\xi_s^\ell = (\xi_{s,1}^\ell, \dots, \xi_{s,d}^\ell)^T$. Let $\mathbf{V}_t = (\{X_{t,j}\}, \{\mathcal{H}_{t,j}^{i,N}\}, \{R_t^{(1,j)}\}, \{R_t^{(2,j,k)}\}, \{\xi_{t,j}^\ell\})^T$ be the \mathbb{R}^{2dN+d^2+2d} -dimensional vector corresponding to the system of SDEs (6.2.6). Then we observe that there exist functions $\Pi_1 : \Delta_T^2 \times \mathbb{R}^{2dN+d^2+2d} \rightarrow \mathbb{R}^{2dN+d^2+2d}$ and $\Pi_2 : \Delta_T^2 \times \mathbb{R}^{2dN+d^2+2d} \rightarrow \mathbb{R}^{2dN+d^2+2d} \otimes \mathbb{R}^{d^2}$ such that

$$\mathbf{V}_t = \mathbf{V}_0 + \int_0^t \Pi_1((t,s), \mathbf{V}_s) ds + \int_0^t \Pi_2((t,s), \mathbf{V}_s) d\mathbf{W}_s,$$

where $\mathbf{W} := (W^{1,1}, \dots, W^{1,d}, \dots, W^{d,1}, \dots, W^{d,d})^T$. (Note that the dependence on the evolving time t in Π_1 and Π_2 is due to the processes $R^{(1,j)}$ and $R^{(2,j,k)}$.) For any $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$, there exists some $C > 0$ such that for any $\mu_1, \mu_2 \in \mathcal{P}_2(\mathbb{R}^d)$,

$$\begin{aligned} \sup_{s \in [0, T]} |\mathcal{V}^\Phi((s, 0), \mu_1) - \mathcal{V}^\Phi((s, 0), \mu_2)| &\leq \|\Phi\|_{\text{Lip}} \sup_{s \in [0, T]} W_2(\mathcal{L}(X_s^{0, \mu_1}), \mathcal{L}(X_s^{0, \mu_2})) \\ &\leq C \|\Phi\|_{\text{Lip}} W_2(\mu_1, \mu_2), \end{aligned} \quad (6.2.7)$$

where the final inequality follows from the proof of Lemma 3.1 in [9]. Moreover, by the Lipschitz property of σ , (6.2.5) and the fact that $\mathcal{V}^\Phi((T, \cdot), \cdot) \in \mathcal{M}_4([0, T] \times \mathcal{P}_2(\mathbb{R}^d))$ for any $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$, it is clear that the map

$$x \mapsto \sigma(x, \mu_u^X)^T \partial_\mu \mathcal{V}^\Phi((t, u), \mu_u^X)(x)$$

is locally Lipschitz continuous, uniform in t and u , for any $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$. Combining with (6.2.7), we deduce that there exists some real number $C > 0$ (depending on N and d) such that for any $(t, s) \in \Delta_T^2$ and $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^{2dN+d^2+2d}$,

$$\left| \Pi_1((t, s), \mathbf{x}_1) \right|^2 + \left| \Pi_2((t, s), \mathbf{x}_1) \right|^2 \leq C(1 + |\mathbf{x}_1|^2).$$

Furthermore, there exists a sequence of positive integers $\{C_k\}_{k \in \mathbb{N}}$ (depending on k , N and d) such that for any $(t, s) \in \Delta_T^2$ and $\mathbf{x}_1, \mathbf{x}_2 \in \mathbb{R}^{2dN+d^2+2d}$ with $|x_1|, |x_2| \leq k$,

$$\left| \Pi_1((t, s), \mathbf{x}_1) - \Pi_1((t, s), \mathbf{x}_2) \right|^2 + \left| \Pi_2((t, s), \mathbf{x}_1) - \Pi_2((t, s), \mathbf{x}_2) \right|^2 \leq C_k |\mathbf{x}_1 - \mathbf{x}_2|^2.$$

By these two estimates, we can proceed via the classical argument of Picard iteration to show the existence of a strong solution. Uniqueness also follows from these two estimates. (See, for example, the proof of Theorem 2.3.4 in [50] for details.) Finally, (6.2.4) follows from standard arguments involving L^p estimates. (See, for example, the proof of Theorem 2.4.1 in [50] for details.) \square

Next, we state the result on the strong error between $\mathcal{H}^{i,N}$ and $Y^{i,N}$.

Theorem 6.2.2. *Assume (Int), (Structure), (Reg-B and Σ) and $(\mathcal{M}_4\text{-}\Phi^{(1)}$ and $\Phi^{(2)})$. Then*

$$\sup_{t \in [0, T]} \mathbb{E} |\mathcal{H}_t^{i,N} - Y_t^{i,N}|^2 \leq \frac{C}{N^2},$$

for some constant $C > 0$ that does not depend on N .

Proof. To begin, we observe from Lemma 5.2.2 (for the initial conditions) and the equations of $X_{t,j}$ and $\mathcal{H}_{t,j}^{i,N}$ in (6.2.3) that

$$\sup_{t \in [0, T]} \mathbb{E} |X_{t,j}^i - \mathcal{H}_{t,j}^{i,N}|^4 \lesssim \frac{1}{N^2}, \quad \text{for each } j \in \{1, \dots, d\},$$

which implies that

$$\sup_{t \in [0, T]} \mathbb{E} |X_t^i - \mathcal{H}_t^{i, N}|^4 \lesssim \frac{1}{N^2}. \quad (6.2.8)$$

By (5.3.3), subtracting $\mathcal{H}_{t,j}^{i, N}$ by $Y_{t,j}^{i, N}$ gives

$$\begin{aligned} \mathcal{H}_{t,j}^{i, N} - Y_{t,j}^{i, N} &= \int_0^t \left[(B_j(\mathcal{H}_s^{i, N}) - B_j(Y_s^{i, N})) + (\Phi_j^{(1)}(\mu_s^X) - \Phi_j^{(1)}(\mu_s^{Y, N})) \right. \\ &\quad + \left[\mathcal{V}^{\Phi_j^{(1)}} \left((s, 0), \frac{1}{N} \sum_{\ell=1}^N \delta_{\xi_\ell} \right) - \mathcal{V}^{\Phi_j^{(1)}}((s, 0), \nu) \right. \\ &\quad \left. \left. + \frac{1}{N} \sum_{\ell=1}^N \int_0^s \sigma(\mathcal{H}_u^{\ell, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^{\Phi_j^{(1)}}((s, u), \mu_u^X)(\mathcal{H}_u^{\ell, N}) \cdot dW_u^\ell \right] ds \right. \\ &\quad + \sum_{k=1}^m \int_0^t \left[(\Sigma_{j,k}(\mathcal{H}_s^{i, N}) - \Sigma_{j,k}(Y_s^{i, N})) + (\Phi_{j,k}^{(2)}(\mu_s^X) - \Phi_{j,k}^{(2)}(\mu_s^{Y, N})) \right. \\ &\quad + \left[\mathcal{V}^{\Phi_{j,k}^{(2)}} \left((s, 0), \frac{1}{N} \sum_{\ell=1}^N \delta_{\xi_\ell} \right) - \mathcal{V}^{\Phi_{j,k}^{(2)}}((s, 0), \nu) \right. \\ &\quad \left. \left. + \frac{1}{N} \sum_{\ell=1}^N \int_0^s \sigma(\mathcal{H}_u^{\ell, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^{\Phi_{j,k}^{(2)}}((s, u), \mu_u^X)(\mathcal{H}_u^{\ell, N}) \cdot dW_u^\ell \right] dW_s^{i,k} \right. \\ &= \int_0^t \left[(B_j(\mathcal{H}_s^{i, N}) - B_j(Y_s^{i, N})) \right. \\ &\quad - \int_0^s \frac{1}{2N^2} \sum_{i=1}^N \text{Tr} \left(a(Y_u^{i, N}, \mu_u^{Y, N}) \partial_\mu^2 \mathcal{V}^{\Phi_j^{(1)}}((s, u), \mu_u^{Y, N})(Y_u^{i, N}, Y_u^{i, N}) \right) du \\ &\quad - \frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(Y_u^{i, N}, \mu_u^{Y, N})^T \partial_\mu \mathcal{V}^{\Phi_j^{(1)}}((s, u), \mu_u^{Y, N})(Y_u^{i, N}) \cdot dW_u^i \\ &\quad + \frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(\mathcal{H}_u^{i, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^{\Phi_j^{(1)}}((s, u), \mu_u^X)(\mathcal{H}_u^{i, N}) \cdot dW_u^i \Big] ds \\ &\quad + \sum_{k=1}^m \int_0^t \left[(\Sigma_{j,k}(\mathcal{H}_s^{i, N}) - \Sigma_{j,k}(Y_s^{i, N})) \right. \\ &\quad - \int_0^s \frac{1}{2N^2} \sum_{i=1}^N \text{Tr} \left(a(Y_u^{i, N}, \mu_u^{Y, N}) \partial_\mu^2 \mathcal{V}^{\Phi_{j,k}^{(2)}}((s, u), \mu_u^{Y, N})(Y_u^{i, N}, Y_u^{i, N}) \right) du \\ &\quad - \frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(Y_u^{i, N}, \mu_u^{Y, N})^T \partial_\mu \mathcal{V}^{\Phi_{j,k}^{(2)}}((s, u), \mu_u^{Y, N})(Y_u^{i, N}) \cdot dW_u^i \\ &\quad \left. \left. + \frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(\mathcal{H}_u^{i, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^{\Phi_{j,k}^{(2)}}((s, u), \mu_u^X)(\mathcal{H}_u^{i, N}) \cdot dW_u^i \right] dW_s^{i,k}. \right. \end{aligned} \quad (6.2.9)$$

Take any $\Phi \in \mathcal{M}_4(\mathcal{P}_2(\mathbb{R}^d))$. By (6.2.8), we observe that

$$\begin{aligned} &\mathbb{E} \left[\left(\frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(X_u^i, \mu_u^X)^T \partial_\mu \mathcal{V}^\Phi((s, u), \mu_u^X)(X_u^i) \cdot dW_u^i \right. \right. \\ &\quad \left. \left. - \frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(\mathcal{H}_u^{i, N}, \mu_u^X)^T \partial_\mu \mathcal{V}^\Phi((s, u), \mu_u^X)(\mathcal{H}_u^{i, N}) \cdot dW_u^i \right)^2 \right] \lesssim \frac{1}{N^2}. \end{aligned} \quad (6.2.10)$$

On the other hand, a combination of (5.3.5) and (5.3.7) gives

$$\mathbb{E} \left[\left(\frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(Y_u^{i,N}, \mu_u^{Y,N})^T \partial_\mu \mathcal{V}^\Phi((s, u), \mu_u^{Y,N})(Y_u^{i,N}) \cdot dW_u^i - \frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(X_u^i, \mu_u^X)^T \partial_\mu \mathcal{V}^\Phi((s, u), \mu_u^X)(X_u^i) \cdot dW_u^i \right)^2 \right] \lesssim \frac{1}{N^2}. \quad (6.2.11)$$

Therefore, a combination of (6.2.10) and (6.2.11) gives

$$\mathbb{E} \left[\left(\frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(Y_u^{i,N}, \mu_u^{Y,N})^T \partial_\mu \mathcal{V}^\Phi((s, u), \mu_u^{Y,N})(Y_u^{i,N}) \cdot dW_u^i - \frac{1}{N} \sum_{i=1}^N \int_0^s \sigma(\mathcal{H}_u^{i,N}, \mu_u^X)^T \partial_\mu \mathcal{V}^\Phi((s, u), \mu_u^X)(\mathcal{H}_u^{i,N}) \cdot dW_u^i \right)^2 \right] \lesssim \frac{1}{N^2}. \quad (6.2.12)$$

Finally, a combination of (6.2.9), (6.2.12) and the Lipschitz property of B_j and $\Sigma_{j,k}$, $j, k \in \{1, \dots, d\}$, gives

$$\mathbb{E}(\mathcal{H}_{t,j}^{i,N} - Y_{t,j}^{i,N})^2 \lesssim \int_0^t \mathbb{E}|\mathcal{H}_s^{i,N} - Y_s^{i,N}|^2 ds + \frac{1}{N^2}, \quad j \in \{1, \dots, d\},$$

which concludes the result, by summing j over 1 to d , along with an application of Gronwall's inequality. \square

Chapter 7

Conclusion and Future Works

For the bulk of the thesis, most of the results rely on the regularity of function \mathcal{V} defined in Theorem 3.5.2, which is a mere generalisation of Theorem 7.2 of [9]. Accordingly, most theorems are formulated under the strong hypothesis of class \mathcal{M}_k . This inevitably excludes many interesting examples, such as the Burger's equation, whose drift is the Heaviside function (recall (2.2.3) and Example 2.2.2). The only occasion where the condition of uniform boundedness of \mathcal{V} is needed is when we apply Theorem 3.3.7 to conclude that the p th order linear functional derivative of a function has p th order polynomial growth if the function is in \mathcal{M}_p . Nonetheless, Theorem 3.3.7 is no longer needed and Theorem 3.5.2 can be applied to a much more general setting if Theorem 3.5.2 is formulated in terms of linear functional derivatives. This might be possible by following the approach of PDE analysis of forward-backward systems in [11].

There are also several potential results upon generalisation of Theorem 3.5.2. Firstly, if one can obtain full control over the L-derivatives of \mathcal{V} in Theorem 3.5.2 over $[0, \infty)$, then the results in Chapters 4-6 can be extended to the case of unbounded time horizon. Work can also be done to investigate McKean-Vlasov SDEs and particle systems beyond the respective forms of (2.1.5) and (2.2.4), which can have potential applications in Lagrangian models and mean-field games.

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