Regularised Variational Schemes for non-Gradient Systems, and Large Deviations for a Class of Reflected McKean-Vlasov SDE.

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Abstract

This thesis consists of two parts. The first part constructs entropy regularised variational schemes for a range of evolutionary partial differential equations (PDEs), not necessarily in gradient flow form, with a focus on kinetic models. The second part obtains Freidlin-Wentzell large deviation principles and exit times for a class of reflected McKean-Vlasov stochastic differential equations (SDEs).

The theory of Wasserstein gradient flows in the space of probability measures has made enormous progress over the last twenty years. It constitutes a unified and powerful framework in the study of dissipative PDEs, providing the means to prove well-posedness, regularity, stability and quantitative convergence to the equilibrium. The recently developed entropic regularisation technique paves the way for fast and efficient numerical methods for solving these gradient flows. However, many PDEs of interest do not have a gradient flow structure and, a priori, the theory is not applicable. In the first part of the thesis, we develop time-discrete entropy regularised, (one-step and two-step), variational schemes for general classes of non-gradient PDEs. The convergence of the schemes is proved as the time-step and regularisation strength tend to zero. For each scheme we illustrate the breadth of the proposed framework with concrete examples.

In the second part of the thesis we study reflected McKean-Vlasov diffusions over a convex, non-bounded domain with self-stabilizing coefficients that do not satisfy the classical Wasserstein Lipschitz condition. For this class of problems we establish existence and uniqueness results and address the propagation of chaos. Our results are of wider interest: without the McKean-Vlasov component they extend reflected SDE theory, and without the reflective term they extend the McKean-Vlasov theory. Using classical tools from the theory of Large Deviations, we prove a Freidlin-Wentzell type Large Deviation Principle for this class of problems. Lastly, under some additional assumptions on the coefficients, we obtain an Eyring-Kramer's law for the exit time from subdomains contained in the interior of the reflecting domain. Our characterization of the rate function for the exit-time distribution is explicit.

Lay Summary

A gradient flow describes an evolution equation, whereby the dynamics evolve by moving in the direction of steepest descent of some energy functional. To fully describe a gradient flow, one needs: an initial condition, the energy functional, and a geometry of the space which the dynamics take place in (this defines a notion of gradient). In part I of this thesis we study gradient flows in the space of probability measures. The geometry of this space is determined by a certain distance function, arising from the theory of optimal transport, called the Wasserstein metric. In particular we discretise time, and study a variational numerical scheme that approximates the gradient flow. In the Wasserstein space, these schemes are called JKO schemes. It turns out that in nature there are many systems which are not gradient flows, but still have an associated Lyapunov functional (a functional which decreases along the trajectory of the dynamics). For such systems the 'vanilla JKO schemes' are not applicable, our work goes towards extending this classical theory. As well as dealing with non-gradient dynamics, we also regularise the schemes, which makes them easier to implement numerically.

The material in Part II of this thesis is substantially different to that in Part I. In Part II, we study particle systems which are confined to a convex domain by reflecting barriers. These particle systems can be used to model a variety of real world phenomena in which the dynamics are prescribed to stay in some given domain. The term 'particle system' is taken in broad terms, this real world phenomena can range anywhere from gas molecules (living in a container), to stock prices (bounded below by zero). We model these systems as being governed by general forces, as well as some random perturbations. When the number of particles in the system tends to infinity, we can describe the entire system of equations by a single equation, called the mean field limit or McKean-Vlasov equation. In this thesis we prove the well-posedness of such equations, as well as the convergence of the particle system to the mean field limit (this is called the propagation of chaos). After this, we study the systems fluctuations as the strength of the random perturbations tends to zero, in the literature these results are called Freidlin-Wentzell Large Deviations. Lastly, we investigate the first time at which a particle exits a subdomain (which is fully contained in the interior of the reflecting domain).

Contents

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Declaration of Originality

I declare that this dissertation 'Regularised Variational Schemes for non-Gradient Systems, and Large Deviations for a Class of Reflected McKean-Vlasov SDE' is my own and was composed solely by myself, except where explicitly stated in the text. Moreover, to the best of my knowledge this dissertation is not substantially the same as any qualification or piece of work which has been (or currently is being) submitted to any university or related institution.

In particular, Part I contains two research articles [DAdR22, ADR22] (to appear in the SIAM Journal on Mathematical Analysis (SIMA) and in Discrete and Continuous Dynamical Systems (DCDS) respectively). These two articles were a collaborative effort between Gonçalo dos Reis[1], Manh Hong Duong[2], and myself. The collaboration was initiated by Gonçalo dos Reis and Hong Duong. The research theme in [DAdR22] was suggested by Hong Doung, whilst I proposed the line of research in [ADR22].

Part II is based on our article [ADRR$^+$22] (published in Stochastic Processes and their Applications), which was a collaboration between Gonçalo dos Reis, Romain Ravaille[3], William Salkeld[4], Julian Tugaut[3] and myself. The research problem as well as the collaboration was suggested by Gonçalo dos Reis and Julian Tugaut. I wrote the propagation of chaos result, and the section on large deviation principles, and contributed to the introduction and the well-posedness results.

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How to Read this Thesis

In this thesis appendices appear after each chapter. References are made throughout and listed together for all chapters in a general bibliography given at the end. Equations are numbered by chapter, for example in the third section of Chapter 2, the first equation would be numbered "(2.3.1)". Parts I and II are separate research projects and either can be read without the other.

When reading Part I, Chapter 1 should be read first since it provides an overview of the subject matter and the notation used throughout Part I. The reader can then choose to either read Chapters 2 and 3 (which are based on splitting schemes) together, or skip to Chapter 4 (based on single step schemes). Chapters 2 and 3 should be read together and in order, since the proofs in Chapter 3 follow similarly, and in many cases are quoted from, those in Chapter 2. The general strategy and structure of Chapters 2-4 is similar. For example, the proofs of well-posedness (of the scheme) in Chapters 2-4 are substantially the same, and so the reader is suggested to only go through one of these in detail. The main point of difference is that Chapters 2 and 3 more clearly demonstrate how to exploit the conservative-dissipative structure, in particular the cost functions there are explicit (whilst in Chapter 4 they are not). Another point of difference is that the addition of entropic regularisation is treated more thoroughly in Chapter 4. Part II contains a single chapter and is completely self contained.

Part I

Entropy Regularised Variational Schemes for non-Gradient Systems

Chapter 1

Introduction

The mathematics contained in this chapter is not new, we just lay the foundation for Part I of this thesis. The organisation of this chapter is as follows: we start with a brief introduction to Wasserstein gradient flows in Section 1.1 and then immediately turn our attention on their associated discrete variational schemes (which are the focus of this part of the thesis) in Section 1.2, in Section 1.3 we explain the themes of our research and some limitations of the existing theory. Lastly, Section 1.4 sets in place any notation that will be universal throughout Part I.

1.1 Gradient flows in continuous time

A gradient flow describes a trajectory which follows the direction of steepest descent of some functional, which for now we will just call an energy functional[1] A gradient flow consists of three components: an initial value (it's an initial value problem), an energy functional, and a geometry on the underlying space. Knowing the geometry of the underlying space is essential, without it there is no meaning to the notion of 'direction of steepest descent'. For an initial value x_0, an energy functional $\mathcal{F}$ and a notion of gradient "grad", one can write a gradient flow as

$$\partial_t x(t) = -\mathrm{grad}\mathcal{F}(x(t)), \qquad x(0) = x_0. \tag{1.1.1}$$

The most well-known situation is when the underlying space is $\mathbb{R}^d$, that is

$$\frac{d}{dt}x(t) = -\nabla\mathcal{F}(x(t)), \qquad x(0) = x_0 \in \mathbb{R}^d, \tag{1.1.2}$$

where $\mathcal{F} : \mathbb{R}^d \to \mathbb{R}$ and ∇ is the usual gradient operator in Euclidean space. In fact, the terminology 'gradient flow' stems from the finite-dimensional case, since in this case we are studying *the flow* of the vector field $-\nabla\mathcal{F}(x(t))$. When the state space is a Hilbert space, $(\mathcal{H}, \langle\cdot,\cdot\rangle_{\mathcal{H}})$ with $\mathcal{F} : \mathcal{H} \to \mathbb{R}$, one can automatically define the gradient: indeed if $\mathcal{F}'_x : \mathcal{H} \to \mathbb{R}$ is the Fréchet derivative of $\mathcal{F}$ at x, then by the Riesz representation theorem there exists a unique element in $z \in \mathcal{H}$ such that

$$\mathcal{F}'_x(y) = \langle y, z\rangle_{\mathcal{H}}, \quad \forall y \in \mathcal{H}.$$

The gradient $\mathrm{grad}\mathcal{F}(x)$ is then set to be z. An example of a gradient flow on an infinite dimensional space, is the heat equation as a gradient flow of the Dirichlet energy

$$\mathcal{F}(\rho) := \frac{1}{2}\int_{\mathbb{R}^d} \|\nabla\rho\|^2 dx,$$

[1] We may also call this functional a free energy functional or a Lyapunov function. In the literature it can also be referred to as an entropy functional, but we reserve the terminology of entropy functional to mean the Boltzmann entropy or the relative entropy.

in the Hilbert space $L^2(\mathbb{R}^d)$. Note, by an integration by parts

$$\frac{d}{dt}\mathcal{F}(\rho) = -\big\langle \partial_t \rho, \Delta\rho \big\rangle_{L^2(\mathbb{R}^d)}, \tag{1.1.3}$$

i.e. $\mathcal{F}$ decreases fastest along solutions of $\partial_t \rho = \Delta\rho$. However, this theory is somewhat classical, and over the last 20 years or so there has been a renaissance in the field of gradient flows. The celebrated book [AGS08] of Ambrosio, Gigli, and Savaré developed an entire theory of gradient flows in metric spaces. Of course, there is inherently less structure in a metric space compared to a Hilbert space (in particular it is not a vector space), so that notions like $\partial_t x$ and grad$\mathcal{F}$ require careful definitions. A general idea to overcome this is to construct analogous (generally not equivalent) notions of a gradient flow in Euclidean space, which will then serve as appropriate definitions in a metric space. One option is to define a gradient flow through an EDE (*Energy Dissipation Equality*) as follows: for a differentiable function $\mathcal{F} : \mathbb{R}^d \to \mathbb{R}$ and a smooth curve $\rho : \mathbb{R} \to \mathbb{R}^d$, we have, by the Cauchy-Schwarz inequality and Young's inequality (for real numbers),

$$\mathcal{F}(\rho(s)) - \mathcal{F}(\rho(t)) = \int_s^t -\frac{d}{dr}\mathcal{F}(\rho(r))dr = \int_s^t -\nabla\mathcal{F}(\rho(r))\cdot\partial_r\rho(r)dr \le \int_s^t \big(\frac{1}{2}\|\nabla\mathcal{F}(\rho(r))\|^2 + \frac{1}{2}\|\partial_r\rho(r))\|^2\big)dr,$$

with equality if and only if $\partial_r\rho(r) = -\nabla\mathcal{F}(\rho(r))$. Therefore, $\rho = -\nabla\mathcal{F}(\rho)$ almost everywhere in (s,t), is equivalent to the *Energy Dissipation Equality* :

$$\mathcal{F}(\rho(s)) - \mathcal{F}(\rho(t)) = \int_s^t \big(\frac{1}{2}\|\nabla\mathcal{F}(\rho(r))\|^2 + \frac{1}{2}\|\partial_r\rho(r))\|^2\big)dr. \tag{1.1.4}$$

Note (1.1.4) does not require a definition of gradient, it only requires a definition of the modulus of $\nabla\mathcal{F}$. It turns out that the quantities appearing in (1.1.4) have a metric counterpart (see [San15, Section 3]), that is, in a metric space the modulus of the gradient, as well as the metric derivative $\|\partial_t\rho\|$, are well defined. Therefore, the metric analogue of the EDE serves as one appropriate definition of a gradient flow in a metric space. There is another characterisation of gradient flows in metric spaces which is well suited to deal with uniqueness and stability results. This characterisation is called the *Evolution Variational Inequality* (EVI) and requires 'geodesic convexity' (convexity along geodesics) of the functional. Neither the EDE or EVI will play a role in our work, for a further discussion on these notions of gradient flow the reader is referred to [AGS08, San15]. It is also the case that, if the metric of the gradient flow is a Riemannian metric, one can use the standard form of a dissipative system under the GENERIC framework [Ött05, ÖG97, GÖ97] as a definition of gradient flow. The GENERIC formalism will also not be used in this thesis, except in Chapter 3 to study pre-GENERIC diffusion processes, where it is stated in a function space setup [DO21].

In this thesis we consider the problem from a *discrete perspective.* From this perspective one views a gradient flow as an interpolation of a *minimising movement scheme* [DG93] (as some parameter to be thought of as a time-step tends to zero). We introduce this concept of a gradient flow in Section 1.2.

1.1.1 Wasserstein gradient flows

The Wasserstein metric. We now turn our attention on a specific metric space, the Wasserstein space $(\mathcal{P}_2(\mathbb{R}^d), W_2)$. This is the space $\mathcal{P}_2(\mathbb{R}^d)$ of Borel probability measures on $\mathbb{R}^d$ with finite 2nd moments, equipped with the Wasserstein metric W_2. The metric (between two measures ρ_0 and ρ_1) is most intuitively defined using a *transport map* $\mathcal{T} : \mathbb{R}^d \to \mathbb{R}^d$, such that $\mathcal{T}_\#\rho_0 = \rho_1$, which minimises

$$\int_{\mathbb{R}^d} \|\mathcal{T}(x) - x\|^2 d\rho_0(x). \tag{1.1.5}$$

The interpretation here is that $d\rho_0(x)$ determines how much mass is at $x \in \mathbb{R}^d$, $\mathcal{T}$ transports this mass from ρ_0 to ρ_1, and $\|\mathcal{T}(x) - x\|^2$ determines the cost of that transport (with respect to the Euclidean distance squared). The Wasserstein metric, between ρ_0 and ρ_1, is then taken as the square root of (1.1.5). The problem of finding a $\mathcal{T}$ that minimises (1.1.5) was first considered by Gaspard Monge in the late 1700s, the problem is usually referred to as the 'Monge Problem'. This formalism is quite restrictive, for instance, consider the problem when $\rho_0 = \delta_{x_1}$ and $\rho_1 = \frac{1}{2}(\delta_{y_1} + \delta_{y_2})$, then there does not exist a mapping $\mathcal{T}$ such that $\mathcal{T}_\# \rho_0 = \rho_1$, and the Monge problem is ill-posed. In the above sense, the Monge problem does not allow for 'mass to be split'. Another drawback of Monge's formalisation is that the set of transport maps (the constraint set) is not closed in any useful topology. It was not until the late 1900s that the problem was put on firmer ground, by Leonid Vitaliyevich Kantorovich. Kantorovich's formulation uses a *transport plan*, i.e. an element of the set

$$\Pi(\rho_0, \rho_1) := \{\gamma \in \mathcal{P}(\mathbb{R}^d \times \mathbb{R}^d), \ : \ \gamma(A \times \mathbb{R}^d) = \rho_0(A), \ \gamma(\mathbb{R}^d \times A) = \rho_1(A), \ \forall \text{ Borel } A \subset \mathbb{R}^d\},$$

and defines the total transport cost as

$$\inf_{\Pi(\rho_0,\rho_1)} \int_{\mathbb{R}^{2d}} \|x - y\|^2 d\gamma(x, y). \tag{1.1.6}$$

The Kantorovitch formulation has many advantages

- There always exists a transport plan: the product measure $\rho_0 \times \rho_1$.
- The set $\Pi(\rho_0, \rho_1)$ is tight.
- Transport maps induce transport plans: if $\mathcal{T}_\# \rho_0 = \rho_1$, then $(\mathrm{id}, \mathcal{T})_\# \rho_0$ is a transport plan.
- It admits a very useful dual problem.
- The map $\gamma \mapsto \int_{\mathbb{R}^{2d}} \|x - y\|^2 d\gamma(x, y)$ is linear and continuous with respect to the weak topology.

Define $W_2^2(\rho_0, \rho_1)$ as the minimal cost (1.1.6). $W_2(\cdot, \cdot)$ defines a metric on $\mathcal{P}_2(\mathbb{R}^d)$, In fact, the Wasserstein has many useful properties [Vil08, page 110], possibly, the most widely used of these is that it metrizes weak convergence [Vil08, Theorem 6.9]. Moreover, the Wasserstein metric induces a geometry on the space of probability measures which really captures the idea of transportation of mass. This can be seen by studying geodesics in this space, which move the mass continuously from say ρ_0 to ρ_1, unlike what happens when we take averages between densities in $L^2(\mathbb{R}^d)$, whereby the height of the densities is just re-scaled. Lastly, we mention the Benamou-Brenier formula

$$W_2^2(\rho_0, \rho_1) = \inf \Big\{ \int_0^1 \int_{\mathbb{R}^d} \|v(t, x)\|^2 d\rho(t, x) dt, \ : \ \partial_t \rho = \mathrm{div}(\rho v), \ \rho(0) = \rho_0, \ \rho(1) = \rho_1 \Big\}, \tag{1.1.7}$$

which is a reformulation of the Wasserstein optimal transport problem into a PDE fluid flow problem. The interpretation is that the optimal curve $\rho : [0, 1] \to \mathcal{P}(\mathbb{R}^d)$ in (1.1.7) flows ρ_0 into ρ_1, whilst minimising the kinetic energy $\|v\|^2$ of each particle mass. This formula was proved by Jean-David Benamou and Yann Brenier [BB00] with the intention of using it as a computational tool, however it has proved to be a fundamental theoretical result and will play a key role when we view the Wasserstein space as a Riemannian manifold. The form (1.1.6) is usually referred to as the static problem and (1.1.7) as the dynamic problem, these ideas have been extended to more general transport problems, see the survey [Bra12].

Gradient flows in the Wasserstein space. Part I of this thesis will focus on Wasserstein gradient flows (WGF), i.e. gradient flows in the space of probability measures equipped with the Wasserstein metric. Out of all the metric space gradient flows, WGF have undoubtedly received the most attention (see [AGS08, Part II] and [San17, Chapter 4]), this is due to: their links to optimal transport, their solvability via structure preserving numerical schemes, the perspective they provide to study a wide range of fundamental evolutionary PDE, and their derivation via microscopic dynamics. One formally calls a solution of

$$\partial_t \rho = \mathrm{div}\Big[\rho \nabla \Big(\frac{\delta \mathcal{F}}{\delta \rho}\Big)\Big], \quad \rho(0) = \rho_0 \in \mathcal{P}_2(\mathbb{R}^d), \tag{1.1.8}$$
$$\mathcal{F} : \mathcal{P}_2(\mathbb{R}^d) \to \mathbb{R}, \ \ (\mathcal{P}_2(\mathbb{R}^d), W_2),$$

a Wasserstein gradient flow of the functional $\mathcal{F}$, and views $-\mathrm{div}\Big[\rho\nabla\Big(\frac{\delta\mathcal{F}}{\delta\rho}\Big)\Big]$ as the Wasserstein gradient. In (1.1.8) $\frac{\delta\mathcal{F}}{\delta\rho}$ is the variational derivative, see Section 1.4 for precise definitions. The interest in WGF came at the turn of the century, sparked by the seminal work of Jordan, Kinderlehrer, and Otto [JKO98] (the most downloaded article in the SIAM Journal on Mathematical Analysis). They identified a Wasserstein gradient flow structure (1.1.8) in the Fokker-Planck equation. Their work realised this structure through a minimising movement scheme, see Section 1.2. Around the same time, Felix Otto [Ott01] showed that the Wasserstein space inherits a formal Riemannian geometry, and that the gradient flow (1.1.8) can be stated in this framework. The starting point is to view the space of probability measures $\mathcal{P}_2(\mathbb{R}^d)$, as a Riemannian manifold with metric tensor $\langle\cdot,\cdot\rangle_\rho$ on the 'tangent space' $T_\rho\mathcal{P}_2(\mathbb{R}^d)$, defined as

$$\begin{cases} \langle s_1, s_2\rangle_\rho := \int_{\mathbb{R}^d}\rho(x)\nabla p_1(x)\cdot\nabla p_2(x)dx, \\ s_i + \mathrm{div}(\rho\nabla p_i) = 0, \text{ for } i = 1,2. \end{cases} \tag{1.1.9}$$

If $\rho : [0,1] \to \mathcal{P}_2(\mathbb{R}^d)$ is a curve, then its velocity $\partial_t\rho(t)$ is viewed as a tangent vector, and the quantity $\|\partial_t\rho(t)\|_{\rho(t)}$ is the length of that vector. Therefore the integral over $[0,1]$ of the function $t \mapsto \|\partial_t\rho(t)\|_{\rho(t)}$ gives the length of the curve ρ in the 'manifold' $\mathcal{P}_2(\mathbb{R}^d)$. Now note that the Benamou-Brenier formula (1.1.7) tells us that the Wasserstein metric coincides with the notion of Riemannian distance induced by the choice of metric tensor (1.1.9). In this way one can formally view the Wasserstein space $(\mathcal{P}_2(\mathbb{R}^d), W_2)$ as a Riemannian manifold. This is just half the story though, we now argue why $-\mathrm{div}(\rho\nabla\frac{\delta\mathcal{F}}{\delta\rho})$ can be viewed as the Wasserstein gradient of $\mathcal{F}$ at ρ. Denote by grad_W the gradient induced from the metric tensor (1.1.9). Then by the definition of the gradient in a Riemannian manifold, we have for any smooth curve ρ such that $\rho(0) = \bar{\rho}$,

$$\big\langle \mathrm{grad}_W(\mathcal{F}(\bar{\rho})), \partial_t|_{t=0}\rho(t)\big\rangle_{\bar{\rho}} = \frac{d}{dt}\Big|_{t=0}\mathcal{F}(\rho(t)) = \int_{\mathbb{R}^d}\frac{\delta\mathcal{F}}{\delta\rho}(\bar{\rho})\partial_t|_{t=0}\rho(t)dx.$$

Letting p solve $\partial_t|_{t=0}\rho + \mathrm{div}(\bar{\rho}\nabla p) = 0$, gives

$$\begin{aligned} \big\langle \mathrm{grad}_W(\mathcal{F}(\bar{\rho}), \partial_t|_{t=0}\rho(t)\big\rangle_{\bar{\rho}} &= -\int_{\mathbb{R}^d}\frac{\delta\mathcal{F}(\bar{\rho})}{\delta\rho}\mathrm{div}(\bar{\rho}\nabla p)dx \\ &= \int_{\mathbb{R}^d}\bar{\rho}\nabla\frac{\delta\mathcal{F}(\bar{\rho})}{\delta\rho}\cdot\nabla p dx. \end{aligned} \tag{1.1.10}$$

Now (1.1.10) in combination with the definition of the metric tensor (1.1.9) lets us claim that

$$\mathrm{grad}_W(\mathcal{F}(\bar{\rho})) = -\mathrm{div}\Big(\bar{\rho}\nabla\frac{\delta\mathcal{F}(\bar{\rho})}{\delta\rho}\Big).$$

The above construction is only formal, rigorous definitions of WGF are suggested in [AGS08, page 279], this thesis is only conerned with the first of those: a definition via the 'minimising movement' approach.

Since the analysis of the Fokker-Planck equation [JKO98], the theory of WGF has made enormous progress, spanning research activity in various branches of mathematics including partial differential equations, probability theory, and optimal transport. The theory constitutes a powerful framework in the study of dissipative PDEs providing the means to prove well-posedness, regularity, stability and quantitative convergence to the equilibrium, [AGS08, Vil08, San15, ABS21]. For different choices of $\mathcal{F}$, many dissipative evolutionary PDEs, modeling phenomena in biology, chemistry, and physics, have been analysed via this framework, see the discussion in [San15, Section 8.4.2] or [San17, Section 4.3], and the literature cited below.

Dissipative systems analysed under the above framework

Fokker-Planck equation [JKO98, Ber18]	$\partial_t \rho = \mathrm{div}(\rho \nabla f) + \Delta \rho.$
Non-linear diffusion [Ott01, Lis09, CDPS17]	$\partial_t \rho = \mathrm{div}\big(\rho \nabla \big(f + u'(\rho)\big)\big).$
Advection-diffusion-interaction [CMV03, CMV06, BCC08, Lab17]	$\partial_t \rho = \mathrm{div}\big(\rho \nabla (f + u'(\rho) + K * \rho)\big).$
DLSS/simplified quantum drift-diffusion [GST09a, JM07, MMS09]	$\partial_t \rho = -\mathrm{div}(\rho D(\rho^{\alpha-1}\Delta\rho^{\alpha})),$ $1/2 \leq \alpha \leq 1.$
The relativistic heat equation [MS20b, MP09]	$\partial_t \rho = \mathrm{div}\Big(\rho \frac{\nabla \log \rho}{\sqrt{1 + \|\nabla \log \rho\|^2}}\Big).$
Fourth-order thin-film equations [GO01, Ott98, GO03]	$\partial_t \rho = -\partial_x(\rho \partial_x^3 \rho).$
Non-local interaction equations without diffusion [CDF+11, FT22]	$\partial_t \rho = \mathrm{div}\big(\rho \nabla (f + K * \rho)\big).$

The above examples are by no means exhaustive. The theory has been extended to a variety of different settings including: general metric spaces, [AGS08], models of crowd motion [MRCS10, MS16], Riemannian manifolds [Zha07], and discrete structures [CHLZ12, Maa11, Mie13, EPSS21]. We now move on to the focal point of this part of the thesis: the discretisation (in time) of the WGF (1.1.8).

1.2 Gradient flows in discrete time, the JKO scheme

Consider an implicit Euler scheme for the gradient flow in Euclidean space (1.1.2), where given x_h^n we solve the implicit equation for x_h^{n+1}

$$\frac{x_h^{n+1} - x_h^n}{h} = -\nabla \mathcal{F}(x_h^{n+1}),$$

that is

$$\nabla\Big(\frac{\|x - x_h^n\|^2}{2h} + \mathcal{F}(x)\Big)\Big|_{x = x_h^{n+1}} = 0.$$

Now if $\mathcal{F}$ is convex then $x \mapsto \frac{\|x - x_h^n\|^2}{2h} + \mathcal{F}(x)$ is strictly convex, and we have that the implicit Euler scheme is equivalent to

$$x_h^{n+1} = \operatorname*{argmin}_{x \in \mathbb{R}^d} \Big\{ \frac{\|x - x_h^n\|^2}{2h} + \mathcal{F}(x) \Big\}. \tag{1.2.1}$$

This gives a weak formulation of the gradient flow (1.1.2), in the sense that its well-posedness only requires weak assumptions of $\mathcal{F}$, e.g. bounded from below and lower semi-continous, and doesn't require any differentiability. By defining a sequence $\{x_h^n\}$ through (1.2.1), for a given x^0, and constructing the interpolation $x_h(t) := x_h^{n+1}$ for $t \in [tn, t(n+1))$, one would hope that x_h will converge to the gradient flow (1.1.2) as $h \to 0$. This observation motivates a new definition of gradient flow in a general metric space $(\mathbf{M}, \mathbf{d})$ as the limit, as $h \to 0$, of the analogous interpolation of the iterates

$$x_h^{n+1} = \operatorname*{argmin}_{x \in \mathbf{M}} \Big\{ \frac{\mathbf{d}(x_h^n, x)^2}{2h} + \mathcal{F}(x) \Big\}.$$

The first term is the distance between current and new states, whilst the second term encourages a reduction of the functional. This construction was first made by De Georgi [DG93, DGMT80], in which the limit of the interpolation x_h was called a minimising movement of $\mathcal{F}$ with respect to $\mathbf{d}$ (or generalised minimising movement if the time-step is not uniform). These ideas have since been developed, see [AG08, Chapter 2] and [San15, Chapter 8.1]. Most notable is the application of this approach in the Wasserstein space [JKO98], which we discuss in more detail next.

1.2.1 The JKO scheme

Discrete time gradient flow/minimising movement/variational schemes in the Wasserstein space have been coined under the umbrella term of 'JKO schemes'. We will usually refer to the schemes studied in our work as variational schemes, or JKO schemes[2]. Here, we introduce these classical schemes for gradient systems, keeping in mind that the following chapters aim to extend this theory to non-gradient systems.

Consider the linear Fokker-Planck equation (FPE)

$$\partial_t \rho = \operatorname{div}(\rho \nabla f) + \Delta \rho, \quad \rho(0) = \rho_0, \tag{1.2.2}$$

which is the forward Kolmogorov equation of the overdamped Langevin dynamics

$$dX(t) = -\nabla f(X(t))\, dt + \sqrt{2} dW(t), \quad X(0) \sim \rho_0. \tag{1.2.3}$$

Noting that, for the free energy function

$$\mathcal{F}_{\text{fpe}}(\rho) := \int_{\mathbb{R}^d} \big(\rho(x) \log \rho(x) + f(x)\rho(x)\big) dx. \tag{1.2.4}$$

$\frac{\delta \mathcal{F}_{\text{fpe}}}{\delta \rho} = f + \log(\rho) + 1$, the dynamics (1.2.2)-(1.2.3) is a Wasserstein gradient flow in the sense of (1.1.8).

In their seminal work [JKO98] Jordan, Otto and Kinderlehrer showed that the solution of the FPE, over the time interval $[0, T]$, can be approximated by the following iterative minimising movement (steepest descent) scheme. Given a time-step $h > 0$ and defining $\rho_h^0 := \rho_0$, then determine ρ_h^{n+1}, $n = 1, ..., \lfloor \frac{T}{h} \rfloor$, as the unique minimiser of the minimisation problem

$$\rho_h^{n+1} := \underset{\rho \in \mathcal{P}_2(\mathbb{R}^d)}{\operatorname{argmin}} \Big\{ \frac{W_2^2(\rho_h^n, \rho)}{2h} + \mathcal{F}_{\text{fpe}}(\rho) \Big\}. \tag{1.2.5}$$

Then, defining the piecewise constant interpolation $\rho_h(t) := \rho_h^{n+1}$, for $t \in [tn, t(n+1))$, [JKO98] prove the convergence of ρ_h to the weak solution of (1.2.2) over $[0, T]$, as the time-step $h \to 0$. The convergence is weak in $L^1(\mathbb{R}^d)$ for each fixed t, and strong in $L^1(\mathbb{R}^d \times [0, T])$. In (1.2.4), the free energy functional $\mathcal{F}_{\text{fpe}}$ is the sum of the (negative) Boltzmann entropy functional and external energy functional. Hence, the scheme moves ρ^n to minimise the potential energy and maximise the Boltzmann entropy, with W_2 controlling how far it can move in a time-step h. It is useful to note that $\mathcal{F}_{\text{fpe}}(\rho)$ can be written as $H(\rho|\mu) + C$, where $H(\cdot|\cdot)$ is the relative entropy, and μ is the Gibbs distribution $\mu \propto e^{-f}$, and C is a constant independent of ρ. So that, we can replace $\mathcal{F}_{\text{fpe}}$ by $H(\cdot|\mu)$ in (1.2.5) without altering the solution, and the dynamics (1.2.2) can be seen as a dissipation of the relative entropy.

Over the last twenty years, many PDEs have been shown to fit into a similar framework to that discovered in [JKO98]. That is, for a Wasserstein gradient flow (1.1.8) of a general energy function $\mathcal{F}$, one can associate the discrete scheme

$$\rho_h^{n+1} := \underset{\rho \in \mathcal{P}_2(\mathbb{R}^d)}{\operatorname{argmin}} \Big\{ \frac{W_2^2(\rho_h^n, \rho)}{2h} + \mathcal{F}(\rho) \Big\}. \tag{1.2.6}$$

As explained above, (1.2.6) should really be viewed as an implicit Euler scheme: the analogue to (1.2.1) in the Wasserstein space. The well-posedness of (1.2.6) can usually be tackled by the direct method of calculus of variations, in this case that is:

- For a given ν, establish that the functional $\frac{W_2^2(\nu, \cdot)}{2h} + \mathcal{F}(\cdot)$ is bounded from below.
- Show that, with respect to some topology (in this work the weak convergence of probability measures), a minimising sequence has a convergent subsequence in $\mathcal{P}_2(\mathbb{R}^d)$.

[2] Arguably more appropriate terminology might be 'JKO-like schemes' since most of the schemes we study are not WGF, and JKO is reserved for gradient flows.

- Use the lower semi-continuity of $\frac{W_2^2(\nu,\cdot)}{2h} + \mathcal{F}(\cdot)$ to identify this limit as the minimiser.

This is exactly the method that we use to obtain the well-posedness of the schemes we construct in the following chapters.

The most distinguished feature of the JKO scheme is that it preserves the structural information of the continuous time evolution to which it is approximating. Firstly, each iteration $\rho_h^n \in \mathcal{P}(\mathbb{R}^d)$ remains a probability distribution (mass and non-negativity are preserved). Secondly, and most notably, the free energy functional $\mathcal{F}$ decreases along the sequence $\{\rho_h^n\}$, this is easy to see by comparing ρ_h^n as a competitor to ρ_h^{n+1} in (1.2.6), giving

$$\frac{W_2^2(\rho_h^n, \rho^{n+1})}{2h} + \mathcal{F}(\rho_h^{n+1}) \leq \mathcal{F}(\rho_h^n),$$

i.e. $\mathcal{F}(\rho_h^{n+1}) \leq \mathcal{F}(\rho_h^n)$. This is particularly favorable: the WGF structure (1.1.8) is revealing explicitly the physically relevant energy functional, whilst the discrete scheme (1.2.6) is preserving that structure.

The scheme (1.2.6) will be the cornerstone of Part I of this thesis. Before introducing our objectives (the construction of similar schemes, but for non-gradient systems), we review some of the existing theory of the JKO scheme.

A heuristic argument for (1.2.6)**.** Here we provide the heuristic argument (see [San17, page 121]) for why the interpolation of (1.2.6) should converge to (1.1.8). Since the scheme (1.2.6) is mass preserving, one can expect the interpolation of the densities ρ^n to converge to the solution of a continuity equation

$$\partial_t \rho + \operatorname{div}(\rho v) = 0, \tag{1.2.7}$$

for a velocity $v : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d$ that determines the flow of mass. Consider the optimality condition [San15, Proposition 7.20] for the JKO scheme at iteration n, then ρ_h^{n+1} almost everywhere

$$\frac{1}{2h} \frac{\delta W_2^2}{\delta \rho}(\rho_h^n, \rho_h^{n+1}) + \frac{\delta \mathcal{F}}{\delta \rho}(\rho_h^{n+1}) = C, \tag{1.2.8}$$

for some constant C. The variational derivative $\frac{\delta \mathcal{F}}{\delta \rho}$ will be problem dependent. The variational derivative of the Wasserstien $\frac{\delta W_2^2}{\delta \rho}(\rho_h^n, \rho_h^{n+1})$ is given [San15, Proposition 7.17] by $2\phi_h^n$, where ϕ_h^n is the Kantorovich potential related to the cost $\frac{1}{2}\|x-y\|^2$ between ρ_h^{n+1} and ρ_h^n. So that differentiating (1.2.8) gives

$$\frac{\nabla \phi_h^n}{h} + \nabla \frac{\delta \mathcal{F}}{\delta \rho}(\rho_h^{n+1}) = 0,$$

and by Breniers theorem [ABS21, Theorem 5.2] $\mathcal{T}_n^h(x) = x - \nabla \phi_h^n$, where $\mathcal{T}_n^h$ is the transport map between ρ_h^{n+1} and ρ_h^n, so

$$\frac{x - \mathcal{T}_n^h(x)}{h} = -\nabla \frac{\delta \mathcal{F}}{\delta \rho}(\rho_h^{n+1}). \tag{1.2.9}$$

The left hand side of (1.2.9) is the displacement between ρ_h^n and ρ_h^{n+1} divided by the time-step, i.e. it can be interpreted as a velocity. So that, as $hn \to t \in [0,T]$, one hopes that $\frac{x-\mathcal{T}_n^h(x)}{h}$ will tend towards the velocity field $v(t)$ in (1.2.7), whilst $\frac{\delta \mathcal{F}}{\delta \rho}(\rho_h^{n+1})$ will converge to $\frac{\delta \mathcal{F}}{\delta \rho}(\rho(t))$.

The scheme is widely applicable. The JKO scheme (1.2.6), and similar variational schemes inspired by it, provide a powerful tool to obtain existence of weak solutions to a variety of PDEs. Variational schemes in the W_2 transport cost are by far the most common: the pioneering work [JKO98] dealt with the Fokker-Planck equation and 20 years later [ST22] study the same equation obtaining stronger convergence results, [AGS08, Chapters 2 and 3] laid out a general strategy for proving convergence of these schemes for a more general class of energy functionals, [CDF+11] relaxes convexity assumptions on the driving functional in their study of non-local interaction equations with finite-time aggregation, [MRCS10] also relaxes convexity assumptions when studying a model crowd motion, [BCC08, BCK+15] develops the framework for the Keller-Segel system, [Ott01] proved convergence of the JKO scheme for the Porous Medium equation, [AS08, AMS11] applies the theory to a model of superconductivity and accounts for signed measures,

[CG04] builds a conditioned scheme for the kinetic Fokker-Planck equation, [MO14] performs a full (spatio-temporal) discretization for a non-linear diffusion equation, [DFF13] uses a 'freezing method' to construct a JKO scheme for equations with a non-symmetric interaction potential but do not include diffusion, [CG03] employs a scheme that conditions on the spatial variables to solve the nonlinear kinetic Fokker-Planck equation, in [CL17, CFSS18] splitting methods are used combining ODEs with variational schemes, see [GST09b] for a scheme solving the Quantum Drift-Diffusion equation, also the related works [MMS09, MR22] on higher order gradient flows, as well as the studies of Hele-Shaw type gradient flows [DMC20, GO01, GO03].

Many similar variational schemes have been built with perturbed optimal transport distances. For instance [LLW20, CDPS17] develops schemes with regularised (by the Fisher information and entropy respectively) transport problems. [Lis09] extends the general theory for non-linear diffusion equations by allowing for non-isotropic inhomogeneous diffusion matrices. [MP09, Agu05] following the ideas of [Ott96] generalise these notions of gradient flow to more general cost functions. In [Hua00, DPZ14] large deviation principles are used to induce suitable transport problems for the kinetic Fokker-Planck, the same ideas are applied in [HJ00] to the regularised Vlasov-Poisson-Fokker-Planck equation. A convex combination of transport distances is used in [DJ19] to solve the time-fractional Fokker-Planck equation. [PRV13] adds an additional functional to be minimised in their scheme, this is to account for decay in their Fokker-Planck equation. Lastly, see [FG10] for a new transport distance associated to gradient flows with Dirichlet boundary conditions.

Each of the works above uses the convergence of a variational scheme, inspired by the framework (1.2.6), to obtain existence of solutions to a PDE.

A microscopic justification. Here we will be discussing large deviation principles (LDPs), the reader is referred to [DZ98] or [dH00] for a review of that theory and precise statements.

We reiterate that our perspective is to study the PDE (1.1.8) as a gradient flow in the Wasserstein space, in a sense this is a choice. It turns out that a single deterministic differential equation can have multiple gradient flow formulations. As we mentioned, one could alternatively view the heat equation as a gradient flow of the Dirichlet energy[3], see (1.1.3). In a similar vein, different microscopic stochastic processes can, as the number of particles tends to infinity, give rise to the same macroscopic deterministic equation. It has been conjectured (for instance in [ADPZ13]) that gradient flow structures are determined by the large deviations of the underlying stochastic processes. The work [PRV14] demonstrates exactly this by showing that different stochastic particle systems, modelling the heat equation, give rise to distinct gradient flow structures. When the heat equation is viewed as the diffusion equation, i.e. derived from the model of a diffusing particle (Brownian motion), the induced gradient flow structure is a Wasserstein gradient flow of the Boltzmann entropy [ADPZ11]. We now detail this connection. Consider a system of independent Brownian Particles, $X_1(t), \dots, X_N(t) \in \mathbb{R}^d$, with independent identically distributed initial condition ρ_0, each has the transition kernel[4]

$$p_t(x, y) = p_t(x - y) = \frac{1}{(4\pi t)^{d/2}} e^{-\frac{\|x-y\|^2}{4t}}.$$

The empirical measure of the system is defined as

$$L_N(t) := \frac{1}{N} \sum_{i=1}^{N} \delta_{X_i(t)},$$

and satisfies the following (Law of Large Numbers) result

$$L_N(t) \underset{N\to\infty}{\overset{\text{almost surely}}{\longrightarrow}} \rho_0 * p_t. \tag{1.2.10}$$

[3]Other examples of spaces and functionals for which the heat equation is a gradient flow can be found in [PRV14, Page 2].

[4]Note this is the kernel for a Brownian particle with generator Δ, usually in the literature Brownian particles have generator $\frac{1}{2}\Delta$.

Hence, in the many particle limit, this system is a microscopic[5] approximation of the diffusion equation, since $\rho_0 * p_t$ is the solution of the diffusion equation at time t with initial condition ρ_0. Loosely speaking, the Large Deviation Principle (LDP) for $L_N(t)$ tells us at what exponential rate we have the convergence (1.2.10), paraphrasing it reads

$$\mathbb{P}(L_N(h) \approx \rho | L_N(0) = \rho_0) \underset{N\to\infty}{\approx} e^{-NI_h(\rho_0,\rho)},$$

where the rate function is

$$I_h(\rho_0, \rho) := \inf_{\gamma\in\Pi(\rho_0,\rho)} H(\gamma|\rho_0 * p_h).$$

The following result, first proved in [ADPZ11], ties the rate function to the gradient flow functional (for the diffusion equation), through the notion of $\Gamma-$convergence[6], it reads

$$I_h(\rho_0,\cdot) - \frac{1}{4h} W_2^2(\rho_0,\cdot)) \xrightarrow[h\to 0]{\Gamma} \frac{1}{2}\big(H(\cdot) - H(\rho_0)\big),$$

or paraphrasing

$$I_h(\rho_0,\cdot) \underset{h\to 0}{\approx} \frac{1}{4h} W_2^2(\rho_0,\cdot) + \frac{1}{2}\big(H(\cdot) - H(\rho_0)\big). \tag{1.2.11}$$

In-fact, the lower order result $hI_h(\rho_0,\cdot) \approx \frac{1}{4}W_2^2(\rho_0,\cdot)$ was first proved in [Léo07]. If we multiply the right hand side of (1.2.11) by 2, it is the WGF functional, with the addition of $H(\rho_0)$[7], for the diffusion equation. Note that the minimisers of the right hand side are equal to that of $\frac{1}{2h}W_2^2(\rho_0,\cdot) + H(\cdot)$, since scaling and adding constants will not alter the minimiser. The left hand side of (1.2.11) is the rate functional for the LDP, and since $H(\cdot|\rho_0 * p_h)$ is the entropy relative to $\rho_0 * p_h$, we have $I_h(\rho_0,\rho) = 0$ (is minimised) if and only if $\rho = \rho_0 * p_h$. In this way, we can see that the minimiser of the WGF functional is tending towards the exact solution of the diffusion equation as $h \to 0$. This is as expected since the JKO scheme is only an approximation to the true solution, as $h \to 0$. The above observations are schematically summarised in [ADPZ11, Equation (4)]. Since the work of [ADPZ11], it has been shown that for many systems, the Wasserstein gradient flow structure arises from large deviation principles of the underlying stochastic processes, see the articles [ADPZ13, DLR13, DPZ13, EMR15] as well as the thesis [Ren13] for the precise results. The links between Wasserstein gradient flows and large deviation principles not only explain the origin and interpretation of such structures but also give rise to new gradient-flow structures [MPR14].

Benefits of the JKO scheme. To summarise, the framework (1.2.6) has many favorable properties:

- The variational scheme does not require the functional $\mathcal{F}$ to satisfy too strong regularity or convexity assumptions.
- The JKO scheme is structure preserving, this property is rare among numerical schemes.
- These schemes are broadly applicable, they provide a tool to prove the existence of solutions to many fundamental non-linear, non-local, evolutionary PDE.
- There is a well studied microscopic justification, via the theory of Large Deviations, for the structure of Wasserstein gradient flows.
- The regularised versions of these schemes can be solved efficiently using variants of Sinkhorns matrix scaling algorithm, see Section 1.3.2.

Motivated by the success of the JKO scheme, the next section lays out our objectives to extend these results beyond the classical theory.

[5]It is microscopic in the sense that the position of each particle in the system is observed, in comparison to the "macroscopic" approach of studying their density.

[6]Recall the fundamental theorem of $\Gamma-$convergence: 'minimisers converge to minimisers', [DM12, Chapter 7].

[7]It is also interesting to note that the right hand side frequently appears in a priori estimates for JKO schemes, e.g. Lemma 3.4.6

1.3 Our objectives.

The next three chapters are devoted to constructing variational schemes for general evolution equations. In this work we consider evolution equations of the form

$$\partial_t \rho = \mathscr{L}' \rho, \qquad \rho|_{t=0} = \rho_0, \tag{1.3.1}$$

where $\mathscr{L}'$ is the formal (linear or non-linear) adjoint operator of the generator $\mathscr{L}$ of a Markov process on a state space $\mathbb{R}^d$ and the unknown ρ is a time-dependent probability measure on $\mathbb{R}^d$, i.e. $\rho : [0,T] \to \mathcal{P}(\mathbb{R}^d)$. Thus Equation (1.3.1) can be viewed as the forward Kolmogorov equation associated to the Markov process describing the time-evolution of ρ. Equation (1.3.1) arises naturally in statistical mechanics for which $\rho(t,x)\,dx$ often models the probability of finding a particle, evolving according to the Markov process, at state x and time t. The specific forms of $\mathscr{L}'$ will be given at start of each of the following chapters. As described above there is a well established theory of JKO schemes for many gradient systems. The objectives of our work which go towards extending this general theory are

1. To develop variational schemes for conservative-dissipative systems with degenerate diffusion matrices.

2. To show the schemes converge when entropic regularisation is added to the optimal transport problem.

We now explore the meaning of these objectives separately.

1.3.1 Conservative-dissipative degenerate systems

Many fundamental PDEs are not gradient flows but still posses a Lyapunov functional[8]. Due to the presence of the Lyapunov functional, developing a variational formulation akin to the JKO-minimising movement scheme (1.2.5) for these non-gradient systems is a natural question, but it is still mostly open. A prototypical example of a degenerate evolution equation containing both conservative and dissipative dynamics[9] is the (generalized[10]) Kramers' (or kinetic Fokker-Planck) equation [Kra40, Ris89],

$$\partial_t \rho = \underbrace{\Big(- \operatorname{div}_q(\rho p) + \operatorname{div}_p(\rho \nabla_q V) \Big)}_{\text{conservative part}} + \underbrace{\Big(\operatorname{div}_p(\rho \nabla_p F) + \Delta_p \rho \Big)}_{\text{dissipative part}}, \tag{1.3.2}$$

for a density ρ depending on $t \in \mathbb{R}_+, q, p \in \mathbb{R}^d$. In the above equation, we use the notation div_q and similarly ∇_q to indicate that the differential operator acts only on one variable. The Kramers equation is the forward Kolmogorov equation of the underdamped Langevin dynamics

$$d \begin{pmatrix} Q \\ P \end{pmatrix} = \underbrace{\begin{pmatrix} P \\ -\nabla V(Q) \end{pmatrix} dt}_{\text{conservative dynamics}} + \underbrace{\begin{pmatrix} 0 \\ -\nabla F(P)\,dt + \sqrt{2}\,dW_t \end{pmatrix}}_{\text{dissipative dynamics}}. \tag{1.3.3}$$

The Langevin dynamics (1.3.3) describes the movement of a particle (with unity mass) at position Q and with momentum P under the influence of three forces: an external force field $(-\nabla V(Q))$, a (possibly non-linear) friction $(-\nabla F(P))$ and a stochastic noise $(\sqrt{2}dW_t)$. The Kramers equation (1.3.2) characterizes the time evolution of the probability of finding the particle at time t at position q and with momentum p. Unlike the Fokker-Planck equation (1.2.2), which is purely dissipative, the Kramers equation (1.3.2) is a mixture of both conservative and dissipative dynamics. The first part in (1.3.3) is a deterministic Hamiltonian system with Hamiltonian energy $\mathcal{H}(q,p) = p^2/2 + V(q)$. The evolution of this part is reversible and conserves the Hamiltonian. Correspondingly, the first part of (1.3.2) is also reversible and conserves the expectation of $\mathcal{H}$,

$$\mathbb{E}[\mathcal{H}(Q,P)] := \int_{\mathbb{R}^{2d}} \rho(q,p)\mathcal{H}(q,p)\,dqdp.$$

[8] We use the term "Lyapunov functional" to mean a functional which decreases along the tracjectory of the dynamics.

[9] By "conservative and dissipative dynamics" we just mean that there is an associated functional which is invariant under the 'conservative part' of the dynamics and is non-increasing under the 'dissipative part' of the dynamics.

[10] In the classical Kramers equation, $F(p) = \frac{p^2}{2}$.

On the other hand, the second part of (1.3.3) is an overdamped Langevin dynamics (cf. (1.2.3)), but only in the p-variable. The corresponding part in (1.3.2) is precisely a Fokker-Planck equation in p-variable (cf. (1.2.2)), which is a Wasserstein gradient flow in the p-variable. Because of the mixture of both conservative and dissipative effects, the full Kramers equation (1.3.2) is not a gradient flow, and the theory of Wasserstein gradient flows, in particular the JKO-minimizing movement scheme (1.2.6), is not directly applicable.

Developing structure-preserving[11] schemes for such equations with mixed dynamics is currently of great interest both theoretically and computationally, according to [Ött18] "an important challenge for the future is how the structure of thermodynamically admissible evolution equations can be preserved under time-discretization, which is a key to successful numerical calculations". In general, more work is required for classical discretisation methods to retain the structural properties inherent to each model. For example, for the preservation of a Lyapunov/dissipative structure in the Euler-Maruyama method see [MSH02, BSTT22] and for Runge-Kutta methods see [JS15, CG17], and references therein. On the other-hand, retaining the features of the continuous time system is a celebrated trademark of the JKO construction (1.2.6). Therefore, it seems reasonable that an adaptation of this method will be well suited to persevering the conservative-dissipative structure described above.

Another challenging feature of the dynamics we consider is that they are degenerate diffusions, in the sense that they are governed by a diffusion matrix which is only positive semi-definite. This property is present in kinetic models, like Kramers equation above, i.e. in (1.3.2) the Laplacian operator acts only on the velocity variable, or equivalently in (1.3.3) there is only Brownian noise in the velocity variable. This is also a feature of other models we consider, such as higher order degenerate diffusions (see Section 4.3.3), and the hypocoercive Ornstein-Uhlenbeck process (see Section 3.3). Degeneracy is a classical problem, it is well known that noise smooths solutions, so that to have enough regularity the noise must permeate through the system, this is the theory of hypoellipticity [Hör67]. For us the degeneracy, in particular the non-invertibility of the diffusion matrix, means that we cannot perform a simple change of variables in the transport problem to account for the non-isotropic diffusion [12].

It is worth mentioning now that many of the examples we consider in this work belong to the general class of non-gradient systems, namely GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) systems [Ött05]. We will discuss this framework more in Chapter 3.

Part I of this thesis builds variants of the JKO scheme adapted to degenerate evolution equations with mixed dynamics. The two features, degeneracy and mixed dynamics, are treated simultaneously. This is done by either constructing a *one-step, purely variational scheme* (Chapter 4) or a *two-step splitting scheme* (Chapters 2 and 3).

One-step schemes. After an appropriate Lyapunov functional is identified, the idea in constructing one-step schemes is to adapt the cost functional in the optimal transport problem to make up for the degenerate mixed dynamics. The main difficulty is to find an appropriate (optimal transport) cost function, which is often non-homogeneous, time-step dependent and does not induce a metric. Nonetheless, for the kinetic Fokker-Planck equation, several schemes have been built, in which the corresponding cost functions are found based on either the fundamental solution or the conservative part [DPZ14, Hua00], see also [HJ00] for a similar approach for the non-linear Vlasov-Poisson-Fokker-Planck equation. Other interesting examples include the class of Lagrangian systems with local transport [FGY11] and a class of degenerate diffusions of Kolmogorov type [DT18]. In these examples the cost functions are derived respectively from the underlying Lagrangian structure and the large deviation rate functional. The relationship with the large deviation rate functionals was discussed in Section 1.2. We stress that there does not yet exist (nor have we found) a fool-proof formula for deriving a suitable cost function associated to a system with mixed dynamics.

two-step schemes. If one's objective is to develop a unified approach for tackling systems with mixed dynamics, then it may be desirable to develop operator-splitting methods that reflect the same division

[11] The structures we look to preserve are: the conservation of mass, the non-negativity, and the Lyapunov structure.
[12] An isotropic diffusion is one in which the diffusion matrix is a constant times the identity.

between conservative and dissipative effects. The reason for this is that by splitting the dynamics the identification of the cost function is almost immediate. For the Kramers equation, such a splitting scheme is introduced in [DPZ14]. However, the scheme [DPZ14, Scheme 2c] uses a complicated optimal transport cost functional for the dissipative part which does not capture the fact that it is simply a Wasserstein gradient flow in the momentum variable. More recently in [CL17] the authors introduce an operator-splitting scheme for a non-degenerate non-local-nonlinear diffusion equation

$$\partial_t \rho + \operatorname{div}\big(\rho b[\rho]\big) = \Delta P(\rho) + \operatorname{div}\big(\rho \nabla f\big),$$

where $b[\rho]$ is a divergence-free vector field for each ρ, and P is the non-linear pressure function. The above equation does not cover the Kramers equation since the latter is a degenerate diffusion, in which the Laplacian only acts on the momentum variables. A natural question arises

Can we develop structure preserving operator-splitting schemes for non-local, degenerate conservative-dissipative systems?

In our splitting schemes we deal with the degeneracy via a regularisation by noise, see Chapters 2 and 3 for the details.

1.3.2 Entropic regularisation of the JKO scheme

There has been a growing interest in developing structure-preserving numerical methods for Wasserstein-type gradient flows using the JKO scheme [BFS12, CCP19, CM10]. However, from a computational point of view, implementing the JKO scheme (1.2.6) directly is expensive since at each iteration it requires the resolution of a convex optimisation problem involving a Wasserstein distance to the position at the previous step. The entropic regularisation technique developed in [Cut13] overcomes this difficulty by transforming the transport problem into a strictly convex problem that can be solved more efficiently with Sinkhorn's matrix scaling algorithm [SK67]. This regularisation technique has found applications in a variety of domains such as machine learning, image processing, graphics and biology, see the recent monograph [PC19] for a great detailed account of the topic. By replacing the usual Wasserstein distance W_2 in the JKO scheme (1.2.6) by its entropy smoothed approximation $W_{2,\epsilon}$, defined as

$$W_{2,\epsilon}(\mu,\nu) := \Big(\inf_{\gamma \in \Pi(\mu,\nu)} \int_{\mathbb{R}^{2d}} \|x-y\|^2 d\gamma(x,y) + \epsilon H(\gamma) \Big)^{1/2}, \tag{1.3.4}$$

one obtains a regularised scheme (with regularisation strength $\epsilon > 0$) for the Wasserstein gradient flow. Notice the term in the infimum (1.3.4) can be written as a relative entropy/Kullback-Leibler divergence of γ against the Gaussian transition kernel. The regularised scheme leverages the reformulation of this optimisation problem as a Kullback-Leibler projection and makes use of Dykstra's algorithm to attain a fast and convergent numerical scheme [CDPS17, Pey15]. Similar ideas have been applied to other evolutionary equations such as flux-limited gradient flows [MS20b] and a tumour growth model of Hele-Shaw type [DMC20].

When implementing a JKO scheme numerically, it is usually implicitly regularised by the programmer. However, this procedure should be rigorously justified, i.e. the regularised version of (1.2.6) should be proven to converge, as $\epsilon, h \to 0$ in some suitable way. This was first done in [CDPS17] for a class of WGF, under the scaling $\epsilon|\log\epsilon| \le Ch^2$. In this thesis we show that (under the same scaling between ϵ, h) regularisation can be incorporated into more general variational schemes, involving general cost functions and splitting procedures. We believe the scaling assumption to be optimal due to the convergence rates of optimal transport costs [CPT22, Theorem 1.1], we do not manage to prove its optimality or relax the scaling assumption.

Lastly we should mention that entropic regularisation is not without its drawbacks. In particular the regularisation introduces error, which is reduced as $\epsilon \to 0$. However, taking a small regularisation strength causes an increase in the convergence time of Sinkhorns algorithm, and can cause numerical underflow. This is discussed in more detail in Section 4.4 and of course in [PC19].

1.4 Notation

The notation contained here will be fixed throughout Part I of the thesis.

Throughout $d \in \mathbb{N}$ will be the dimension of the space. A fixed $T > 0$ denotes the length of the time interval we consider. Throughout, C denotes a constant whose value may change without indication and depends on the problem's involved constants, but, critically, it is independent of key parameters of this work, namely the time-step $h > 0$, the number of iterates $N \in \mathbb{N}$, and the regularisation strength $\epsilon > 0$, of the schemes we study. The Euclidean inner product between two vectors $x, y \in \mathbb{R}^d$ will be written as $x \cdot y$ or sometimes $\langle x, y\rangle$. We write $\|\cdot\|$ as the Euclidean norm on $\mathbb{R}^d$, and $|\cdot|$ when $d = 1$. The symbol $\|\cdot\|$ is also used as the 2-norm on $\mathbb{R}^{d\times d}$. For a matrix A let A^T be its transpose, and denote its trace by $\mathrm{Trace}(A)$. Let $\mathbb{R}_+$ be the set of non-negative real numbers.

Function spaces: Let $\Omega \subseteq \mathbb{R}^d$, we write $|\Omega|$ as its $d-$dimensional Lebesgue measure. The space of Lebesgue $m-$integrable functions on Ω is denoted by $L^m(\Omega)$. The Sobolev space of functions in $L^1(\Omega)$ with first weak derivatives also in $L^1(\Omega)$ is denoted $W^{1,1}(\Omega)$. We say that $f \in L^1_{\text{loc}}(\mathbb{R}^d)$ if $f \in L^1(\Omega)$ for any compact $\Omega \subset \mathbb{R}^d$. We define the space $f \in W^{1,1}_{\text{loc}}(\mathbb{R}^d)$ similarly. The supremum norm $\|\cdot\|_{\infty,\Omega}$ of a vector field $\phi : \Omega \to \mathbb{R}^d$, or a function $\phi : \Omega \to \mathbb{R}$, is used to denote $\sup_{x\in\Omega} \|\phi(x)\|$, $\sup_{x\in\Omega} |\phi(x)|$ respectively, when $\Omega = \mathbb{R}^d$ we just write $\|\cdot\|_\infty$. Let $A, B \subseteq \mathbb{R}^d$, define $C^k(A; B)$ as the k-times continuously differentiable functions from A to B with continuous k^{th} derivative. Define $C_c^\infty(A; B)$ as the set of infinitely differentiable functions from A to B with compact support. We specifically write $C_c^\infty(\mathbb{R}^d)$ to denote infinitely differentiable functions from $\mathbb{R}^d$ to $\mathbb{R}$ with compact support. Let $C_b(\mathbb{R}^d)$ be the set of continuous bounded functions from $\mathbb{R}^d$ to $\mathbb{R}$. We call 'id' the identity map on any space.

Probability spaces and entropy: Denote the space of Borel probability measures on $\mathbb{R}^d$ as $\mathcal{P}(\mathbb{R}^d)$. The 2nd moment M of a measure $\rho \in \mathcal{P}(\mathbb{R}^d)$ is defined as

$$\mathcal{P}(\mathbb{R}^d) \ni \rho \mapsto M(\rho) := \int_{\mathbb{R}^d} \|x\|^2 \rho(dx). \tag{1.4.1}$$

The set of probability measures with finite 2nd moments is denoted $\mathcal{P}_2(\mathbb{R}^d)$,

$$\mathcal{P}_2(\mathbb{R}^d) := \{\rho \in \mathcal{P}(\mathbb{R}^d) \ : \ M(\rho) < \infty\}. \tag{1.4.2}$$

Define $\mathcal{P}_2^r(\mathbb{R}^d)$ as those $\rho \in \mathcal{P}_2(\mathbb{R}^d)$ which are absolutely continuous. Throughout, when a measure is said to be 'absolutely continuous' we implicitly mean with respect to the Lebesgue measure (unless stated otherwise). We will use the same symbol ρ to denote a measure $\rho \in \mathcal{P}_2^r(\mathbb{R}^d)$ as well as its associated density. Define H to be the negative of Boltzmann entropy,

$$\mathcal{P}(\mathbb{R}^d) \ni \rho \mapsto H(\rho) := \begin{cases} \int_{\mathbb{R}^d} \rho \log \rho, & \text{if } \rho \in \mathcal{P}_2^r(\mathbb{R}^d) \\ +\infty, & \text{otherwise} \end{cases}, \tag{1.4.3}$$

which throughout we will just refer to as the entropy. Also define the positive part of the entropy as

$$\mathcal{P}(\mathbb{R}^d) \ni \rho \mapsto H_+(\rho) := \begin{cases} \int_{\mathbb{R}^d} \max\{\rho \log \rho, 0\}, & \text{if } \rho \in \mathcal{P}_2^r(\mathbb{R}^d) \\ +\infty, & \text{otherwise} \end{cases}, \tag{1.4.4}$$

and the negative part of the entropy as

$$\mathcal{P}(\mathbb{R}^d) \ni \rho \mapsto H_-(\rho) := \begin{cases} \int_{\mathbb{R}^d} |\min\{\rho \log \rho, 0\}|, & \text{if } \rho \in \mathcal{P}_2^r(\mathbb{R}^d) \\ +\infty, & \text{otherwise} \end{cases}. \tag{1.4.5}$$

The set of transport plans between given measures $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ is denoted by $\Pi(\mu, \nu) \subset \mathcal{P}_2(\mathbb{R}^{2d})$. That is, for $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$, $\gamma \in \Pi(\mu, \nu)$ if $\gamma(\mathcal{B} \times \mathbb{R}^d) = \mu(\mathcal{B})$ and $\gamma(\mathbb{R}^d \times \mathcal{B}) = \nu(\mathcal{B})$ for all Borel subsets of $\mathcal{B} \subset \mathbb{R}^d$. Lastly, the 2-Wasserstein distance between two measures $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ is denoted by $W_2(\mu, \nu)$, i.e.

$$W_2(\mu, \nu) := \Big(\inf_{\gamma\in\Pi(\mu,\nu)} \int_{\mathbb{R}^{2d}} \|x - y\|^2 d\gamma(x, y)\Big)^{1/2}.$$

We analogously define the p-Wasserstein distance and space of Borel probability measures with finite $p-$moments, denoted W_p and $\mathcal{P}_p(\mathbb{R}^d)$ respectively. For any two subsets $P, Q \subset \mathcal{P}_2(\mathbb{R}^d)$ we denote $\Pi(P,Q)$ as the set of transport plans whose marginals lie in P and Q respectively. For any probability measure γ and function c on $\mathbb{R}^{2d}$ we write

$$(c,\gamma) := \int_{\mathbb{R}^{2d}} c(x,y)d\gamma(x,y).$$

For a vector field $\eta : \mathbb{R}^d \to \mathbb{R}^d$ and measure $\mu \in \mathcal{P}(\mathbb{R}^d)$ we write $(\eta)_{\#}\mu$ as the push-forward of μ by η. We use the symbol $*$ to denote the convolution, that is for a vector field $K : \mathbb{R}^{d_1} \to \mathbb{R}^{d_1}$ and a measure $\rho \in \mathcal{P}(\mathbb{R}^{d_2})$, $K * \rho : \mathbb{R}^{d_1} \to \mathbb{R}^{d_1}$ is defined as

$$K * \rho(x) := \int_{\mathbb{R}^{d_2}} K(x - x')\rho(x', z)dx'dz, \tag{1.4.6}$$

where $x, x' \in \mathbb{R}^{d_1}$ and $z \in \mathbb{R}^{d_2-d_1}$.

Differentials: Let $\nabla\phi$, $\Delta\phi$, and $\nabla^2\phi$ be the gradient, Laplacian, and Hessian respectively, of a sufficiently smooth function $\phi : \mathbb{R}^d \to \mathbb{R}$. For a sufficiently smooth vector field $\eta : \mathbb{R}^d \to \mathbb{R}^d$ let $\operatorname{div}(\eta)$, and $J\eta$ be its divergence and Jacobian respectively. For a variable $t \in \mathbb{R}$, ∂_t denotes the partial derivative with respect to that variable. Likewise, subscripts attached to other differential operators (e.g. ∇_v) also denote differentiation only with respect to that variable. Given a functional $\mathcal{G} : \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}$, we denote its variational derivative at $\rho \in \mathcal{P}(\mathbb{R}^d)$ by $\frac{\delta\mathcal{G}}{\delta\rho}(\rho)$, defined as the function such that $\frac{d}{d\epsilon}\mathcal{G}(\rho + \epsilon\chi)|_{\epsilon=0} = \int_{\mathbb{R}^d} \frac{\delta\mathcal{G}}{\delta\rho}(\rho)d\chi$, for a suitable class[13] of perturbations χ such that $\rho + \epsilon\chi \in \mathcal{P}(\mathbb{R}^d)$ for all $\epsilon > 0$ small enough. For a curve $\nu : [0,T] \to \mathbf{M}$ in a metric space $(\mathbf{M}, \mathbf{d})$, its metric derivative at t is defined as

$$|\nu'|(t) := \lim_{h\to 0} \frac{\mathbf{d}(\nu(t), \nu(t+h))}{h},$$

provided the limit exists.

Landau notation: We use an enhanced version of the Landau "big-O" and "small-o" notation in the following way: The "big-O" notation $\phi(h) = O(\varphi(h))$, for functions $\phi, \varphi : \mathbb{R}_+ \to \mathbb{R}$ denotes that there exists $C, h_0 > 0$ such that $|\phi(h)| \le C\varphi(h)$ for all $h < h_0$ and we say a matrix $B \in \mathbb{R}^{d\times d}$ is $O(h)$ if $\max_{i,j} |B_{i,j}| \le Ch$ – critically, the constants C, h_0 are independent of any other parameter/variable of interest that ϕ or B may depend on (otherwise such dependence is made explicit). Further we use the Landau "little-o" notation $\phi(h) = o(\varphi(h))$ to mean $\lim_{h\to 0} \frac{\phi(h)}{\varphi(h)} = 0$.

[13] We need to restrict to a suitable class of perturbations χ which make $\mathcal{G}$ finite, see [San15, Chapter 7] for more details.

Chapter 2

A Conservative-Dissipative Splitting Scheme

The work contained here is taken from our paper [ADR22].

2.1 Introduction

In this chapter we consider a general class of degenerate, non-local, conservative-dissipative evolutionary equations of the form

$$\partial_t \rho + \operatorname{div}\big(\rho b[\rho]\big) = \operatorname{div}\big(D\big(\nabla \rho + \rho \nabla f\big)\big), \qquad \rho(0,\cdot) = \rho_0(\cdot), \tag{2.1.1}$$

where the unknown ρ is a time dependent probability distribution on $[0,T]\times\mathbb{R}^d$, $D \in \mathbb{R}^{d\times d}$ is a semi-positive definite (symmetric) matrix (possibly degenerate), $f : \mathbb{R}^d \to \mathbb{R}$ a given energy potential, $b : \mathcal{P}(\mathbb{R}^d)\times\mathbb{R}^d \to \mathbb{R}^d$ a divergence free non-local vector field, and the probability density $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ is the initial condition. Equation (2.1.1) can be viewed as the forward Kolmogorov equation describing the time evolution of the distribution ρ associated to the stochastic process X satisfying the following SDE of McKean type

$$dX(t) = b[\rho(t)](X(t))dt - D\nabla f(X(t))dt + \sqrt{2}\sigma dW(t), \qquad \rho(t) = \operatorname{Law}(X(t)), \tag{2.1.2}$$

for a constant diffusion matrix σ, with $\sigma\sigma^T = D$. This serves as a general model for the dynamic limit of weakly interacting particles, evolving under the influence of an interaction force $b[\rho]$ depending on the law of the process itself, and a potential drift ∇f, whilst being perturbed by Brownian noise $W(t)$. Like the Kramers equation (see Section 1.3.1), (2.1.1) contains both conservative and dissipative effects. The conservative part is represented via the divergence-free vector field (the transport part in the left-hand side of (2.1.1)), in particular implying that the entropy will be preserved under this part. On the other hand, the dissipative part is given by the right hand side of (2.1.1), which resembles a D-Wasserstein gradient flow [Lis09] (but note that D can be degenerate). The aim of this chapter is to develop operator-splitting schemes, which capture the conservative-dissipative splitting and take into account the degeneracy of the diffusion matrix, for solving (2.1.1).

Our operator-splitting scheme can be summarised as follows (details follow in Section 2.2).

The operator-splitting scheme. We split the dynamics described in (2.1.1) by two phases:

1. *Conservative (transport) phase*: for a given ρ, we solve the conservative part, which is simply a transport equation, using the method of characteristics

   $$\partial_t \rho + \operatorname{div}\big(\rho b[\rho]\big) = 0$$

   The existence of a solution to the above equation under a transport/push-forward map is guaranteed by DiPerna-Lions theory [DL89].

2. *Dissipative (diffusion) phase*: we solve the dissipative (diffusion) part using a JKO-miminimizing movement scheme
$$\partial_t \rho = \operatorname{div}\big(D\big(\nabla \rho + \rho \nabla f\big)\big). \tag{2.1.3}$$
We emphasize again that we allow the diffusion matrix D to be degenerate. Because of the degeneracy of D, the JKO-scheme using the D-weighted Wasserstein matrix developed in [Lis09] is not applicable. To overcome this difficulty, we use a simple idea, that is to use a small perturbation of D to get a symmetric positive definite matrix. The key novelty here is that we perturb D by $D_h := D + hI$ where h is the time-step in the discretisation scheme. Thereby, we solve the dissipative (diffusion) equation iteratively using the minimizing movement scheme: ρ_h^{n+1} is determined as the unique minimizer of the minimization problem
$$\min_{\rho} \Big\{ \frac{1}{2h} W_{c_h}(\rho, \rho_h^n) + \int_{\mathbb{R}^d} \big(f\rho + \rho \log \rho\big) dx \Big\},$$
where
$$W_{c_h}(\mu, \nu) = \inf_{\gamma \in \Pi(\mu,\nu)} \int_{\mathbb{R}^{2d}} \big\langle\, (D + hI)^{-1}(x-y), (x-y) \,\big\rangle\, d\gamma(x,y).$$

Our main result, Theorem 2.2.5, establishes the convergence of the above splitting-scheme to a weak solution of (2.1.1) as the time-step h tends to zero. Our operator-splitting scheme is simple and natural capturing the conservative-dissipative splitting of the dynamics, in particular the fact that the dissipative part is a D-weighted Wasserstein gradient flow. Furthermore, motivated by the efficiency of entropic regularisation methods in computational performances, in Theorem 2.4.2 we also provide an entropic regularisation of the above scheme. We expect that the entropy regularised scheme will be useful when one performs numerical simulations although we do not pursue it here. Our result offers a unified approach to establish existence results for a wide class of degenerate, non-local, conservative-dissipative systems. In fact, the class of (2.1.1) is rich and includes many cases of interest: the linear and kinetic Fokker-Planck [Ris89], the (regularised) Vlasov Poisson Fokker-Planck [HJ13], and higher-order degenerate diffusions approximating the generalised Langevin and generalised Vlasov equations [OP11, Duo15]. We will discuss in details these concrete applications in Section 2.5.

Comparison to existing literature. There is a vast literature on operator-splitting methods for solving PDEs, see e.g. [GO16]. We now compare our work with the most relevant literature where the dissipative dynamics involves a Wassertein-type gradient flow. The closest articles to ours are [CL17, Ber18] where the authors consider equations of the form (2.1.1) and introduce similar operator-splitting schemes. However, these papers are limited to non-degenerate diffusion matrices D ($D = I$ in these papers). In fact, [Ber18] does not deal with mixed dynamics, the splitting is carried out at the level of the gradient flow. In [YB13], the authors implement a numerical method that splits an aggregation-diffusion equation, where they exploit its transport structure using a Lagrangian method for the aggregation part, and employ an implicit finite-difference scheme for the diffusion part. Our splitting method is of a different nature, in that we would treat [YB13, Equation (1.1)] as a dissipative equation with no conservative dynamics. Other works that also develop operator-splitting schemes for degenerate PDEs are [CG04, MS20a], however these works only deal with a linear, local conservative dynamics, and are more involved since they require the calculation of conditional distributions (on which they perform the gradient step) at each iteration. Several papers including [Hua00, DPZ14, DT18] (see Chapter 4) also develop JKO-type minimizing movement schemes for degenerate diffusion equations; however these papers use one-step schemes where the cost functions are often non-homogeneous, time-step dependent and do not induce a metric. We also mention recent works in which operator-splitting methods have been investigated for partial differential equations containing a Wasserstein gradient flow part and a non-Wasserstein part. The papers [BA15, DL19] construct operator-splitting schemes for fractional Fokker-Planck equations, in which the transport phase is solved by a JKO-type minimizing movement scheme while the fractional diffusion is solved exactly by convolution with the fractional heat kernel. More recently, [LWW21] builds operator-splitting scheme for reaction-diffusion systems with detailed balanced based on an energetic variational formulation of the systems.

Outlook for future work. From a modelling perspective the non-local term b captures the interactions between a large ensemble of particles. In this case, it takes the form of a convolution between the density distribution and a certain kernel, and our assumptions require the kernel to be uniformly bounded and

Lipschitz. However, many fundamental models of interacting particle systems contain terms which are composed of singular interaction kernels [JW18, Ser20]. This leads to the natural and challenging question: can our method be generalized to deal with singular interaction kernels? In this chapter, we demonstrate via the regularised Vlasov-Poisson-Fokker-Planck equation that our method is applicable when one regularises the Coulomb interaction (see Section 2.5.2). A criticism of the method we present is that it is only partially discretised. Firstly, only one half (the dissipative part) of our splitting is a discretisation in time, for the conservative part we have left it as an exact equation, it might be desirable to also discretise these dynamics (note there is an exact solution for the linear KFPE with no external potential). Secondly, for the dissaptive part, we have only made a discretisation in time, when it comes to implementing the Sinkhorn algorithm one needs to make a spatial discretisation as-well. With this in mind it would be preferable to obtain the convergence of a fully discretised split step scheme, although it is beyond the scope of this thesis, we leave it for future work. Another interesting question is whether we can use the variational structure developed in this chapter to study exponential convergence to the equilibrium of degenerate PDEs of the form (2.1.1). This is related to the hypocoercivity theory introduced by Villani [Vil09], further highlighting these variational structures would provide more insight to that theory. After writing this chapter it came to our attention that strengthening the assumptions would allow us to view (2.1.1) in linear hypocoercive form. We explore this in Chapter 3.

Organisation of the chapter. In Section 2.2 we present the operator-splitting scheme, assumptions, and the main result of this chapter. The proof of the main result is given in Section 2.3. In Section 2.4 we show how the scheme can be regularised. Section 2.5 provides several explicit examples to which our work can be applied to. Finally, the Appendix contains some detailed computations and proofs which guarantee the well-posedness of the JKO step.

2.2 The operator-splitting scheme, assumptions and our main result

In this section, we introduce the operator-splitting scheme for solving (2.1.1), and state our assumptions, and finally, give the main result of this chapter, Theorem 2.2.5. Denote the free energy $\mathcal{F} : \mathcal{P}_2^r(\mathbb{R}^d) \to \mathbb{R}$ as the sum of the potential energy and the entropy

$$\mathcal{F}(\rho) := F(\rho) + H(\rho),$$

where

$$F(\rho) := \int_{\mathbb{R}^d} \rho f dx, \quad \text{and} \quad H(\rho) := \int_{\mathbb{R}^d} \rho \log(\rho) dx.$$

The following properties of the entropy functional are well known.

Lemma 2.2.1 ([JKO98, Proposition 4.1])**.** There exists a $0 < \alpha < 1$, $C > 0$, such that

$$H(\mu) \geq -C(M(\mu)+1)^{\alpha}, \quad \text{and} \quad H_{-}(\mu) \leq C(M(\mu)+1)^{\alpha}, \tag{2.2.1}$$

for all $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$. Moreover, H is weakly lower semi-continuous under uniformly bounded moments, i.e., if $\{\mu_k\}_{k\in\mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^d)$, $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ with $\mu_k \rightharpoonup \mu$, and there exists $C > 0$ such that $M(\mu_k), M(\mu) < C$ for all $k \in \mathbb{N}$, then

$$H(\mu) \leq \liminf_{k\to\infty} H(\mu_k). \tag{2.2.2}$$

Operator-splitting scheme: Let $T > 0$ denote the terminal time and $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ be given, with $\mathcal{F}(\rho_0) < \infty$. Let $h > 0$, $N \in \mathbb{N}$ be such that $hN = T$, and let $n \in \{0, \dots, N-1\}$. Set $\rho_h^0 = \tilde{\rho}_h^0 = \rho_0$. Given ρ_h^n, our operator-splitting to determine ρ_h^{n+1} consists of two phases

1. *Conservative (transport) phase*: first we perform a push forward by the conservative dynamics as

$$\tilde{\rho}_h^{n+1} = X_h^n(h,\cdot)_{\#}\rho_h^n, \tag{2.2.3}$$

   where $X_h^n : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}^d$ is the flow of b

$$\begin{cases} \partial_t X_h^n = b[\rho_h^n] \circ X_h^n, \\ X_h^n(0,\cdot) = \text{id}. \end{cases} \tag{2.2.4}$$

2. *Dissipative (diffusion) phase*: next, define ρ_h^{n+1} as the minimizer of the following JKO-type optimal transport minimization problem

$$\rho_h^{n+1} = \operatorname*{argmin}_{\rho \in \mathcal{P}_2^r(\mathbb{R}^d)} \Big\{ \frac{1}{2h} W_{c_h}(\tilde\rho_h^{n+1}, \rho) + \mathcal{F}(\rho) \Big\}, \tag{2.2.5}$$

where W_{c_h} is a Kantorovich optimal transport cost functional, defined for $h > 0$ as

$$W_{c_h}(\mu, \nu) := \inf_{\gamma \in \Pi(\mu,\nu)} \int c_h(x, y) d\gamma(x, y), \tag{2.2.6}$$

with the cost function $c_h : \mathbb{R}^{2d} \to \mathbb{R}$ given by

$$c_h(x, y) := \big\langle D_h^{-1}(x - y), (x - y)\big\rangle, \tag{2.2.7}$$

for the matrix $D_h \in \mathbb{R}^{d\times d}$ defined as

$$D_h := D + hI. \tag{2.2.8}$$

Note that since D is symmetric positive semi-definite, the addition of hI to D guarantees that D_h is symmetric positive definite (see Lemma 2.3.3). Hence, c_h is well defined for all $h > 0$ and $\sqrt{c_h}$ defines a metric on $\mathbb{R}^d$, which in-turn means $W_{c_h}^{1/2}$ defines a metric on $\mathcal{P}_2(\mathbb{R}^d)$ (see [Vil08, Chapter 6]). This is precisely a D_h-weighted Wasserstein distance [Lis09]. The above perturbation can be also effectively achieved by adding small noise to the SDE (2.1.2). We mention that if the matrix D is invertible then there is no need to perform the perturbation. Instead we can adopt the scheme with $c_h(x, y) = c(x, y) := \big\langle D^{-1}(x - y), (x - y)\big\rangle$ and all results would remain true. Moreover, it may be overkill to add h on each diagonal, especially when implementing this numerically, in this case one should just perturb D enough to make it invertible.

For each $n \in \{0, \ldots, N\}$ we denote $\tilde\gamma_h^{n,c}, \tilde\gamma_h^n \in \Pi(\tilde\rho_h^n, \rho_h^n)$, as the following optimal couplings (respectively)

$$W_{c_h}(\tilde\rho_h^n, \rho_h^n) = \int_{\mathbb{R}^{2d}} c_h(x, y) d\tilde\gamma_h^{n,c}(x, y), \qquad W_2^2(\tilde\rho_h^n, \rho_h^n) = \int_{\mathbb{R}^{2d}} \|x - y\|^2 d\tilde\gamma_h^n(x, y), \tag{2.2.9}$$

and for $n \in \{0, \ldots, N-1\}$ we define $\gamma_h^n \in \Pi(\rho_h^n, \tilde\rho_h^{n+1})$ as the optimal coupling

$$W_2^2(\rho_h^n, \tilde\rho_h^{n+1}) = \int_{\mathbb{R}^{2d}} \|x - y\|^2 d\gamma_h^n(x, y). \tag{2.2.10}$$

The optimal couplings in (2.2.9) and (2.2.10) are all well defined, see Lemma 2.A.2. Throughout this work we will adopt the notation that $t_n = nh$ for $n \in \{0, \ldots, N\}$. Consider the following piecewise constant in time interpolations of $\{\rho_h^n\}_{n=0}^N$

$$\rho_h(t, \cdot) := \rho_h^{n+1} \text{ for } t \in [t_n, t_{n+1}), \tag{2.2.11}$$

and of $\{\tilde\rho_h^n\}_{n=0}^N$

$$\tilde\rho_h(t, \cdot) := \tilde\rho_h^{n+1} \text{ for } t \in [t_n, t_{n+1}), \tag{2.2.12}$$

and consider the interpolation of $\{\tilde\rho^n\}_{n=0}^N$, which continuously follows the conservative dynamics

$$\rho_h^\dagger(t, \cdot) := \big(X_h^n(t - t_n, \cdot)\big)_\# \rho_h^n \text{ for } t \in [t_n, t_{n+1}), \tag{2.2.13}$$

so that for $t \in [t_n, t_{n+1})$, $\rho_h^\dagger(t) = \mu(t - t_n)$ where μ is the solution of the continuity equation (see Lemma 2.3.1)

$$\begin{cases} \partial_t \mu(t, \cdot) + \operatorname{div}\big(\mu(t, \cdot) b[\rho_h^n]\big) = 0 \\ \mu(0, \cdot) = \rho_h^n. \end{cases} \tag{2.2.14}$$

We now introduce assumptions on the potential f, the non-local vector field b, and the diffusion matrix D. Under these assumptions we will prove the well-posedness of the splitting scheme and the convergence of the interpolations (2.2.11)-(2.2.13) to a weak solution of (2.1.1).

Assumption 2.2.2. The potential energy $f \in C^1(\mathbb{R}^d)$ is assumed to be non-negative $f(x) \geq 0$, and Lipschitz, that is there exists a constant $C > 0$ such that for any $x, y \in \mathbb{R}^d$

$$|f(x) - f(y)| \leq C\|x - y\|.$$

For the non-local drift $b : \mathcal{P}(\mathbb{R}^d) \times \mathbb{R}^d \to \mathbb{R}^d$, we assume that there exists $C > 0$ such that for any $\mu \in \mathcal{P}_2(\mathbb{R}^d)$

$$\|b[\mu](x)\| \leq C\big(1 + \|x\|\big),\ \forall x \in \mathbb{R}^d, \quad b[\mu] \in W^{1,1}_{\text{loc}}(\mathbb{R}^d), \qquad \operatorname{div}(b[\mu]) = 0. \tag{2.2.15}$$

Moreover, we assume there exists $C > 0$ for all $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$

$$\int_{\mathbb{R}^d} \|b[\nu](x) - b[\mu](x)\|^p d\nu(x) \leq C W_p^p(\nu, \mu),\ p \in \{1, 2\}. \tag{2.2.16}$$

Lastly assume the constant matrix $D \in \mathbb{R}^{d \times d}$ is semi-positive definite (symmetric).

Remark 2.2.3 (Commenting on the assumptions)*.* The Lipschitz assumption on f is standard when working on the space of probability measures with finite 2nd moments, particularly ensuring that the free energy functional is well-defined. In terms of the assumptions on the non-local vector field b, (2.2.15) implies well-posedness of the transport problem via DiPerna-Lions theory [DL89]. Moreover, imposing the regularity in the measure component (2.2.16) allows us to obtain upper-bounds for some error terms when proving the convergence of the scheme to a weak solution of (2.1.1). Note that when b takes the form of a convolution with an interaction kernel, (2.2.16) is satisfied when the kernel is uniformly bounded, Lipschitz and differentiable, which are the cases for the examples in Section 2.5. Note that the above assumptions have been also made in [CL17].

We now make the definition of a weak solution to (2.1.1) precise.

Definition 2.2.4 (Weak solution)**.** The curve $\rho : [0, T] \to \mathcal{P}_2^r(\mathbb{R}^d)$, $t \mapsto \rho(t, \cdot)$, is called a weak solution to the general evolution equation (2.1.1) if for all $\varphi \in C_c^\infty([0, T) \times \mathbb{R}^d)$ we have

$$\int_0^T \int_{\mathbb{R}^d} \rho\Big(\partial_t \varphi + \big(b[\rho] - D\nabla f\big) \cdot \nabla\varphi + \operatorname{div}\big(D\nabla\varphi\big)\Big) dx dt + \int_{\mathbb{R}^d} \rho^0(x)\varphi(0, x) dx = 0. \tag{2.2.17}$$

The main (abstract) result of this work is the following theorem which gives the existence of weak solutions of the evolution equation (2.1.1). We do not deal with uniqueness here, but in principle, it can be obtained via displacement convexity arguments and an exponential in time contraction on the W_2 distance between two solutions started from different initial data, cf. [Lab17].

Theorem 2.2.5. Let ρ be a weak solution of the evolution equation (2.1.1) in the sense of Definition 2.2.4. Let $h > 0$, $N \in \mathbb{N}$ with $hN = T$, and let $\{\rho_h^n\}_{n=0}^N, \{\tilde{\rho}_h^n\}_{n=0}^N$ be the solution of the scheme (2.2.3)-(2.2.5). Define the piecewise constant interpolations $\rho_h, \tilde{\rho}_h$ by (2.2.11)-(2.2.12) and the continuous interpolation $\rho_h^\dagger$ by (2.2.13). Suppose that Assumption 2.2.2 holds. Then

(i) for each $t \in [0, T]$ as $h \to 0$ ($N \to \infty$ abiding by $hN = T$) we have

$$\rho_h(t, \cdot), \tilde{\rho}_h(t, \cdot), \rho_h^\dagger(t, \cdot) \underset{h \to 0}{\longrightarrow} \rho(t) \quad \text{weakly in} \quad L^1\big(\mathbb{R}^d\big). \tag{2.2.18}$$

(ii) Moreover, there exists a map $[0, T] \ni t \mapsto \rho(t, \cdot)$ in $\mathcal{P}_2^r(\mathbb{R}^d)$ such that for all $1 \leq p < 2$

$$\lim_{h \to 0} \sup_{t \in [0,T]} \max\Big\{W_p(\rho_h(t, \cdot), \rho(t, \cdot)), W_p(\tilde{\rho}_h(t, \cdot), \rho(t, \cdot)), W_p(\rho_h^\dagger(t, \cdot), \rho(t, \cdot))\Big\} = 0. \tag{2.2.19}$$

The convergence is understood as being taken up to a subsequence if necessary.

Note that the convergence (2.2.18) is stronger than weak $L^1((0,T)\times\mathbb{R}^d)$ convergence, indeed let $\psi \in L^\infty((0,T)\times\mathbb{R}^d)$ then

$$\lim_{h\to 0}\int_0^T \underbrace{\int_{\mathbb{R}^d}\rho_h(t,x)\psi(t,x)dx}_{=:G_h(t)}\,dt = \int_0^T \lim_{h\to 0} G_h(t)dt = \int_0^T\int_{\mathbb{R}^d}\rho(t,x)\psi(t,x)dxdt,$$

where in the first equality we have used Lebesgue Dominated Convergence Theorem on G_h, note $|G_h(t)| \le T\sup_{s\in[0,T],x\in\mathbb{R}^d}\psi(s,x)$ for all $t\in[0,T]$, and in the second equality we have used the convergence in (2.2.18). Section 2.3 is devoted to proving the above Theorem 2.2.5.

Remark 2.2.6. If one were to instead consider the evolution equation, for a non-linear function P,

$$\partial_t\rho + \operatorname{div}(\rho b[\rho]) = \operatorname{div}\Big(D\big(\nabla P(\rho) + \rho\nabla f\big)\Big),$$

then following the strategy in [CL17], to deal with the non-linear term, we expect one could construct a similar scheme to the one detailed above by adjusting the free energy functional $\mathcal{F}$. We leave this for now to not over complicate the presentation.

2.3 Proof of the main result

The objective of this section is to prove the main result, Theorem 2.2.5. Once a suitable optimal transport cost functional has been identified, the proof of the convergence of the discrete variational approximation scheme to a weak solution of the evolutionary equation is now a well-established procedure following the celebrated strategy of [JKO98]: firstly we prove the well-posedness of the scheme, then we derive discrete Euler-Lagrange equations for the minimisers of (2.2.5) and necessary a priori estimates, and finally we prove the convergence of the scheme to a weak solution of (2.1.1). An additional step in our proof for the constructed operator-splitting scheme is to combine the two (conservative and dissipative) phases together. Since the outcome of the conservative phase $\tilde\rho_h^{n+1}$ becomes an input of the dissipative phase, we need to show that the 2nd moments, the free-energy functionals and the distances involved, with respect to this density are controllable. This is where we make use of the divergence-free property and the other assumptions of the non-local vector field b.

Recall from Section 2.2 the definitions of the sequences $\rho_h^n, \tilde\rho_h^n$, interpolations $\rho_h, \tilde\rho_h, \rho_h^\dagger$, and optimal couplings $\tilde\gamma_h^{n,c}$, $\tilde\gamma_h^n$, γ_h^n. Also recall that the constant $C>0$ that appears will be independent of h and $n\in\{0,\dots N\}$, but may depend on the final time T. The following results hold under the assumptions of Theorem 2.2.5, and for all $0<h<1$ small enough, note that we are ultimately interested in the case where $h\to 0$.

2.3.1 Preliminary results and well-posedness

The main result here is that the scheme proposed in Section 2.2 is well-posed. We also make some preliminary observations on the matrix D_h, and on solutions to the continuity equation which will be useful later on.

The transport equation. By our assumptions on b, we can use DiPerna-Lions theory [DL89] to conclude that there exists a solution to the ODE (2.2.4), which when pushing forward the initial density solves the continuity equation (2.2.14). Moreover, we note that the conservative dynamics preserves the entropy H.

Lemma 2.3.1. Let $\rho_h^n \in \mathcal{P}_2^r(\mathbb{R}^d)$. Then the following results hold for any $n\in\{0,\dots,N-1\}$.

(i) There exists a unique $X_h^n:\mathbb{R}_+\times\mathbb{R}^d\to\mathbb{R}^d$, such that for a.e. $x\in\mathbb{R}^d$ the map $t\mapsto X_h^n(t,x)$ solves (2.2.4),

$$X_h^n(t,x) = x + \int_0^t b[\rho_h^n]\circ X_h^n(s,x)ds.$$

Moreover, $\mathbb{R}^d \ni x \mapsto X_h^n(\cdot, x) \in L^1_{\mathrm{loc}}(\mathbb{R}^d; C(\mathbb{R}))$, and for a.e. $x \in \mathbb{R}^d$ the map $\mathbb{R}_+ \ni t \mapsto X_h^n(t,x) \in C^1(\mathbb{R})$. In particular, X_h^n satisfies the properties of a flow, i.e. $X_h^n(0,\cdot) = \mathrm{id}$ and $X_h^n(t+s,x) = X_h^n(t, X_h^n(s,x))$, and hence X_h^n is a bijection.

(ii) For $t \in [t_n, t_{n+1})$, $\rho_h^\dagger(t,\cdot)$ solves the continuity equation (2.2.14) over the interval $[0,h)$.

(iii) We have the following entropy preservation identities

$$H\big(\rho_h^\dagger(t,\cdot)\big) = H(\rho_h^n) \ \forall t \in [t_n, t_{n+1}), \qquad H(\tilde{\rho}_h^{n+1}) = H(\rho_h^n). \tag{2.3.1}$$

Proof. Since $b[\rho_h^n]$ satisfies Assumption 2.2.2, (i) and (ii) follow by [DL89, Theorem III.1]. In regard to (iii), note that for all $t \geq 0$ the map $X_h^n(t,\cdot)$ preserves the Lebesgue measure since b is a divergence free vector field. The result is thus immediate. □

The following lemma bounds the change of the distribution under the Hamiltonian dynamics, in a time-step h, by its 2nd moment.

Lemma 2.3.2. The following result holds for any $n \in \{0, \dots, N-1\}$. Let $\rho_h^n \in \mathcal{P}_2^r(\mathbb{R}^d)$. Let μ be the solution of (2.2.14) over the interval $[0,h]$ and let $0 \leq s_1 \leq s_2 \leq h$. Then

$$W_2^2(\mu(s_1,\cdot), \mu(s_2,\cdot)\big) \leq Ch \int_{s_1}^{s_2} \big(1 + M(\mu(s,\cdot))\big) ds. \tag{2.3.2}$$

Moreover, for any $t \in [t_n, t_{n+1})$, $M(\rho_h^\dagger(t,\cdot)), M(\tilde{\rho}_h(t,\cdot)) < C\big(M(\rho_h^n) + 1\big)$.

Proof. Let μ solve (2.2.14). For any $0 \leq s_1 \leq s_2 \leq h$, from the Benamou-Brenier formula [AGS08, Chapter 8] and (2.2.15), we have

$$\begin{aligned} W_2^2\big(\mu(s_1,\cdot), \mu(s_2,\cdot)\big) \leq & (s_2 - s_1) \int_{s_1}^{s_2} \int_{\mathbb{R}^d} \|b[\rho_h^n](x)\|^2 \mu(s,x) dx ds \\ \leq & (s_2 - s_1) C \int_{s_1}^{s_2} \int_{\mathbb{R}^d} \big(1 + \|x\|^2\big) \mu(s,x) dx ds \leq hC \int_{s_1}^{s_2} \big(1 + M(\mu(s,\cdot))\big) ds, \end{aligned}$$

which is (2.3.2). Now consider

$$\begin{aligned} \partial_t M(\mu(t,\cdot)) = \partial_t \int_{\mathbb{R}^d} \|X_h^n(t,x)\|^2 \rho_h^n(x) dx =& 2 \int_{\mathbb{R}^d} X_h^n(t,x) \cdot \partial_t X_h^n(t,x) \rho_h^n(x) dx \\ =& 2 \int_{\mathbb{R}^d} X_h^n(t,x) \cdot b[\rho_h^n] \circ X_h^n(t,x) \rho_h^n(x) dx \\ \leq & C \int_{\mathbb{R}^d} \big(1 + \|X_h^n(t,x)\|^2\big) \rho_h^n(x) dx \\ =& C \int_{\mathbb{R}^d} \big(1 + \|x\|^2\big) d\big(X_h^n(t,\cdot)_\# \rho_h^n\big)(x) = C\big(1 + M(\mu(t,\cdot))\big). \end{aligned}$$

Employing Grönwall's inequality, we have for any $t \in [0,h]$ (recalling that throughout this article $h \leq T$)

$$M(\mu(t,\cdot)) \leq C\big(M(\mu(0,\cdot)) + 1\big) = C\big(M(\rho_h^n) + 1\big). \tag{2.3.3}$$

For $t \in [t_n, t_{n+1})$, recall $\rho_h^\dagger(t,\cdot)$ is equal to the solution of (2.2.14) over the interval $[0,h)$. Hence for any $t \in [t_n, t_{n+1})$, by (2.3.3),

$$M(\rho_h^\dagger(t,\cdot)) \leq C(M(\rho_h^n) + 1).$$

Moreover, for all $t \in [t_n, t_{n+1})$ we have $\tilde{\rho}_h(t,\cdot) = \tilde{\rho}_h^{n+1} = \mu(h,\cdot)$, where again μ solves (2.2.14), and hence by (2.3.3)

$$M(\tilde{\rho}_h(t,\cdot)) = M(\tilde{\rho}_h^{n+1}) = M(\mu(h,\cdot)) \leq C(M(\rho_h^n) + 1),$$

for any $t \in [t_n, t_{n+1})$. This completes the proof. □

The optimal transport problem. In this section we discuss the well-posedness of the minimization problem (2.2.5). It is natural to achieve well-posedness of the scheme through finiteness, lower semi-continuity, and convexity of the functionals which appear in it. First observe that D_h is indeed positive definite.

Lemma 2.3.3 (The cost function)**.** The matrix D_h defined in (2.2.8) is positive definite (i.e., invertible) which implies,

$$\|x-y\|^2 \le C c_h(x,y), \quad \forall x,y \in \mathbb{R}^d. \tag{2.3.4}$$

Proof. This is well-known.

□

The next result addresses the existence of a unique minimiser to (2.2.5). This type of result is classical and can be shown using the direct method of calculus of variations with respect to the weak topology. For completeness the details of the proof can be found in Appendix 2.A.

Proposition 2.3.4. Let $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$ with $\mathcal{F}(\mu) < \infty$. Then, there exists a unique $\nu^* \in \mathcal{P}_2^r(\mathbb{R}^d)$ such that

$$\nu^* = \underset{\nu\in\mathcal{P}_2^r(\mathbb{R}^d)}{\operatorname{argmin}} \Big\{ \frac{1}{2h} W_{c_h}(\mu,\nu) + \mathcal{F}(\nu) \Big\}. \tag{2.3.5}$$

2.3.2 Discrete Euler-Lagrange equations

The following results are by now classical [JKO98, Proposition 4.1], so we state them without proof.

Lemma 2.3.5. Let $\eta \in C_c^\infty(\mathbb{R}^d;\mathbb{R}^d)$, and let Φ be the solution of the following ODE:

$$\partial_s \Phi_s = \eta(\Phi_s), \;\; \Phi_0 = \mathrm{id}.$$

Then for any $\nu \in \mathcal{P}_2^r(\mathbb{R}^d)$ we have

$$\delta\mathcal{F}(\nu,\eta) := \frac{d}{ds}\mathcal{F}\big((\Phi_s)_\#\nu\big)\Big|_{s=0} = \int_{\mathbb{R}^d} \nu(y)\eta(y)\cdot\nabla f(y)dy - \int_{\mathbb{R}^d} \nu(y)\mathrm{div}(\eta(y))dy. \tag{2.3.6}$$

Lemma 2.3.6. Let $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$. Let ν be the optimal solution in (2.3.5), and let γ be the corresponding optimal plan in $W_{c_h}(\mu,\nu)$. Then, for any $\eta \in C_c^\infty(\mathbb{R}^d;\mathbb{R}^d)$ we have

$$0 = \frac{1}{2h}\int_{\mathbb{R}^{2d}} \Big\langle \eta(y), \nabla_y c_h(x,y) \Big\rangle d\gamma(x,y) + \delta\mathcal{F}(\nu,\eta).$$

In particular, for any $\varphi \in C_c^\infty(\mathbb{R}^d)$, by choosing $\eta(x) = D_h\nabla\varphi(x)$, and $\tilde\gamma_h^{n+1,c}$ defined in (2.2.9), we have

$$0 = \frac{1}{h}\int_{\mathbb{R}^{2d}} \Big\langle y-x, \nabla\varphi(x) \Big\rangle d\tilde\gamma_h^{n+1,c}(x,y) + \delta\mathcal{F}(\rho_h^{n+1}, D_h\nabla\varphi). \tag{2.3.7}$$

2.3.3 A priori estimates

In this section we establish a priori estimates which will allow us to prove the convergence of the scheme to a weak solution of (2.1.1) in Section 2.3.4. More precisely, we will show the uniform boundedness of the 2nd moments and of free energies of the minimization iterations (2.2.5). These uniform bounds are preserved under the conservative dynamics, this is explained in the next lemma.

Lemma 2.3.7. Let $n \in \{0,1,\ldots,N-1\}$. If there exists a constant $C_1 > 0$, independent of h and n, such that $M(\rho_h^n), \mathcal{F}(\rho_h^n) < C_1$, then $\tilde\rho_h^{n+1}$ obtained from (2.2.3) satisfies

$$M(\tilde\rho_h^{n+1}), \mathcal{F}(\tilde\rho_h^{n+1}) < C.$$

As usual, the constant C appearing is also independent of h and n, but will depend on C_1.

Proof. The bound for the moments clearly hold by Lemma 2.3.2. For the free energy functional, we have $\mathcal{F}(\tilde{\rho}_h^{n+1}) = F(\tilde{\rho}_h^{n+1}) + H(\rho_h^n)$ by the conservation of entropy in Lemma 2.3.1. Therefore, since f is Lipschitz

$$\begin{aligned}\mathcal{F}(\tilde{\rho}_h^{n+1}) = \int_{\mathbb{R}^d} f(x)\tilde{\rho}_h^{n+1}(x)dx + H(\rho_h^n) &\leq C\int_{\mathbb{R}^d} \big(\|x\|+1\big)\tilde{\rho}_h^{n+1}(x)dx + H(\rho_h^n)\\ &\leq C(M(\tilde{\rho}_h^{n+1})+1) + H(\rho_h^n) \leq C(M(\tilde{\rho}_h^{n+1})+1) + \mathcal{F}(\rho_h^n) \leq C.\end{aligned}$$

□

The following lemma controls the sum of the optimal transport costs of the JKO steps, by using $\tilde{\rho}_h^{n+1}$ as a competitor to ρ_h^{n+1} in (2.2.5). This estimate is of a similar type to [JKO98, Equation (46)], however, because of the splitting nature of our scheme, we don't use ρ_h^n as a competitor in (2.2.5), making the estimate more involved.

Lemma 2.3.8. For an $0 < \alpha < 1$, and any $n \in \{1, \dots, N-1\}$ it holds that

$$\sum_{i=0}^{n-1} W_{c_h}(\tilde{\rho}_h^{i+1}, \rho_h^{i+1}) \leq Ch\Big(1 + \mathcal{F}(\rho^0) + \big(M(\rho_h^n)+1\big)^\alpha\Big). \tag{2.3.8}$$

The $C > 0$ appearing here does not depend on the initial condition ρ^0.

Proof. Let $n \in \{0, 1, \dots, N-1\}$. Since ρ_h^{n+1} attains the infimum in (2.2.5) we can compare it against $\tilde{\rho}_h^{n+1}$. This gives

$$\frac{1}{2h}W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \leq \mathcal{F}(\tilde{\rho}_h^{n+1}) - \mathcal{F}(\rho_h^{n+1}).$$

Using Lemma 2.3.1 for the entropy, the above is equivalent to

$$\frac{1}{2h}W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \leq F(\tilde{\rho}_h^{n+1}) - F(\rho_h^{n+1}) + H(\rho_h^n) - H(\rho_h^{n+1}). \tag{2.3.9}$$

Recall now that $(c_h, \tilde{\gamma}_h^{n+1,c}) = W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1})$. Using that f is Lipschitz and Young's inequality with $\sqrt{\sigma}$ for some $\sigma > 0$, we can see

$$\begin{aligned}F(\tilde{\rho}_h^{n+1}) - F(\rho_h^{n+1}) = \int_{\mathbb{R}^{2d}} (f(x) - f(y))d\tilde{\gamma}_h^{n+1,c}(x,y) &\leq C\int \|x-y\| d\tilde{\gamma}_h^{n+1,c}(x,y)\\ &\leq \frac{C}{2\sigma}\int \|x-y\|^2 d\tilde{\gamma}_h^{n+1,c}(x,y) + \frac{C\sigma}{2}\\ &\leq \frac{C}{2\sigma}\int c_h(x,y) d\tilde{\gamma}_h^{n+1,c}(x,y) + \frac{C\sigma}{2},\end{aligned}$$

where in the last step we used (2.3.4). Substituting this into (2.3.9) yields

$$\frac{1}{2h}W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \leq \frac{C}{2\sigma}\int c_h(x,y) d\tilde{\gamma}_h^{n+1,c}(x,y) + \frac{C\sigma}{2} + H(\rho_h^n) - H(\rho_h^{n+1}).$$

Choosing $\sigma = 2Ch$ leads to

$$\frac{1}{2h}W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \leq \frac{1}{4h}W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) + Ch + H(\rho_h^n) - H(\rho_h^{n+1}).$$

After rearranging we finally conclude

$$W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \leq C\Big(h^2 + h\big(H(\rho_h^n) - H(\rho_h^{n+1})\big)\Big). \tag{2.3.10}$$

The sum of (2.3.10) over $i \in \{0, \dots, n-1\}$ contains a telescopic component which allows for the simplified expression

$$\sum_{i=0}^{n-1} W_{c_h}(\tilde{\rho}_h^{i+1}, \rho_h^{i+1}) \leq Ch\Big(1 + H(\rho^0) - H(\rho_h^n)\Big),$$

where we have used that $Nh = T$. We employ (2.2.1) to deal with $-H(\rho_h^n)$ in the above expression, while to make $\mathcal{F}(\rho^0)$ appear we use the positivity of f. This leads to

$$\sum_{i=0}^{n-1} W_{c_h}(\tilde{\rho}_h^{i+1}, \rho_h^{i+1}) \leq Ch\Big(1 + \mathcal{F}(\rho^0) + \big(M(\rho_h^n) + 1\big)^{\alpha}\Big).$$

□

The next Lemma provides uniform bounds in n and h for the 2nd moments, free energy functionals, and positive part of the entropy functionals of the solutions from the scheme (2.2.3) - (2.2.5). The proof is inspired by the procedure found in [DPZ14, Hua00], first obtaining bounds locally and then extending them over the full time interval.

Lemma 2.3.9 (Boundedness of the energy functionals, 2nd moments and the positive part of the entropy functionals)**.** For all $n \in \{0, 1, \dots, N\}$, we have

$$M(\rho_h^n), \mathcal{F}(\rho_h^n), H_+(\rho_h^n) \leq C \qquad \text{and} \qquad M(\tilde{\rho}_h^n), \mathcal{F}(\tilde{\rho}_h^n), H_+(\tilde{\rho}_h^n) \leq C.$$

Proof. Throughout this proof the constant $\bar{C}$ will change from line to line, and importantly it is independent of ρ^0. For the sake of notational clarity we omit the dependence of the iterates $\rho_n^h, \tilde{\rho}_h^n$ on h for this proof.

For any $n \in \{1, \dots, N\}$ we have that (by Cauchy-Schwarz inequality)

$$\begin{aligned} M(\rho^n) \leq 2\Big(M(\rho^0) + W_2^2(\rho^0, \rho^n)\Big) \leq& 2\Big(M(\rho^0) + n\sum_{i=0}^{n-1} W_2^2(\rho^i, \rho^{i+1})\Big) \\ \leq& 4\Big(M(\rho^0) + n\sum_{i=0}^{n-1} W_2^2(\rho^i, \tilde{\rho}^{i+1}) + W_2^2(\tilde{\rho}^{i+1}, \rho^{i+1})\Big) \\ \leq& 4\Big(M(\rho^0) + n\sum_{i=0}^{n-1} W_2^2(\rho^i, \tilde{\rho}^{i+1}) + \bar{C}W_{c_h}(\tilde{\rho}^{i+1}, \rho^{i+1})\Big). \end{aligned} \tag{2.3.11}$$

From Lemma 2.3.2 we have $4TW_2^2(\rho^i, \tilde{\rho}^{i+1}) \leq \bar{C}h^2(1 + M(\rho^i))$ for a constant $\bar{C}$ (independent of the initial condition), substituting this, and the bound (2.3.8) into (2.3.11), we have, whilst noting $hN = T$,

$$\begin{aligned} M(\rho^n) \leq& 4\Big(M(\rho^0) + \bar{C}\big(1 + \mathcal{F}(\rho^0)\big)\Big) + \bar{C}\Big((1 + M(\rho^n))^{\alpha} + h\sum_{i=0}^{n-1}(1 + M(\rho^i))\Big) \\ \leq& C + \bar{C}\Big((1 + M(\rho^n))^{\alpha} + h\sum_{i=0}^{n-1}(1 + M(\rho^i))\Big) \\ \leq& C + \bar{C}\Big((1 + M(\rho^n))^{\alpha} + h\sum_{i=0}^{n-1} M(\rho^i)\Big), \end{aligned} \tag{2.3.12}$$

for a constant C depending only on $\mathcal{F}(\rho^0)$ and $M(\rho^0)$, and constant $\bar{C}$ independent of ρ^0. Since the $\bar{C}$ appearing in (2.3.12) is fixed and independent of the initial condition, we can find $h_0 > 0, N_0 \in \mathbb{N}$ (independent of the initial condition) such that for all $h \leq h_0$ we have $hN_0\bar{C} \leq \frac{1}{2}$. Set $M_{N_0} := \max_{n=1,\dots,N_0} M(\rho^n)$. Then (2.3.12) implies

$$\begin{aligned} M_{N_0} \leq& C + \bar{C}\Big((1 + M_{N_0})^{\alpha} + hN_0 M_{N_0}\Big) \\ \leq& C + \bar{C}(1 + M_{N_0})^{\alpha} + \frac{1}{2}M_{N_0}, l \end{aligned}$$

which implies

$$M_{N_0} \leq 2\big(C + \bar{C}(1 + M_{N_0})^{\alpha}\big), \tag{2.3.13}$$

from which we can conclude $M(\rho^n) \leq C$, for all $n = 1, \ldots, N_0$, and all $h \leq h_0$. For the free energy, note that by definition of ρ^{i+1}, we have that

$$\mathcal{F}(\rho^{i+1}) - F(\tilde{\rho}^{i+1}) - H(\tilde{\rho}^{i+1}) \leq 0,$$

adding and subtracting $F(\rho^i)$, and recalling that $H(\rho^i) = H(\tilde{\rho}^{i+1})$, implies

$$\mathcal{F}(\rho^{i+1}) - \mathcal{F}(\rho^i) \leq |F(\rho^i) - F(\tilde{\rho}^{i+1})|. \tag{2.3.14}$$

Summing (2.3.14) from $i = 0, \ldots, n-1$, using that f is Lipschitz, and applying Young's inequality for some $\sigma > 0$, we have

$$\mathcal{F}(\rho^n) - \mathcal{F}(\rho^0) \leq \sum_{i=0}^{n-1} |F(\rho^i) - F(\tilde{\rho}^{i+1})| \leq C \sum_{i=0}^{n-1} \int_{\mathbb{R}^{2d}} \|x - y\| d\gamma^i(x, y) \leq C \sum_{i=0}^{n-1} \Big(\frac{1}{\sigma} W_2^2(\rho^i, \tilde{\rho}^{i+1}) + \sigma\Big). \tag{2.3.15}$$

Now let N_0, h_0 be chosen as before, and let $n = 1, \ldots, N_0$. We know, by Lemma 2.3.2 and the bounded moments just proved, that $W_2^2(\rho^i, \tilde{\rho}^{i+1}) \leq Ch^2(1 + M(\rho^i)) \leq Ch^2$ for $i \leq n$. Therefore, choosing $\sigma = h$ in (2.3.15) implies the uniform bounded energies $\mathcal{F}(\rho^n) \leq C$. Note that $\mathcal{F}(\rho^n) \leq C$ implies $H(\rho^n) \leq C$ (since $f \geq 0$), moreover, (2.2.1) and the uniform bounds on $M(\rho^n)$ imply that $H_-(\rho^n) \leq C$, therefore we have that $H_+(\rho^n) \leq C$. So far we have established the uniform bounds

$$M(\rho^n), \mathcal{F}(\rho^n), H_+(\rho^n) \leq C, \qquad \forall n = 1, \ldots, N_0,\ h \leq h_0. \tag{2.3.16}$$

Since the N_0 and h_0 we have chosen are independent of the initial data we can extend the bound (2.3.16) to all $n \in \{1, \ldots, N\}$ similarly as has been done in [Hua00, Lemma 5.3] or [DPZ14], see also the end of the proof of Lemma 4.6.4 in Chaper 4. The uniform bounds $M(\rho^n), \mathcal{F}(\rho^n), H_+(\rho^n) \leq C$, Lemma 2.3.7, and another application of (2.2.1) establishes $M(\tilde{\rho}^n), \mathcal{F}(\tilde{\rho}^n), H_+(\tilde{\rho}^n) \leq C$, completing the proof.

□

Lemma 2.3.9 states the uniform bounds for the discrete elements of our schemes. The following Lemma induces those bounds for the interpolations (2.2.11), (2.2.12) and (2.2.13).

Lemma 2.3.10 (A priori estimates for the interpolations)**.** For all $n \in \{0, 1, \ldots, N\}$, the moments, free-energies and the positive part of the entropies are uniformly bounded (in n, h, t), namely,

$$M(\rho_h(t,\cdot)), M(\tilde{\rho}_h(t,\cdot)), M(\rho_h^{\dagger}(t,\cdot)) \leq C, \qquad \mathcal{F}(\rho_h(t,\cdot)), \mathcal{F}(\tilde{\rho}_h(t,\cdot)), \mathcal{F}(\rho_h^{\dagger}(t,\cdot)) \leq C,$$

$$\text{and} \qquad H_+(\rho_h(t,\cdot)), H_+(\tilde{\rho}_h(t,\cdot)), H_+(\rho_h^{\dagger}(t,\cdot)) \leq C.$$

Proof. These results for the interpolations follow easily from Lemma 2.3.9. Indeed, it is immediate from their definitions how this is inferred for the interpolations $\rho_h(t,\cdot), \tilde{\rho}_h(t,\cdot)$. For $\rho_h^{\dagger}(t,\cdot)$, just notice from Lemma 2.3.2 that we have $M(\rho_h^{\dagger}(t,\cdot)) \leq C$. This uniform moment bound gives us the other two bounds for $\rho_h^{\dagger}(t,\cdot)$: for the free energy one follows the argument in Lemma 2.3.7 (using the bounded energy of ρ_h^n), and for the positive entropy one uses again (2.2.1). □

The uniform bounds established in Lemma 2.3.9 allow us to control the transport cost (w.r.t to both cost functions c_h and $\|\cdot\|^2$) of the JKO step.

Lemma 2.3.11 (Estimates of the sum of optimal transport costs)**.** We have

$$\sum_{n=0}^{N-1} W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \leq Ch, \quad \text{and} \quad \sum_{n=0}^{N-1} W_2^2(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \leq Ch. \tag{2.3.17}$$

Proof. The estimate (2.3.8), together with the uniform bounds of Lemma 2.3.9, gives the first result of (2.3.17). The second result is immediate from the first and (2.3.4), since

$$\sum_{n=0}^{N-1} W_2^2(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \leq C \sum_{n=0}^{N-1} W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \leq Ch.$$

□

The uniform moment bounds, in conjunction with the preliminary observation of Lemma 2.3.2, allow us to control the Wasserstein cost of the conservative phase.

Lemma 2.3.12 (Estimates of the sum of optimal transport costs for the conservative dynamics)**.** We have

$$\sum_{n=0}^{N-1} W_2^2(\rho_h^n, \tilde{\rho}_h^{n+1}) \leq Ch. \tag{2.3.18}$$

Proof. We recall (2.3.2), implying that for any $n = 0, \dots, N-1$, $W_2^2(\rho_h^n, \tilde{\rho}_h^{n+1}) \leq Ch^2(1 + M(\rho_h^n))$, the uniform bounded moment estimates then give the result. □

2.3.4 Convergence of the operator-splitting scheme

Having obtained a priori estimates, in this section we prove the main theorem, Theorem 2.2.5, that is the convergence of the time-interpolations of the discrete solutions constructed from the operator-splitting scheme in Section 2.2 to a weak solution of the main evolutionary equation (2.1.1). The following Lemma shows that these interpolations converge to limits which are equal almost everywhere to some curve $[0,T] \ni t \mapsto \rho(t,\cdot) \in \mathcal{P}_2^r(\mathbb{R}^d)$, and moreover, the sequences $\rho_h(t,\cdot), \tilde{\rho}_h(t,\cdot), \rho_h^\dagger(t,\cdot)$ converge in W_p (for $1 \leq p < 2$) to ρ, uniformly in time.

Lemma 2.3.13. [Convergence of the time-interpolations] Let $1 \leq p < 2$. There exists a curve $[0,T] \ni t \mapsto \rho(t,\cdot) \in \mathcal{P}_2^r(\mathbb{R}^d)$, such that

$$\lim_{h\to 0} \sup_{t\in[0,T]} \max\left\{W_p(\rho_h(t,\cdot), \rho(t,\cdot)), W_p(\tilde{\rho}_h(t,\cdot), \rho(t,\cdot)), W_p(\rho_h^\dagger(t,\cdot), \rho(t,\cdot))\right\} = 0, \tag{2.3.19}$$

where the convergence $h \to 0$ is done taking subsequences if necessary.

Proof. The proof follows an adapted version of [AGS08, Theorem 11.1.6]. We provide the argument for ρ_h only, the approach for $\tilde{\rho}_h, \rho_h^\dagger$ is similar. To obtain the uniform convergence we set up an Arzela-Ascoli argument for continuous functions between metric spaces [BS18, Theorem 1.1.11]. Since the paths ρ_h are not continuous we introduce the continuous concatenation of $\{\rho_h^n\}_n$ by geodesics. Let $n \in \{1, \dots, N-1\}$. Fix any $s, t \in [0,T]$, define the path $\nu_h : [0,T] \to \mathcal{P}_2(\mathbb{R}^d)$ by concatenating ρ_h^{n-1} and ρ_h^n on $[t_{n-1}, t_n]$ by a constant speed geodesic. Then for $t \in [t_{n-1}, t_n)$

$$\begin{aligned} W_2(\nu_h(t), \rho_h(t)) = W_2(\nu_h(t), \rho_h^n) =& W_2(\nu_h(t), \nu_h(t_n)) \\ \leq& W_2(\rho_h^{n-1}, \rho_h^n)(t - t_{n-1}) \leq W_2(\rho_h^{n-1}, \rho_h^n)h \leq Ch. \end{aligned}$$

Its not hard to see that for each $t \in [0,T]$, $M(\nu_h(t))$ is uniformly bounded, and hence $\{\nu_h(t)\}_h$ is tight. Therefore by Prokhorov's theorem, there exists $[0,T] \ni t \mapsto \rho(t) \in \mathcal{P}_2(\mathbb{R}^d)$, and a subsequence (not relabelled) such that $\nu_h(t) \rightharpoonup \rho(t) \in \mathcal{P}_2(\mathbb{R}^d)$ for all $t \in [0,T]$ as $h \to 0$. The uniformly integrable 2nd moments implies

$$\int_{B_r(0)} \|x\|^p d\nu_h(t) \leq \frac{1}{r^{2-p}} \int_{B_r(0)} \|x\|^2 d\nu_h(t) \leq C\frac{1}{r^{2-p}} \underset{r\to\infty}{\longrightarrow} 0. \tag{2.3.20}$$

(2.3.20) in combination with the weak convergence implies the sequence of continuous functions $\{\nu_h\}_h$ converges point-wise in $(\mathcal{P}_p(\mathbb{R}^d), W_p)$ (for $1 \leq p < 2$) [AGS08, Proposition 7.1.5]. We now show that this sequence is also uniformly equicontinuous. Recall that since ν_h is a concatenation of constant speed geodesics, so that for all $r \in [t_n, t_{n+1}]$, the metric derivative $|\nu_h'|(r)$ is such that (see [San17, Section 2])

$$|\nu_h'|(r) = \frac{W_2(\rho_h^n, \rho_h^{n+1})}{h}. \tag{2.3.21}$$

Now by Hölder's inequality

$$W_2(\nu_h(t), \nu_h(s)) \le \int_s^t |\nu_h'(r)| dr \le (t-s)^{1/2} \Big(\int_s^t |\nu_h'|^2(r) dr \Big)^{1/2},$$

and from (2.3.21), (2.3.17), and (2.3.18)

$$\int_0^T |\nu_h'|^2(r) dr = h \sum_{n=0}^{N-1} \Big(\frac{W_2(\rho_h^n, \rho_h^{n+1})}{h} \Big)^2 \le \frac{C}{h} \sum_{n=0}^{N-1} \big(W_2^2(\rho_h^n, \tilde{\rho}_h^{n+1}) + W_2^2(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \big) \le C.$$

Hence

$$W_2(\nu_h(t), \nu_h(s)) \le C(t-s)^{1/2},$$

i.e. ν_h is uniformly (in h) $\frac{1}{2}-$Hölder continuous with respect to the $2-$Wasserstein metric. By Jensen's inequality it is clear that $W_p \le W_q$ for $p \le q$, so that in particular for $1 \le p < 2$, $W_p(\nu_h(t), \nu_h(s)) \le C(t-s)^{1/2}$, and the family $\{\nu_h\}_{h>0}$ is equicontinuous from $[0,T]$ to $(\mathcal{P}_p(\mathbb{R}^d), W_p)$. Then an application of Arzela-Ascoli gives the uniform convergence (taking subsequences if necessary)

$$\lim_{h\to 0} \sup_{t\in[0,T]} W_p\big(\nu_h(t), \rho(t)\big) = 0.$$

We are then able to deduce the uniform convergence of ρ_h to ρ from that of ν_h, namely

$$\begin{aligned}
\lim_{h\to 0} \sup_{t\in[0,T]} W_p(\rho_h(t), \rho(t)) &\le \lim_{h\to 0} \sup_{t\in[0,T]} \Big(W_p\big(\rho_h(t), \nu_h(t)\big) + W_p\big(\nu_h(t), \rho(t)\big) \Big) \\
&\le \lim_{h\to 0} \Big(Ch + \sup_{t\in[0,T]} W_p\big(\nu_h(t), \rho(t)\big) \Big) = 0.
\end{aligned}$$

Moreover, by the uniform entropy bounds (see Lemma 2.3.10) we have by (2.2.2) that the limit $\rho(t,\cdot) \in \mathcal{P}_2^r(\mathbb{R}^d)$. By an almost identical procedure (this time concatenating geodesics between $\{\tilde{\rho}_h^n\}_n$, and using (2.3.2) for $\rho_h^\dagger$) we get the same convergence of $\tilde{\rho}_h, \rho_h^\dagger$ to some limit path $[0,T] \ni t \mapsto \tilde{\rho}(t) \in \mathcal{P}_2^r(\mathbb{R}^d)$. It remains only to show that $\rho = \tilde{\rho}$ a.e., note we have, for instance using the Dominated Convergence theorem, letting $\varphi \in C_c^\infty([0,T), \mathbb{R}^d)$

$$\begin{aligned}
\int_0^T \int_{\mathbb{R}^d} \big(\tilde{\rho}(t,x) - \rho(t,x)\big)\varphi(t,x) dx dt &= \lim_{h\to 0} \int_0^T \int_{\mathbb{R}^d} \big(\tilde{\rho}_h(t,x) - \rho_h(t,x)\big)\varphi(t,x) dx dt \\
&= \lim_{h\to 0} \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \int_{\mathbb{R}^d} \big(\tilde{\rho}_h^{n+1}(x) - \rho_h^{n+1}(x)\big)\varphi(t,x) dx dt \\
&= \lim_{h\to 0} \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \int_{\mathbb{R}^{2d}} \big(\varphi(t,x) - \varphi(t,y)\big)\tilde{\gamma}^{n+1}(dx,dy) dt,
\end{aligned}$$

where we recall $\tilde{\gamma}^{n+1}$ is the optimal coupling between ρ^{n+1} and $\tilde{\rho}^{n+1}$ in W_2. By Taylor's theorem, Jensen inequality and then Cauchy-Schwarz, we have

$$\begin{aligned}\int_0^T \int_{\mathbb{R}^d} \big(\tilde{\rho}(t,x) - \rho(t,x)\big)\varphi(t,x)dxdt &\leq \lim_{h\to 0} h \sup \|\nabla\varphi\| \sum_{n=0}^{N-1} \int_{\mathbb{R}^{2d}} \|x-y\|\gamma^{n+1}(dx,dy) \\ &\leq \lim_{h\to 0} h \sup \|\nabla\varphi\| \sum_{n=0}^{N-1} W_2(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) \\ &\leq \lim_{h\to 0} h\sqrt{N} \sup \|\nabla\varphi\| \sqrt{\sum_{n=0}^{N-1} W_2^2(\tilde{\rho}_h^{n+1}, \rho_h^{n+1})} \\ &\leq \lim_{h\to 0} Ch\sqrt{T} \sup \|\nabla\varphi\| = 0,\end{aligned}$$

where in the last line we used Lemma 2.3.11. We are then able to conclude that $\tilde{\rho}$ and ρ are equal a.e. □

We can also ascertain the L^1 convergence (2.2.18), i.e. fix $t \in [0,T]$, we show that we have weak $L^1(\mathbb{R}^d)$ convergence of $\rho_h(t,\cdot)$, $\tilde{\rho}_h(t,\cdot)$, and $\rho_h^\dagger(t,\cdot)$ to $\rho(t,\cdot)$ (the same limit as found in the previous Lemma 2.3.13), that is convergence against $L^\infty(\mathbb{R}^d)$ functions not just those in $C_b(\mathbb{R}^d)$. Indeed, since $x \mapsto \max\{x\log x, 0\}$ is a superlinear function, the uniform bounds on the positive entropy (Lemma 2.3.9) implies the families $\{\rho_h(t,\cdot)\}_h, \{\tilde{\rho}_h(t,\cdot)\}_h, \{\rho_h^\dagger(t,\cdot)\}_h$ are equi-integrable, and hence, by the weak convergence of the previous lemma, [San15, Box 8.2 (p301)] implies the weak $L^1(\mathbb{R}^d)$ convergence. Note this convergence is stronger than weak $L^1((0,T)\times\mathbb{R}^d)$ convergence.

The following lemma is a key step in our analysis linking the conservative and the dissipative phases together.

Lemma 2.3.14. For any $\varphi \in C_c^\infty([0,T)\times\mathbb{R}^d)$ we have that

$$\begin{aligned}\sum_{n=0}^{N-1} \int_{\mathbb{R}^d} \Big(\tilde{\rho}_h^{n+1}(x) - \rho_h^{n+1}(x)\Big)\varphi(t_{n+1},x)dx &= \int_0^T \int_{\mathbb{R}^d} \rho_h^\dagger(t,x)\big(\partial_t\varphi(t,x) + b[\rho_h(t-h)](x)\cdot\nabla\varphi(t,x)\big)dxdt \\ &\quad + \int_{\mathbb{R}^d} \rho^0(x)\varphi(0,x)dx. \end{aligned} \tag{2.3.22}$$

Proof. Let $n \in \{0,\dots N-1\}$. First notice that for $t \in [t_n, t_{n+1}]$ by the definition of X_h^n and the chain rule, we have

$$\partial_t\big(\varphi(t, X_h^n(t-t_n,x))\big) = \Big(\partial_t\varphi + b[\rho_n^h]\cdot\nabla\varphi\Big)(t, X_h^n(t-t_n,x)). \tag{2.3.23}$$

Now consider

$$\begin{aligned}&\sum_{n=0}^{N-1} \int_{\mathbb{R}^d} \Big(\tilde{\rho}_h^{n+1}(x) - \rho_h^{n+1}(x)\Big)\varphi(t_{n+1},x)dx - \int_{\mathbb{R}^d} \rho^0(x)\varphi(0,x)dx \\ &= \sum_{n=0}^{N-1} \int_{\mathbb{R}^d} \Big(\tilde{\rho}_h^{n+1}(x)\varphi(t_{n+1},x) - \rho_h^n(x)\varphi(t_n,x)\Big)dx \qquad (2.3.24) \\ &= \sum_{n=0}^{N-1} \int_{\mathbb{R}^d} \rho_h^n(x)\Big(\varphi(t_{n+1}, X_h^n(h,x)) - \varphi(t_n,x)\Big)dx \\ &= \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \int_{\mathbb{R}^d} \rho_h^n(x)\partial_t\big(\varphi(t, X_h^n(t-t_n,x))\big)dxdt \\ &= \sum_{n=0}^{N-1} \int_{t_n}^{t_{n+1}} \int_{\mathbb{R}^d} \rho_h^n(x)\Big(\partial_t\varphi + b[\rho_h^n]\cdot\nabla\varphi\Big)(t, X_h^n(t-t_n,x))dxdt \qquad (2.3.25) \\ &= \int_0^T \int_{\mathbb{R}^d} \rho_h^\dagger(t,x)\Big(\partial_t\varphi + b[\rho_h(t-h,\cdot)]\cdot\nabla\varphi\Big)(t,x)dxdt, \qquad (2.3.26)\end{aligned}$$

where (2.3.24) follows since φ has compact support, in (2.3.25) we have applied (2.3.23), and in (2.3.26) we have used the definitions of the interpolations $\rho_h, \rho_h^\dagger$. $\square$

Now following the classical procedure we can interpolate across the discrete Euler-Lagrange equations (2.3.7).

Lemma 2.3.15. For any $\varphi \in C_c^\infty([0,T) \times \mathbb{R}^d)$ we have

$$\int_0^T \int_{\mathbb{R}^d} \rho_h^\dagger(t,x)\big(\partial_t\varphi(t,x) + b[\rho(t-h,\cdot)](x) \cdot \nabla\varphi(t,x)\big)dxdt + \int_{\mathbb{R}^d} \rho^0(x)\varphi(0,x)dx$$
$$= h\sum_{n=0}^{N-1} \delta\mathcal{F}(\rho_h^{n+1}, D_h\nabla\varphi(t_{n+1},\cdot)) + O(h). \tag{2.3.27}$$

Proof. Let $n \in \{0,\dots,N-1\}$. Recall $\tilde{\gamma}_h^{n,c} \in \Pi(\tilde{\rho}_h^n, \rho_h^n)$, by Taylor's Theorem we have

$$\int_{\mathbb{R}^d} \Big(\rho_h^{n+1}(x) - \tilde{\rho}_h^{n+1}(x)\Big)\varphi(t_{n+1},x)dx = \int_{\mathbb{R}^{2d}} \Big(\varphi(t_{n+1},y) - \varphi(t_{n+1},x)\Big)d\tilde{\gamma}_h^{n+1,c}(x,y)$$
$$= \int_{\mathbb{R}^{2d}} \Big\langle y - x, \nabla\varphi(t_{n+1},y)\Big\rangle d\tilde{\gamma}_h^{n+1,c}(x,y) + \kappa_n(t_{n+1}), \tag{2.3.28}$$

For a remainder term κ_n. By Lemma 2.3.3 we can bound κ_n, namely,

$$|\kappa_n(t)| \le C \sup_{t\in[0,T),z\in\mathbb{R}^d} \|\nabla^2\varphi(t,z)\| \int_{\mathbb{R}^{2d}} \|x-y\|^2 d\tilde{\gamma}_h^{n+1,c}(x,y) \le C\int_{\mathbb{R}^{2d}} c_h(x,y)d\tilde{\gamma}_h^{n+1,c}(x,y). \tag{2.3.29}$$

Using (2.3.28) in combination with the Euler-Lagrange equation (2.3.7) yields the identity

$$\int_{\mathbb{R}^d} \Big(\rho_h^{n+1}(x) - \tilde{\rho}_h^{n+1}(x)\Big)\varphi(t_{n+1},x)dx = \kappa_n(t_{n+1}) - h\delta\mathcal{F}(\rho_h^{n+1}, D_h\nabla\varphi(t_{n+1},\cdot)).$$

Summing the previous expression over $n = 0,\dots,N-1$, gives

$$\sum_{n=0}^{N-1}\int_{\mathbb{R}^d} \Big(\rho_h^{n+1}(x) - \tilde{\rho}_h^{n+1}(x)\Big)\varphi(t_{n+1},x)dx = O(h) - h\sum_{n=0}^{N-1}\delta\mathcal{F}(\rho_h^{n+1}, D_h\nabla\varphi(t_{n+1},\cdot)), \tag{2.3.30}$$

where we have combined (2.3.29) with Lemma 2.3.11 to conclude $|\sum_{n=0}^{N-1}\kappa_n(t_{n+1})| \le Ch$. Finally, using (2.3.22) on the left hand side of (2.3.30), multiplying through by -1, delivers the sought result. $\square$

We are now ready to prove the main theorem, Theorem 2.2.5.

Proof of Theorem 2.2.5. Recall the convergence result of Lemma 2.3.13. To prove Theorem 2.2.5 we need only to argue that (taking subseuqences if necessary) the limit $h \to 0$, $N \to \infty$ in (2.3.27) can be taken. Clearly the error term $O(h)$ in (2.3.27) goes to zero (as $h \to 0$), and for any $\varphi \in C_c^\infty([0,T),\mathbb{R}^d)$ we have

$$\lim_{h\to 0}\int_0^T\int_{\mathbb{R}^d} \rho_h^\dagger(t,x)\partial_t\varphi(t,x)dxdt = \int_0^T\int_{\mathbb{R}^d}\rho(t,x)\partial_t\varphi(t,x)dxdt.$$

We now address the remaining terms of (2.3.27): the free energy and the divergence free part. We start with the free energy term $\delta\mathcal{F}$. Note that we can write

$$h\sum_{n=0}^{N-1}\delta\mathcal{F}\big(\rho_h^{n+1}, D_h\nabla\varphi(t_{n+1},\cdot)\big)$$
$$= \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\Big(\int_{\mathbb{R}^d}\rho_h^{n+1}(x)\big(D_h\nabla\varphi(t_{n+1},x)\cdot\nabla f(x)\big)dx - \int_{\mathbb{R}^d}\rho_h^{n+1}(x)\mathrm{div}\big(D_h\nabla\varphi(t_{n+1},x)\big)dx\Big)dt$$
$$= \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\Big(\int_{\mathbb{R}^d}\rho_h(t,x)\big(D_h\nabla\varphi(t_{n+1},x)\cdot\nabla f(x)\big)dx - \int_{\mathbb{R}^d}\rho_h(t,x)\mathrm{div}\big(D_h\nabla\varphi(t_{n+1},x)\big)dx\Big)dt. \tag{2.3.31}$$

Consider the first term on the right hand side of (2.3.31) (the second term can be dealt with in a similar manner). Adding and subtracting $D_h\nabla\varphi(t,x)$ and $D\nabla\varphi(t,x)$, we get

$$\begin{aligned}\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_{\mathbb{R}^d}&\rho_h^{n+1}\Big(D_h\nabla\varphi(t_{n+1},x)\cdot\nabla f(x)\Big)dxdt\\&=\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_{\mathbb{R}^d}\Bigg(\rho_h\Big(D\nabla\varphi\cdot\nabla f\Big)(t,x)+\rho_h\Big(\big(D_h-D\big)\nabla\varphi\cdot\nabla f\Big)(t,x)\\&\qquad\qquad+\rho_h(t)\Big(D_h\big(\nabla\varphi(t_{n+1})-\nabla\varphi(t)\big)\cdot\nabla f\Big)(x)\Bigg)dxdt.\end{aligned}\tag{2.3.32}$$

Then, as $h\to 0$, the first term tends to $\int_0^T\int_{\mathbb{R}^d}\rho\big(D\nabla\varphi\cdot\nabla f\big)(t,x)dxdt$ by the weak $L^1([0,T]\times\mathbb{R}^d)$ convergence, the second term tends to zero by Cauchy-Schwarz inequality and the fact that $\lim_{h\to 0}\|D_h-D\|=0$ and again the weak $L^1([0,T]\times\mathbb{R}^d)$ convergence. The third term in (2.3.32) also tends to zero as $h\to 0$, since

$$\begin{aligned}&\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_{\mathbb{R}^d}\rho_h(t)\Big(A_h\big(\nabla\varphi(t_{n+1})-\nabla\varphi(t)\big)\cdot\nabla f\Big)(x)dxdt\\\le& C\|A_h\|\sup_{x\in\mathbb{R}^d}\|\nabla f(x)\|\sup_{[u_h,r_h]\subset[0,T),|u_h-r_h|\le h}\ \sup_{s\in[u_h,r_h],x\in\mathbb{R}^d}\|\nabla\varphi(r_h,x)-\nabla\varphi(s,x)\|\underset{h\to 0}{\longrightarrow}0,\end{aligned}$$

where we have used that $\|D_h\|,\sup\|\nabla f\|\le C$, that ρ_h is a probability density, and that $\nabla\varphi$ is uniformly continuous.

Lastly, we address the divergence free term in (2.3.27). Adding and subtracting $\rho_h^\dagger b[\rho_h^\dagger]\cdot\nabla\varphi$ gives

$$\begin{aligned}&\int_0^T\int_{\mathbb{R}^d}\rho_h^\dagger(t,x)b[\rho_h(t-h,\cdot)](x)\cdot\nabla\varphi(t,x)dxdt\\&=\int_0^T\int_{\mathbb{R}^d}\rho_h^\dagger(t,x)\Big(b[\rho_h(t-h,\cdot)]-b[\rho_h^\dagger(t,\cdot)]\Big)(x)\cdot\nabla\varphi(t,x)dxdt+\int_0^T\int_{\mathbb{R}^d}\rho_h^\dagger(t,x)b[\rho_h^\dagger(t,\cdot)](x)\cdot\nabla\varphi(t,x)dxdt.\end{aligned}\tag{2.3.33}$$

The first term in (2.3.33) converges to zero as $h\to 0$ since

$$\begin{aligned}\Big|\int_0^T\int_{\mathbb{R}^d}&\rho_h^\dagger(t,x)\Big(b[\rho_h(t-h,\cdot)](x)-b[\rho_h^\dagger(t,\cdot)](x)\Big)\cdot\nabla\varphi(t,x)dxdt\Big|\\&\le C\int_0^T\Big(\int_{\mathbb{R}^d}\rho_h^\dagger(t,x)\|b[\rho_h(t-h,\cdot)](x)-b[\rho_h^\dagger(t,\cdot)](x)\|^2dx\Big)^{\frac12}dt &(2.3.34)\\&\le C\int_0^T W_2(\rho_h(t-h,\cdot),\rho_h^\dagger(t,\cdot))dt &(2.3.35)\\&=C\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}W_2(\rho_h^n,\rho_h^\dagger(t,\cdot))dt\\&\le CTh, &(2.3.36)\end{aligned}$$

where in (2.3.34) we have used the Cauchy-Schwarz inequality and Jensen's inequality, in (2.3.35) we have used the assumption (2.2.16), and in (2.3.36) we have used (2.3.2) and the bounded moments result of Lemma 2.3.10. The second term on the right hand side of (2.3.33) has already the desired convergence, indeed consider

$$
\begin{aligned}
&\Big|\int_0^T\int_{\mathbb{R}^d}\Big(\rho_h^\dagger(t,x)b[\rho_h^\dagger(t,\cdot)](x)-\rho(t,x)b[\rho(t,\cdot)](x)\Big)\cdot\nabla\varphi(t,x)dxdt\Big|\\
&\qquad\le C\int_0^T\int_{\mathbb{R}^d}\rho_h^\dagger(t,x)\|b[\rho_h^\dagger(t,\cdot)](x)-b[\rho(t,\cdot)](x)\|dxdt \qquad (2.3.37)\\
&\qquad\qquad+\Big|\int_0^T\int_{\mathbb{R}^d}\big(\rho(t,x)-\rho_h^\dagger(t,x)\big)b[\rho(t,\cdot)](x)\cdot\nabla\varphi(t,x)dxdt\Big|\\
&\qquad\le CT\sup_{t\in[0,T]}W_2(\rho_h^\dagger(t,\cdot),\rho(t,\cdot))+\Big|\int_0^T\int_{\mathbb{R}^d}\big(\rho(t,x)-\rho_h^\dagger(t,x)\big)b[\rho(t,\cdot)](x)\cdot\nabla\varphi(t,x)dxdt\Big|, \qquad (2.3.38)
\end{aligned}
$$

where in (2.3.37) we have added and subtracted $\rho_h^\dagger b[\rho]$, used Cauchy-Schwarz inequality, and in (2.3.38) we used again the assumption (2.2.16). The two terms in (2.3.38) go to zero from the convergence established for $\rho_h^\dagger$, and that $b[\rho(t,\cdot)]\cdot\nabla\varphi\in L^\infty((0,T)\times\mathbb{R}^d)$.

Having the above estimates, by passing to the limit $h\to 0$ in (2.3.27) we obtain precisely the weak formulation (2.2.17) of the evolutionary equation (2.1.1). This completes the proof of Theorem 2.2.5. □

2.4 The entropy regularised scheme

Recall Section 1.3.2. In this section, we provide an entropy regularised version of the scheme introduced in Section 2.1. The regularised scheme, presented below, differs only in that we have penalised the weighted Wasserstein distance by an entropy term. The convergence of this new scheme is stated in Theorem 2.4.2, the proof of which is sketched since it only differs slightly to that of Theorem 2.2.5, and the techniques used are similar to those that will appear in Chapter 4. The following assumption introduces a theoretical constraint on the scaling of the time-step and strength of entropic regularisation. It ensures that the error made by the regularisation goes to zero sufficiently fast.

Assumption 2.4.1 (The regularisation's scaling parameters)**.** Take three sequences $\{N_k\}_{k\in\mathbb{N}}\subset\mathbb{N}$, $\{\epsilon_k\}_{k\in\mathbb{N}}\subset\mathbb{R}_+$, and $\{h_k\}_{k\in\mathbb{N}}\subset\mathbb{R}_+$, which, for any $k\in\mathbb{N}$, abide by the following scaling

$$h_kN_k=T,\quad\text{and}\quad 0<\epsilon_k\le\epsilon_k|\log\epsilon_k|\le Ch_k^2, \tag{2.4.1}$$

and are such that $h_k,\epsilon_k\to 0$ and $N_k\to\infty$ as $k\to\infty$.

An entropic regularisation of the operator-splitting scheme. Let the sequences $\{h_k\}_{k\in\mathbb{N}},\{\epsilon_k\}_{k\in\mathbb{N}},\{N_k\}_{k\in\mathbb{N}}$, satisfy Assumption 2.4.1. Throughout the section, for the sake of notational clarity, we have mostly suppressed the dependence of ϵ,h and N on k. Let $\mathcal{F}(\rho_0)<\infty$, and set $\rho_k^0=\tilde\rho_k^0=\rho^0$. Let $n\in\{0,\dots,N_k-1\}$. Given ρ_k^n we find ρ_k^{n+1} as follows, first introduce the push forward of ρ_k^n by the Hamiltonian flow as

$$\tilde\rho_k^{n+1}=X_k^n(h,\cdot)_\#\rho_k^n, \tag{2.4.2}$$

where X_k^n solves

$$\begin{cases}\partial_tX_k^n=b[\rho_k^n]\circ X_k^n,\\ X_k^n(0,\cdot)=\mathrm{id}.\end{cases} \tag{2.4.3}$$

Next define ρ_k^{n+1} as the minimiser of the regularised JKO type descent step

$$\rho_k^{n+1}=\mathrm{argmin}_{\rho\in\mathcal{P}_2^r(\mathbb{R}^d)}\Big\{\frac{1}{2h}W_{c_h,\epsilon}(\tilde\rho_k^{n+1},\rho)+\mathcal{F}(\rho)\Big\}, \tag{2.4.4}$$

where $W_{c_h,\epsilon}$ is the regularised weighted Wasserstein

$$W_{c_h,\epsilon}(\mu,\nu):=\inf_{\gamma\in\Pi(\mu,\nu)}\Big\{\int_{\mathbb{R}^{2d}}c_h(x,y)d\gamma(x,y)+\epsilon H(\gamma)\Big\}, \tag{2.4.5}$$

for the same cost function defined in (2.2.7). Let $\tilde{\gamma}_k^{n,c}$ be the optimal plan associated to $W_{c_h,\epsilon}(\tilde{\rho}_k^n, \rho_k^n)$, and define the interpolations $\rho_k, \tilde{\rho}_k, \rho_k^\dagger$ analogously to the unregularised case but now with respect to the new sequences $\{\rho_k^n\}_{n=0}^N$ and $\{\tilde{\rho}_k^n\}_{n=0}^N$.

The convergence of the above entropic regularised scheme is established in the next result.

Theorem 2.4.2. Assume that f, b and D satisfy Assumption 2.2.2, and let the sequences $\{h_k\}_{k\in\mathbb{N}}, \{\epsilon_k\}_{k\in\mathbb{N}}$ $\{N_k\}_{k\in\mathbb{N}}$ satisfy Assumption 2.4.1. Let $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ satisfy $\mathcal{F}(\rho_0) < \infty$. Let $\{\rho_k^n\}_{n=0}^{N_k}, \{\tilde{\rho}_k^n\}_{n=0}^{N_k}$ be the solution of the regularised scheme (2.4.2)-(2.4.4), with interpolations $\rho_k, \tilde{\rho}_k, \rho_k^\dagger$ as defined above.

Then

(i) for each $t \in [0, T]$ we have

$$\rho_k(t,\cdot), \tilde{\rho}_k(t,\cdot), \rho_k^\dagger(t,\cdot) \underset{k\to\infty}{\longrightarrow} \rho(t) \quad \text{in} \quad L^1\big(\mathbb{R}^d\big). \tag{2.4.6}$$

(ii) Moreover, there exists a map $[0,T] \ni t \mapsto \rho(t,\cdot)$ in $\mathcal{P}_2^r(\mathbb{R}^d)$ such that for all $1 \le p < 2$

$$\sup_{t\in[0,T]} \max \Big\{ W_p\big(\rho_k(t,\cdot), \rho(t,\cdot)\big),\ W_p\big(\tilde{\rho}_k(t,\cdot), \rho(t,\cdot)\big),\ W_p\big(\rho_k^\dagger(t,\cdot), \rho(t,\cdot)\big) \Big\} \underset{k\to\infty}{\longrightarrow} 0, \tag{2.4.7}$$

where the limits ρ appearing above are weak solutions of the evolution equation (2.1.1) in the sense of Definition 2.2.4. The convergence $k \to \infty$ is understood as being taken up to a subsequence if necessary.

The proof does not change much from that of Theorem 2.2.5, so we provide only a sketch, highlighting the parts that are different.

Proof of Theorem 2.4.2. Let $n \in \{0, \ldots, N-1\}$.

The well-posedness. The well-posedness of the regularised scheme relies on the well-posedness of the minimisation problem (2.4.5), the proof is part of the more general well-posedness result Proposition 4.5.1 found in Chapter 4.

A priori estimates. In the proof of Theorem 2.2.5 we compare the quantity $\frac{1}{2h}W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}) + \mathcal{F}(\rho_h^{n+1})$ against $\frac{1}{2h}W_{c_h}(\tilde{\rho}_h^{n+1}, \tilde{\rho}_h^{n+1}) + \mathcal{F}(\tilde{\rho}_h^{n+1})$. The term $W_{c_h}(\tilde{\rho}_h^{n+1}, \tilde{\rho}_h^{n+1})$ is zero, and hence we end up with a control of $W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1})$ in terms of the free energy. However, since $W_{c_h,\epsilon}(\tilde{\rho}_k^{n+1}, \tilde{\rho}_k^{n+1}) \neq 0$, we need to select a new distribution to compare the performance of ρ_k^{n+1} against. We judiciously choose a distribution ρ_ϵ (with optimal plan γ_ϵ) as to make the cost of transporting mass zero, i.e as $\epsilon \to 0$ we aim to have $(c_h, \gamma_\epsilon) \to 0$. We construct such a candidate distribution ρ_ϵ in the following way, let $G \in C_c^\infty(\mathbb{R}^d)$ be a probability density, such that $M(G) = 1$ and $H(G) < \infty$. Define $G_\epsilon(\cdot) := \epsilon^{-2d} G(\frac{\cdot}{\epsilon^2})$, and

$$\gamma_\epsilon(x, y) := \tilde{\rho}_k^{n+1}(x) G_\epsilon\big(y - x\big),$$

as the joint distribution with first marginal $\tilde{\rho}_k^{n+1}$, and second marginal $\rho_\epsilon(y) := \int \gamma_\epsilon(x,y)dx$. One can then calculate/express $H(\gamma_\epsilon), \mathcal{F}(\rho_\epsilon), (c_h, \gamma_\epsilon)$ in terms of $\tilde{\rho}_k^{n+1}$ (see Lemma 4.6.3 of Chapter 4). Comparing the performance of ρ_k^{n+1} against ρ_ϵ in (2.4.4) we get, making use of the scaling (2.4.1) and that $H(\tilde{\gamma}_k^{n+1,c}) \ge H(\rho_k^{n+1}) + H(\tilde{\rho}_k^{n+1})$, the following inequality

$$(c_h, \tilde{\gamma}_k^{n+1,c}) \le Ch^2\Big(M(\tilde{\rho}_k^{n+1}) + 1\Big) - \epsilon H(\rho_k^{n+1}) + 2h\Big(\mathcal{F}(\tilde{\rho}_k^{n+1}) - \mathcal{F}(\rho_k^{n+1})\Big). \tag{2.4.8}$$

We are able to obtain bounded 2nd moments, energy, and entropy estimates in an almost identical fashion as to Lemma 2.3.9, specifically in (2.3.11) we use $(c_h, \tilde{\gamma}_k^{i+1,c})$ in place of $W_{c_h}(\tilde{\rho}^{i+1}, \rho^{i+1})$, and apply (2.4.8). Moreover, summing (2.4.8) and using such estimates, yields the bound

$$\sum_{n=0}^{N-1} (c_h, \tilde{\gamma}_k^{n+1,c}) \le Ch. \tag{2.4.9}$$

It is easy to conclude that we also have

$$\sum_{n=0}^{N-1} W_2^2(\tilde{\rho}_k^{n+1}, \rho_k^{n+1}) \le Ch \quad \text{and} \quad \sum_{n=0}^{N-1} W_2^2(\rho_k^n, \tilde{\rho}_k^{n+1}) \le Ch. \tag{2.4.10}$$

The discrete Euler-Lagrange equation and concluding the convergence. Since ρ_k^{n+1} solves the minimisation problem (2.4.4), the associated discrete Euler-Lagrange equation reads, for any $\varphi \in C_c^\infty(\mathbb{R}^d)$,

$$0 = \frac{1}{h}\int_{\mathbb{R}^{2d}} \Big\langle x-y, \nabla\varphi(y)\Big\rangle d\tilde{\gamma}^{n+1,c}(x,y) + \delta\mathcal{F}(\rho_k^{n+1}, D_h\nabla\varphi) - \frac{\epsilon}{2h}\int_{\mathbb{R}^d} \rho_k^{n+1}(y)\mathrm{div}\big(D_h\nabla\varphi(y)\big)dy. \quad (2.4.11)$$

Therefore, the analogous result to Lemma 2.3.15 is

$$\begin{aligned}&\int_0^T\int_{\mathbb{R}^d} \rho_k^\dagger(t,x)\big(\partial_t\varphi(t,x) + b[\rho(t,\cdot)](x)\cdot\nabla\varphi(t,x)\big)dxdt + \int_{\mathbb{R}^d}\rho^0(x)\varphi(0,x)dx \\ &= \sum_{n=0}^{N-1}\Big(h\delta\mathcal{F}(\rho_k^{n+1}, D_h\nabla\varphi(t_n,\cdot)) - \frac{\epsilon}{2h}\int_{t_n}^{t_{n+1}}\int_{\mathbb{R}^d}\rho_k^{n+1}(y)\mathrm{div}\big(D_h\nabla\varphi(t_n,y)\big)dy\Big) + O(h). \quad (2.4.12)\end{aligned}$$

The convergence claimed in (2.4.6) and (2.4.7) follows by a priori estimates identical to those of Lemma 2.3.13. Hence to complete the proof of Theorem 2.4.2 we need only to deal with the term appearing from the regularisation

$$\sum_{n=0}^{N-1}\frac{\epsilon}{2h}\int_{t_n}^{t_{n+1}}\int_{\mathbb{R}^d}\rho_k^{n+1}(y)\mathrm{div}\big(D_h\nabla\varphi(t_n,y)\big)dy,$$

and show it goes to zero as $\epsilon, h \to 0$. This is clear by a similar argument to that in the end of the proof of Section 2.3.4: using the convergence (2.4.6) of ρ_k and the scaling (2.4.1) which implies that $\frac{\epsilon}{h} \to 0$. □

2.5 Examples

In this section, we present four concrete examples of evolutionary equations that can all be written in the general form (2.1.1): the Vlasov-Fokker-Planck equation, a degenerate non-linear diffusion equation of Kolmogorov-type, the regularised Vlasov-Poisson FPE, and a generalised Vlasov-Langevin equation.

Applicability of Theorems 2.2.5 and 2.4.2 to the examples. In all these examples, we will show explicitly the (non-local) vector field b and the diffusion matrix D. Assuming the drift vector fields and the diffusion matrix are such that Assumption 2.2.2 is satisfied, then Theorem 2.2.5 and/or of Theorem 2.4.2 provides novel operator-splitting variational schemes for solving these evolutionary equations. It will be clear from the explicit formulas that D is symmetric positive semi-definite and $b[\rho]$ is divergence-free. It remains to consider the first and second conditions in (2.2.15), which are assumptions on the growth and regularity of the vector field, and (2.2.16). In all examples, the vector field $b[\rho](x)$ consists of a local part and a non-local part, where the non-local part is a convolution of ρ with an interaction kernel K, namely of the form

$$b_{\text{non-local}}[\rho](x) := (K*\rho)(x) = \int_{\mathbb{R}^d} K(x-x')d\rho(x').$$

When the kernel K is uniformly bounded, Lipschitz, and differentiable the non-local part fulfills Assumption 2.2.2.

Lemma 2.5.1. Suppose that K is uniformly bounded and Lipschitz. Then for all $\rho, \mu \in \mathcal{P}_2(\mathbb{R}^d)$, $z \in \mathbb{R}^d$, we have

$$\int_{\mathbb{R}^d} \|K*\rho(z) - K*\mu(z)\|^p \, d\rho(z) \le CW_p^p(\rho,\mu), \; p \in \{1,2\} \quad (2.5.1)$$

$$\|K*\mu(z)\| \le C(1+\|z\|), \quad (2.5.2)$$

$$K*\mu \in W^{1,1}_{\text{loc}}(\mathbb{R}^d). \quad (2.5.3)$$

Proof. We first prove (2.5.1). We will use the following equivalent formulation of the Wasserstein distance [Vil08, Definition 6.1]

$$W_p^p(\rho,\mu) = \inf\Big[\mathbb{E}(\|X-Y\|^p)\Big], \quad (2.5.4)$$

where the infimum is taken over all couples of $\mathbb{R}^d$ random variables X and Y with $Y \sim \rho$ and $X \sim \mu$. Now let $\mu, \rho \in \mathcal{P}_2(\mathbb{R}^d)$ and take random variables X and Y with $Y \sim \rho$ and $X \sim \mu$. We have for $p \in \{1, 2\}$

$$\begin{aligned}\int_{\mathbb{R}^d} \|K * \rho(z) - K * \mu(z)\|^p \, d\rho(z) &= \int_{\mathbb{R}^d} \| \int_{\mathbb{R}^d} K(z - z')\big(d\rho(z') - d\mu(z')\big)\|^p \, d\rho(z) \\ &= \int_{\mathbb{R}^d} \|\mathbb{E}[K(z - Y) - K(z - X)]\|^p \, d\rho(z) \\ &\leq \int_{\mathbb{R}^d} \mathbb{E}[\|K(z - Y) - K(z - X)\|^p] \, d\rho(z) \\ &\leq C \int_{\mathbb{R}^d} \mathbb{E}[\|Y - X\|^p] \, d\rho(z) = C\mathbb{E}[\|Y - X\|^p].\end{aligned}$$

Taking the infimum over all X and Y and using (2.5.4) yields (2.5.1). Verifying (2.5.2) is straightforward by the uniform bound on K. Finally, we check (2.5.3). Let Ω be an arbitrary compact set in $\mathbb{R}^d$. Firstly it is clear that $K * \mu(z) \in L^1_{\text{loc}}(\mathbb{R}^d)$ since K is uniformly bounded. Let $i, j \in 1, \ldots, d$. It remains to show $\partial_{z_j} K_i * \mu(z) \in L^1_{\text{loc}}(\mathbb{R}^d)$. In fact, since $\|\nabla K_i\| \leq C$, we have

$$\int_\Omega \| \int \partial_{z_j} K_i(z - z') d\mu(z') \| dz \leq \int_\Omega \| \int \nabla K_i(z - z') d\mu(z') \| dz \leq C|\Omega|.$$

This completes the proof of this lemma. □

We now discuss concrete applications of our work.

2.5.1 Vlasov-Fokker-Planck equation (VFPE)

The Vlasov-Fokker-Planck equation, which describes the probability of finding a particle at time t with position $x \in \mathbb{R}^d$ and velocity $v \in \mathbb{R}^d$ moving under the influence of an external potential ∇g, an interaction force K, a frictional force ∇f and a stochastic noise, is given by

$$\partial_t \rho = -v \cdot \nabla_x \rho + \nabla g \cdot \nabla_v \rho + \mathrm{div}_v\big(\rho K * \rho\big) + \mathrm{div}_v\big(\rho \nabla f\big) + \Delta_v \rho.$$

It is the forward Kolmogorov equation of the following stochastic differential equation

$$\begin{cases} dX_t = V_t dt \\ dV_t = -\big(K * \rho(t, X_t) + \nabla g(X_t)\big)dt - \nabla f(V_t)dt + \sqrt{2} dW_t \\ \rho(t) = \mathrm{Law}(X_t, V_t). \end{cases}$$

The VFPE is a special case of (2.1.1) with

$$b[\rho](x, v) = \begin{pmatrix} v \\ -\big(\nabla g(x) + K * \rho(x)\big) \end{pmatrix}, \qquad D = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}, \quad f(x, v) = f(v), \quad (x, v) \in \mathbb{R}^{2d}. \tag{2.5.5}$$

When there is no interaction (i.e., $K = 0$) the VFPE reduces to the Kramers equation. As mentioned in the introduction, various variational schemes have been developed for the Kramers equation [DPZ14, Hua00, CG04, MS20a], see Chapter 4 for extensions of these work to non-linear models. Our work not only provides a novel scheme but also incorporates the interaction force.

2.5.2 Regularized Vlasov-Poisson-Fokker-Planck equation

The Vlasov-Poisson-Fokker-Planck equation is given by

$$\partial_t \rho = -v \cdot \nabla_x \rho + \nabla\big(g(x) + \phi[\rho](x)\big) \cdot \nabla_v \rho - \beta \mathrm{div}_v\big(\rho v\big) + \sigma \Delta_v \rho. \tag{2.5.6}$$

for positive constants σ, β and variables $x, v \in \mathbb{R}^d$, where ϕ solves the Poisson equation

$$\Delta \phi(x) = -\int_{\mathbb{R}^d} \rho(x, v) dv,$$

the solution of which is

$$\phi(x) = \int_{\mathbb{R}^{2d}} \Gamma(x-y)\rho(y,v)dydv, \tag{2.5.7}$$

for Γ defined as

$$\Gamma(r) := \begin{cases} \frac{\omega_d}{\|r\|^{\frac{d-2}{2}}} & \text{for } d>2, \\ \omega_2 \log\|r\| & \text{for } d=2, \end{cases}$$

where ω_d is the surface area of the unit ball in $\mathbb{R}^d$. This equation is of great importance in plasma physics, as it models a cloud of charged particles influencing each other through a Coulomb interaction, whilst subject to deterministic and random forcing. Since Γ is singular our methods can not be directly applied, it is easy to check that (2.2.15) fails to hold. However, if we consider ϕ^ϵ defined analogously to (2.5.7) but with Γ replaced by

$$\Gamma^\epsilon(r) = \begin{cases} \frac{\omega_d}{\left(\|r\|^2+\epsilon\right)^{\frac{d-2}{2}}} & \text{for } d>2, \\ \frac{\omega_d}{2}\log\left(\|r\|^2+\epsilon\right) & \text{for } d=2, \end{cases}$$

then we arrive at the regularised Vlasov-Poisson Fokker-Planck equation

$$\partial_t\rho^\epsilon = -v\cdot\nabla_x\rho^\epsilon + \nabla\big(g(x)+\phi^\epsilon[\rho^\epsilon](x)\big)\cdot\nabla_v\rho^\epsilon - \beta\operatorname{div}_v\big(\rho^\epsilon v\big) + \sigma\Delta_v\rho^\epsilon. \tag{2.5.8}$$

Here we have regularised the Kernel appearing in the convolution (this is different from the regularisation discussed in Section 2.4). For any $\epsilon>0$, Γ^ϵ is no longer singular, and $\|\nabla\Gamma^\epsilon\|$ is uniformly bounded. Moreover, $\nabla\Gamma^\epsilon$ is Lipschitz, indeed, the Hessian is uniformly bounded which can be seen from the following explicit computations, for $d\geq 2$ we have

$$\partial_{x_i}\partial_{x_j}\Gamma^\epsilon(x) = C_d\begin{cases} \frac{1}{(\|x\|^2+\epsilon)^{\frac{d}{2}}} - \frac{dx_i^2}{(\|x\|^2+\epsilon)^{\frac{d+2}{2}}} & \text{if } i=j, \\ -\frac{dx_ix_j}{(\|x\|^2+\epsilon)^{\frac{d+2}{2}}} & \text{if } i\neq j, \end{cases}$$

for some constant C_d depending only on the dimension. Hence by Lemma 2.5.1 assumptions (2.2.15) and (2.2.16) are satisfied.

The solutions ρ^ϵ to (2.5.8) have been shown to converge (as $\epsilon\to 0$) to the solution of the original system (2.5.6) [CS95]. One-step variational schemes (in the space of probability measures) have already been proposed for (2.5.8), see [HJ00]. However, the cost function used in [HJ00] is not a metric, the free energy depends on the time-step *and* contains a mix of conservative and dissipative terms. Our approach naturally splits the conservative and dissipative dynamics.

2.5.3 A generalised Vlasov-Langevin equation

Next we consider the following generalised Vlasov-Langevin equation [OP11, Duo15]

$$\partial_t\rho = -p\cdot\nabla_q\rho + \Big(\mathcal{A}(q) + K*\rho(q) - \sum_{j=1}^m \Lambda^j z^j\Big)\cdot\nabla_p\rho + \sum_{j=1}^m \operatorname{div}_{z^j}\left[(\Lambda^j p + \alpha^j z^j)\rho\right] + \Delta_z\rho. \tag{2.5.9}$$

Note that in the above equation, the coordinates are $(q,p,z)\in\mathbb{R}^{2d+md}$, with $q,p\in\mathbb{R}^d$ and $z\in\mathbb{R}^{md}$ for some $m\in\mathbb{N}$. Equation (2.5.9) is the forward Kolmogorov equation of the SDE system

$$\begin{cases} dQ_t = P_t\,dt, \\ dP_t = -\mathcal{A}(Q_t)\,dt - K*\rho(t,Q_t)\,dt + \sum_{j=1}^m \Lambda^j Z_t^j\,dt, \\ dZ_t^j = -\Lambda^j P_t\,dt - \alpha^j Z_t^j\,dt + \sqrt{2}\,dW_t^j, \qquad j=1,\dots,m. \\ \rho(t) = \mathrm{Law}(Q_t,P_t,Z_t^1,\dots,Z_t^m), \end{cases} \tag{2.5.10}$$

where W_t^j are independent $d-$dimensional Brownian motions, $\mathcal{A}:\mathbb{R}^d\to\mathbb{R}^d$ is an external potential, $K:\mathbb{R}^d\to\mathbb{R}^d$ an interaction kernel, $\Lambda^j,\alpha^j\in\mathbb{R}^{d\times d}$ constant diagonal matrices $\forall j\in\{1,\dots,m\}$. When $\mathcal{A}$ is the gradient of a potential and no kernel is present ($K = 0$), then (2.5.10) can be viewed as the coupling of a deterministic Hamiltonian system (Q_t, P_t) to a heat bath Z_t, the literature on this subject is vast. In this setup, for large m the Markovian system (2.5.10) approximates the Generalised Langevin equation (GLE). The GLE serves as a standard model in non-Markovian non-equilibrium statistical mechanics, where the Hamiltonian system is in contact with one or more heat baths. The heat baths are modeled by the linear wave equation and are initialised according to Gibbs distribution, see [Kup04, OP11, RB06] and references therein. When $K \neq 0$, the mean field term $K * \rho$ models the particle interactions in the underlying deterministic system (via the positions Q_t). In this case, (2.5.10) is the McKean-Vlasov limit of a system of weakly interacting particles [Duo15].

Again the generalised Vlasov-Langevin equation is another example of (2.1.1) where free vector field, diffusion matrix, and potential energy are given by

$$b[\rho](q,p,z) = \begin{pmatrix} p \\ -\mathcal{A}(q) - K * \rho(q) + \sum_{j=1}^m \Lambda^j z^j \\ -\Lambda^1 p \\ \vdots \\ -\Lambda^m p \end{pmatrix}, \quad D = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & I \end{pmatrix}, \quad f(q,p,z) = f(z) = \sum_{j=1}^m \frac{1}{2} \|\alpha^j z^j\|^2,$$

where I is the $md \times md$ identity matrix.

2.5.4 A degenerate diffusion equation of Kolmogorov-type

The final example that we consider is the following non-linear degenerate equation of Kolmogorov type

$$\partial_t \rho = -\sum_{i=2}^n x_i \cdot \nabla_{x_{i-1}} \rho + \mathrm{div}_{x_n}(\nabla f(x_n)\rho) + \Delta_{x_n} \rho. \tag{2.5.11}$$

In the above equation, the coordinates are $\mathbf{x} = \big(x_1, x_2, \ldots, x_{n-1}, x_n\big)^T$, where $x_i \in \mathbb{R}^d$ for each $i \in \{1, \ldots, n\}$. Equation (2.5.11) is the forward Kolmogorov equation of the associated stochastic differential equations

$$\begin{cases} dX_1 = X_2 \, dt \\ dX_2 = X_3 \, dt \\ \quad \vdots \\ dX_{n-1} = X_n \, dt \\ dX_n = -\nabla f(X_n) \, dt + \sqrt{2} \, dW, \end{cases} \tag{2.5.12}$$

where W_t is a d-dimensional Wiener process. System (2.5.12) describes the motion of n coupled oscillators connected to their nearest neighbours with the last oscillator additionally forced by a random noise which propagates through the system. The simplest cases of $n = 1, n = 2$ correspond to the heat equation and Kramers' equation (with no background potential) respectively. When $n > 2$ this type of equations arise as models of simplified finite Markovian approximations of generalised Langevin dynamics [OP11], or harmonic oscillator chains [BL08, DM10]. The recent work [DT17] (see also Section 4.3.3) has constructed a one-step scheme for (2.5.11), however, the cost function used there (the mean squared derivative cost function (4.3.21)), although explicit, does not take a simple form.

Equation (2.5.11) is yet another special case of (2.1.1) with the following divergence free vector field, diffusion matrix, and potential energy

$$b(\mathbf{x}) = (x_2, x_3, \ldots, x_n, 0)^T, \qquad D = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}, \qquad f(\mathbf{x}) = f(x_n), \tag{2.5.13}$$

where, in the matrix D, I is the $d \times d$-dimensional identity matrix, and remaining elements are all 0.

Appendix

2.A Well-posedness of the JKO step

We provide a series of preliminary results, these will aid us in proving the well-posedness of the JKO minimisation step.

Lemma 2.A.1. For any $h > 0$, and any μ and ν in $\mathcal{P}_2(\mathbb{R}^d)$, it is true that

$$M(\nu) \le 2\big(W_2^2(\mu,\nu) + M(\mu)\big) \tag{2.A.1}$$

and

$$M(\nu) \le C\big(W_{c_h}(\mu,\nu) + M(\mu)\big). \tag{2.A.2}$$

Proof. The result (2.A.1) for W_2 is obvious. For (2.A.2) just use (2.A.1) in conjunction with (2.3.4). □

Lemma 2.A.2. Let $h > 0$. Given $\mu, \nu \in \mathcal{P}_2^r(\mathbb{R}^d)$ there exists $\gamma \in \Pi(\mu,\nu)$ such that

$$W_{c_h}(\mu,\nu) = (c_h, \gamma).$$

Moreover, the map $\gamma \mapsto (c_h, \gamma)$ is weakly lower semi-continuous.

Proof. c_h is continuous and non-negative, hence the map $\mathcal{P}(\mathbb{R}^{2d}) \ni \gamma \mapsto (c_h,\gamma)$ is weakly lower semi-continuous by [Vil08, Lemma 4.3]. For the existence see [Vil08, Theorem 4.1]. □

Lemma 2.A.3 (Lower Semi-Continuity of the functionals)**.** Let $\{\nu_k\}_{k\in\mathbb{N}} \subset \mathcal{P}_2^r(\mathbb{R}^d)$, $\mu,\nu \in \mathcal{P}_2^r(\mathbb{R}^d)$, with $\nu_k \rightharpoonup \nu$ as $k \to \infty$. Assume that for all $k \in \mathbb{N}$ the probability measures ν_k, μ, ν have uniformly bounded entropy and 2nd moments. Then

$$\mathcal{F}(\nu) \le \liminf_{k\to\infty} \mathcal{F}(\nu_k), \quad \text{and} \quad W_{c_h}(\mu,\nu) \le \liminf_{k\to\infty} W_{c_h}(\mu,\nu_k). \tag{2.A.3}$$

Proof. Let $\{\nu_k\}, \mu, \nu$ be as assumed above, and $\{\gamma_k\}$ be the associated optimal plans in $W_{c_h,\epsilon}(\mu,\nu_k)$. Note $\{\gamma_k\} \subset \Pi(\mu,\{\nu_k\})$ (see notation, Section 1.4). Since $\{\nu_k\}$ is weakly convergent then it is tight, and [Vil08, Lemma 4.4] implies that $\Pi(\mu,\{\nu_k\})$ is so too. Extracting (and relabelling) a subsequence $\{\gamma_k\}$, we know that (as $k \to \infty$) $\gamma_k \rightharpoonup \gamma \in \mathcal{P}(\mathbb{R}^{2d})$. In fact $\gamma \in \Pi(\mu,\nu)$ since the weak convergence of γ_k implies the weak convergence of its marginals (and we know $\nu_k \rightharpoonup \nu$). Now, the lower semi-continuity described in Lemma 2.A.2 implies that

$$\liminf_{k\to\infty} W_{c_h}(\mu,\nu_k) = \liminf_{k\to\infty} \frac{1}{2h}(c_h,\gamma_k) \ge \frac{1}{2h}(c_h,\gamma) \ge W_{c_h}(\mu,\nu).$$

The lower semi-continuity is proved for a more general class of $\mathcal{F}$ in Chapter 4 (Lemma 4.5.8). □

With the above results in hand we can give the proof of Proposition 2.3.4.

Proof of Proposition 2.3.4. Let $0 < h < 1$ and $\mu, \nu \in \mathcal{P}_2^r(\mathbb{R}^d)$. Define $J_{c_h}(\mu,\nu) := \frac{1}{2h} W_{c_h}(\mu,\nu) + \mathcal{F}(\nu)$, then we have

$$J_{c_h}(\mu,\nu) = \frac{1}{2h} W_{c_h}(\mu,\nu) + M(\mu) + \mathcal{F}(\nu) - M(\mu) \geq W_{c_h}(\mu,\nu) + M(\mu) + \mathcal{F}(\nu) - M(\mu) \tag{2.A.4}$$

$$\geq C_1 M(\nu) + H(\nu) - M(\mu) \tag{2.A.5}$$

$$\geq C_1 M(\nu) - C_2(1 + M(\nu))^\alpha + C_\mu, \tag{2.A.6}$$

where in (2.A.4) we have used that $h < 1$, in (2.A.5) we used Lemma 2.A.1 and the non-negativity of f, and in (2.A.6) we used Lemma 2.2.1. We emphasize that the constants $C_1, C_2 > 0$ are independent of μ, ν and $C_\mu > 0$ is independent of ν. Inequality (2.A.6) implies that $\nu \mapsto J_{c_h}(\mu,\nu)$ is bounded from below. Note that there exists a $\nu \in \mathcal{P}_2^r(\mathbb{R}^d)$ such that $J_{c_h}(\mu,\nu) < \infty$, for example, take $\nu = \mu$ (and the product plan).

Let $\{\nu_k\}$ be a minimising sequence and note that this implies $M(\nu_k), H(\nu_k)$ are uniformly bounded. The uniform boundedness of $M(\nu_k)$ implies tightness of $\{\nu_k\}$, and hence extracting a subsequence we have $\nu_k \rightharpoonup \nu^* \in \mathcal{P}(\mathbb{R}^d)$. Moreover, $\nu^* \in \mathcal{P}_2(\mathbb{R}^d)$ since uniformly bounded 2nd moments and weak convergence of $\{\nu_k\}$ implies that the limit has a bounded 2nd moment as well. Additionally, $\nu^* \in \mathcal{P}_2^r(\mathbb{R}^d)$ by the lower semi-continuity of H, see Lemma 2.2.1. That ν^* is indeed the minimiser of (2.3.5) follows from the lower semi-continuity in Lemma 2.A.3. Finally, the linearity of $F(\cdot)$, convexity of $W_2(\mu,\cdot)$, and the strict convexity of $H(\cdot)$, implies strict convexity of $J_{c_h}(\mu,\cdot)$ and hence uniqueness of minimisers. $\square$

Chapter 3

A Splitting Scheme for Generalised Wasserstein pre-GENERIC Diffusion Processes

At the time of writing, the material contained in this chapter is not published anywhere.

If the assumptions of the last chapter are strengthened, then we can view the setup as a generalised Wasserstein pre-GENERIC splitting, and get a *fully structure preserving scheme.* This alternative perspective provides arguably one of the most natural extensions to the JKO scheme. We stress the main point here, in comparison to the previous chapter: the assumptions are strengthened in such a way that we can use the relative entropy (against an invariant measure) as the free energy functional, the splitting is then natural, and the scheme we construct is *fully structure preserving*, in that the conservative dynamics preserve the free energy.

3.1 Introduction

Recently [DO21] the frameworks of Hypocoercivity Theory and GENERIC were shown to be substantially equivalent. These theories are built for studying stochastic dynamics, more specifically the associated Kolmogorov and Fokker-Planck PDE, for which one can identify a conservative-dissipative splitting structure. The point of this chapter is to illustrate that we can develop fully structure preserving discrete schemes based on this splitting, whereby the dissipative part is solved via a JKO variational scheme. We start with a brief outline of the two frameworks. We warn the reader that, in what follows, we ignore many technical matters concerning the domains of definition of the operators that appear. It should be assumed that these act on an appropriate subset of $L^2(\mathbb{R}^d)$, which is dense in the intersection of the Kolmogorov and Fokker-Planck operators, and on which all the operations are well defined. In Section 3.2, these technical matters are addressed rigorously.

Hypocoercivity. Recall that, the semigroup P_t of a given time-homogeneous Markov process $\{Z_t\}_{t\geq 0}$[1] (say taking values in $\mathbb{R}^d$) acts on $f \in C_b(\mathbb{R}^d)$ and is defined as $(P_t f)(x) := \mathbb{E}[f(Z_t)|Z_0 = x]$. Moreover, for a fixed f, the function $(P_\cdot f)(\cdot) : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}$ solves the (backward) Kolmogorov equation

$$\partial_t u(t,x) = \mathscr{L} u(t,x), \quad u(0,x) = f(x), \tag{3.1.1}$$

where $\mathscr{L}$ is called the Kolmogorov operator of the process $\{Z_t\}_{t\geq 0}$. We may abuse notation and also refer to $\mathscr{L}$ as the generator of the semigroup, however this is only made rigorous once the domains of these operators are identified [BGL+14]. Throughout the chapter we assume the existence of an invariant measure ρ_∞ for

[1] We denote the Markov process by Z_t instead of the usual X_t to not confuse with the flow map X, which appears again in this chapter.

Z_t (equivalently for P_t). The theory of Hypocoercivity[2] developed by Villiani [Vil09] "consists in identifying general structures in which the interplay between a 'conservative part' and a 'degenerate dissipative part' lead to convergence to equilibrium". We focus on processes Z_t which are of linear hypocoercive form, i.e. $\mathscr{L}$ is linear and can be written as

$$\mathscr{L} = B - A^*A. \tag{3.1.2}$$

In (3.1.2) A and B are linear differential operators, and $B^* = -B$ is antisymmetric in $L^2_{\rho_\infty}(\mathbb{R}^d)$[3]. Moreover, A is shorthand for a d-dimensional vector of operators $A = (A_1, \dots, A_d)$, and the expression A^*A should be read as $A^*A = \sum_i^d A_i^* A_i$. Clearly A^*A is symmetric in $L^2_{\rho_\infty}(\mathbb{R}^d)$. The conservative-dissipative split of (3.1.2) is captured by the symmetry (and antisymmetry) of the operators. One way of seeing this is that the $L^2_{\rho_\infty}(\mathbb{R}^d)$ norm of the flow governed by B is preserved, whilst along the flow generated by $-A^*A$ that norm is dissipated (see [DO21, page 11]). The main aim of hypocoercivity is to establish exponentially fast convergence to equilibrium, with explicit convergence rates. One should consult Villani's memoir e.g. [Vil09, Theorem 24] for such results in the setting (3.1.2). Here, we don't study the convergence to equilibrium, instead we only use the linear hypocoercive form (3.1.2) to identify a conservative and gradient flow splitting structure. Although, the long-time behaviour of the schemes we develop would be an interesting unexplored topic to study in the future.

GENERIC. In contrast to Hypocoercivity theory, the GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) framework [Ött05] is devised to study the dual equation of (3.1.1), the Kolmogorov forward/Fokker Planck equation

$$\partial_t \rho(t,x) = \mathscr{L}' \rho(t,x), \quad \rho(0,\cdot) = \rho_0, \tag{3.1.3}$$

where $\mathscr{L}'$ is the (formal) L^2 dual operator of $\mathscr{L}$ associated to the process Z_t, and $\rho(t,\cdot) = \mathrm{Law}(Z_t)$. The GENERIC framework has been used widely in physics and engineering, most notably to derive coarse-grained models. As indicated by its name, GENERIC systems contain both reversible dynamics and irreversible dynamics which are described via two geometric structures (a Poisson structure and a dissipative structure) and two functionals (an energy functional and an entropy functional[4]). These operators and functionals are required to satisfy certain conditions, under which GENERIC systems automatically justify the laws of thermodynamics, namely energy is conserved and entropy is increasing (note that the entropy in mathematical literature is the negative of the entropy in the physics literature). We should point out that in the acronym GENERIC the term 'irreversible' refers to the macroscopic irreversibly (the dissipation of entropy), and the term 'reversible' *does not* refer to the time-reversibility of a stochastic process. For further clarifications on this terminology, we refer the reader to [DO21, Section 2.4] and references therein. We wont actually give the full GENERIC setup here, instead we will focus on *pre-GENERIC* dynamics, in which there is no natural conserved quantity. In particular we study generalised Wasserstein pre-GENERIC, which are evolution's in which $\mathscr{L}'$ takes the form

$$\mathscr{L}'\rho = \mathcal{W}(\rho) - \mathcal{M}_\rho\Big(\frac{1}{2}\frac{\delta \mathcal{S}}{\delta \rho}\Big), \tag{3.1.4}$$

where $\mathcal{M}_\rho(\cdot) = 2A'(\rho A(\cdot))$, for some operator A and $L^2(\mathbb{R}^d)$ dual A' (note $\mathcal{M}_\rho$ is symmetric and positive definite see [DO21, page 20]), and the operator $\mathcal{W}$ and the entropy $\mathcal{S}$ satisfy the degeneracy condition

$$\Big\langle \mathcal{W}(\rho), \frac{\delta \mathcal{S}}{\delta \rho} \Big\rangle = 0. \tag{3.1.5}$$

As a consequence of the above structure, i.e. the positive definiteness of $\mathcal{M}_\rho$ and the degeneracy condition (3.1.5), the solution of (3.1.4) dissipates the entropy $\mathcal{S}$

$$\frac{d\mathcal{S}}{dt}(\rho(t)) = \Big\langle \frac{\delta \mathcal{S}}{\delta \rho}, \partial_t \rho(t) \Big\rangle = \Big\langle \frac{\delta \mathcal{S}}{\delta \rho}, \mathcal{W}(\rho(t)) \Big\rangle + \Big\langle \frac{\delta \mathcal{S}}{\delta \rho}, -\mathcal{M}_{\rho(t)}\Big(\frac{1}{2}\frac{\delta \mathcal{S}}{\delta \rho}\Big) \Big\rangle \le 0.$$

[2]The name hypocoercivity, suggests that it is the study of operators which are 'less than coercive', since hypo is a Greek prefix meaning 'under'.

[3]We use the notation * to denote the dual in $L^2_{\rho_\infty}(\mathbb{R}^d)$ and $'$ the dual in $L^2(\mathbb{R}^d)$.

[4]In the terminology of GENERIC the energy functional is conserved by the dynamics and the entropy functional is dissipated.

Next we make this theory more concrete, in the setting of a general diffusion.

3.2 The setup

In this chapter the homogeneous Markov process Z_t we consider is a general diffusion process

$$dZ_t = b(Z_t)dt + \sqrt{2}\sigma dW_t. \tag{3.2.1}$$

If $\sigma \in \mathbb{R}^{d\times d}$ is constant and $b \in C^1(\mathbb{R}^d;\mathbb{R}^d)$, then as a consequence of Itos Lemma the law of Z_t is absolutely continuous with respect to the Lebesgue measure, and its density $\rho(t)$ satisfies the Kolmogorov-Forward equation

$$\partial_t \rho = \operatorname{div}(D\nabla\rho - b\rho), \tag{3.2.2}$$

where $D = \sigma\sigma^T$. Moreover by [Vil09, Proposition 5], if we assume that (3.2.2) admits an absolutely continuous invariant measure with density $\rho_\infty \in C^2(\mathbb{R}^d)$ which is positive everywhere, then the unknown $p(t,x) = \frac{\rho(t,x)}{\rho_\infty(x)}$ satisfies the modified-Kolmogorov forward equation

$$\partial_t p + Lp = 0, \tag{3.2.3}$$

where $L = B + A^*A$, for $A : \mathcal{D}(A) \supseteq L^2_{\rho_\infty}(\mathbb{R}^d) \to L^2_{\rho_\infty}(\mathbb{R}^d)$, $B : \mathcal{D}(B) \supseteq L^2_{\rho_\infty}(\mathbb{R}^d) \to L^2_{\rho_\infty}(\mathbb{R}^d)$, and $\mathcal{D}(A), \mathcal{D}(B)$ are the domains of A, B respectively. In particular

$$B\rho := (b - D\nabla \log \rho_\infty) \cdot \nabla\rho, \qquad A\rho := \sigma\nabla\rho,$$

and $B^* = -B$. Under Assumption 3.2.1 below, the topological vector space $S(\mathbb{R}^d) \subset \mathcal{D}(A) \cap \mathcal{D}(B)$ (the Schwartz space) is dense in $L^2_{\rho_\infty}(\mathbb{R}^d)$, and hence extending $A_i, B : S(\mathbb{R}^d) \to S(\mathbb{R}^d)$ will guarantee that the operations we perform (i.e. a finite number of applications of A, A^* and B) are authorized.

When L takes the form $L = B + A^*A$, we say that the modified-Kolmogorov equation (3.2.3) is in linear hypocoercive form, or equivalently the Kolmogorov operator $\mathscr{L}$ associated to Z_t is of the form (3.1.2). The recent work [DO21, Section 3] showed that when the modified-Kolmogorov equation is in linear hypocoercvie form, the Kolmogorov forward equation (3.2.2) can be written in Wasserstein pre-GENERIC form,

$$\partial_t \rho = \mathcal{W}\rho - \mathcal{M}_\rho\Big(\frac{1}{2}\frac{\delta H}{\delta\rho}(\rho|\rho_\infty)\Big), \tag{3.2.4}$$

where the operator $\mathcal{W}$ is satisfies (3.1.5) and takes the form $\mathcal{W}\rho = B'\rho = \operatorname{div}(\rho D\nabla \log \rho_\infty - b\rho)$, and $\mathcal{M}_\rho$ is symmetric and positive definite, and is of the form $\mathcal{M}_\rho(\xi) = -2\operatorname{div}(\rho D\nabla\xi)$. Lastly we recall the following observation [DO21, Lemma 2.3] that $B' = B^* = -B$, and hence $\mathcal{W}' = \mathcal{W}^* = -\mathcal{W}$. Note that, since $H(\cdot|\cdot)$ is preserved under coordinate transformation (Lemma 3.A.1), its value will not depend on the choice of coordinates in which we model the dynamics. This fact plays a crucial role in preservation of the structural properties of the system (see Lemma 3.4.1 part (iii)).

The next assumption allows us to make use of the above results to construct a fully structure preserving variational scheme for (3.2.2).

Assumption 3.2.1. We assume that

(i) $\sigma \in \mathbb{R}^{d\times d}$, and $b \in C^1(\mathbb{R}^d;\mathbb{R}^d)$.

(ii) We also assume that (3.2.2) admits a unique absolutely continuous invariant measure with density $\rho_\infty \in C^2(\mathbb{R}^d)$ which is positive everywhere.

(iii) We also assume that b, ρ_∞, D are such that the vector field $b_\infty := -\big(D\nabla \log \rho_\infty - b\big)$ is at most linear $|b_\infty(x)| \le C(1 + |x|)$ for some $C > 0$, and $b_\infty \in W^{1,1}_{\text{loc}}(\mathbb{R}^d)$.

Before giving our scheme we mention that this setting is not 'new', we highlight the article [CS18] which proves a variational principle for non-isotropic diffusion by decomposing the force[5] b into a part which is $D\nabla \log \rho_\infty$ and part which is not. In their work the structural properties are slightly less explicit, in particular they assume that the conservative part is divergence free, whereas for us it is inherent in the setup. Our work can be seen as a discrete version of [CS18, Theorem 5] (without an analysis of the long time behaviour).

Outlook for future work. Similarly to the last chapter, it would be desirable to extend our results to singular interaction kernels, and to fully discretize the scheme. Notice that in the above setup we do not even allow for non-local coefficients. Therefore a strategy for future research is to first identify a wider class of PDE that have the a Wasserstein pre-GENERIC form (3.2.4), and then develop the techniques we use to prove convergence of our scheme to allow for this generalization. In this chapter we prove that over a finite time interval $[0, T]$ our scheme dissipates an energy functional that takes its minimum at the invariant measure ρ_∞. This suggests that, for a fixed time-step, iterating the scheme will give convergence to ρ_∞. A good starting point would be to prove a similar result to [AGS08, Theorem 4.1.2]. Lastly we mention a final line of possible research: can we use two-step schemes to deduce one-step schemes? By this we mean, given the conservative dynamics X of (3.2.5), can we rewrite the transport problem (possibly using the Benamou-Brenier formula) $W_{c_h}(X(h)_\#\mu, \nu) = W_{\tilde{c}_h}(\mu, \nu)$ for some new cost function $\tilde{c}_h$ which incorporates the conservative dynamics X. In particular, we are interested as to how $\tilde{c}_h$ compares to the cost functions which appear in the one-step schemes of the next chapter, Chapter 4.

Organisation of the chapter. In the remainder of this section we construct an operator splitting scheme, and then state the main result of the chapter. Section 3.3 applies this result to the hypocoercive Ornstein-Uhlenbeck process. Finally Section 3.4 proves the main result (following closely the line of argument in the previous chapter).

3.2.1 The scheme

Because of the inherent structure of the Wasserstein pre-GENERIC form (3.2.4) we propose a splitting scheme. The construction is almost identical to Chapter 2.

Let $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ be given, with $H(\rho_0|\rho_\infty) < \infty$. Let $h > 0$, $N \in \mathbb{N}$ be such that $hN = T$, and let $n \in \{0, \ldots, N-1\}$. Set $\rho_h^0 = \tilde{\rho}_h^0 = \rho_0$. Given ρ_h^n we find ρ_h^{n+1} through the following procedure. First we introduce the push forward by the Hamiltonian flow as

$$\tilde{\rho}_h^{n+1} = X(h, \cdot)_\# \rho_h^n, \tag{3.2.5}$$

where $X : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}^d$ (now independent of n, h) the flow of b_∞, solves the ODE

$$\begin{cases} \partial_t X = b_\infty \circ X, \\ X(0, \cdot) = \mathrm{id}. \end{cases} \tag{3.2.6}$$

Next, define ρ_h^{n+1} as the minimiser of the JKO descent step

$$\rho_h^{n+1} = \operatorname*{argmin}_{\rho \in \mathcal{P}_2^r(\mathbb{R}^d)} \Big\{ \frac{1}{2h} W_{c_h}(\tilde{\rho}_h^{n+1}, \rho) + H(\rho|\rho_\infty) \Big\}, \tag{3.2.7}$$

where for the positive semi-definite D, $D_h := D + hI$, and the optimal transport problem W_{c_h}, is defined for $h > 0$ identically to (2.2.6). Also recall from Chapter 2, we have that, for some constant $C > 0$,

$$\|x - y\|^2 \leq C c_h(x, y), \quad \forall x, y \in \mathbb{R}^d, \tag{3.2.8}$$

which implies for any $\mu, \nu \in \mathcal{P}_2(\mathbb{R}^d)$ that

$$M(\nu) \leq C\big(W_{c_h}(\mu, \nu) + M(\mu)\big). \tag{3.2.9}$$

The following result is not hard to prove, we leave the details of it to the Appendix.

[5] In their case the force is denoted ∇f.

Proposition 3.2.2 (The optimal transport problem)**.** If $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$ with $H(\mu|\rho_\infty) < \infty$, then there exists a unique ν^* such that

$$\nu^* = \operatorname*{argmin}_{\nu \in \mathcal{P}_2^r(\mathbb{R}^d)} \Big\{ \frac{1}{2h} W_{c_h}(\mu, \nu) + H(\nu|\rho_\infty) \Big\}. \tag{3.2.10}$$

We again adopt the notation that $t_n = nh$ for $n \in \{0, \dots, N\}$, and define the piecewise constant in time interpolations of $\{\rho_h^n\}_{n=0}^N$

$$\rho_h(t, \cdot) := \rho_h^{n+1}, \text{ for } t \in [t_n, t_{n+1}), \tag{3.2.11}$$

and of $\{\tilde{\rho}_h^n\}_{n=0}^N$

$$\tilde{\rho}_h(t, \cdot) := \tilde{\rho}_h^{n+1}, \text{ for } t \in [t_n, t_{n+1}), \tag{3.2.12}$$

and consider the path which continuously follows the conservative dynamics

$$\rho_h^\dagger(t, \cdot) := \big(X(t - t_n, \cdot)\big)_{\#} \rho_h^n \text{ for } t \in [t_n, t_{n+1}), \tag{3.2.13}$$

so that for $t \in [t_n, t_{n+1})$, $\rho_h^\dagger(t) = \mu(t - t_n)$ where μ is the solution of the continuity equation

$$\begin{cases} \partial_t \mu(t, \cdot) + \operatorname{div}\big(\mu(t, \cdot) b_\infty\big) = 0 \\ \mu(t, \cdot)|_{t=0} = \rho_h^n. \end{cases} \tag{3.2.14}$$

For each $n \in \{0, \dots, N\}$, and $\rho_h^n, \tilde{\rho}_h^n$ defined above, we denote $\tilde{\gamma}_h^{n,c}, \tilde{\gamma}_h^n \in \Pi(\tilde{\rho}_h^n, \rho_h^n)$ and $\gamma_h^n \in \Pi(\rho_h^n, \tilde{\rho}_h^{n+1})$, the optimal plans defined analogously to (2.2.9) and (2.2.10) in the previous chapter. It is important to note that the setup in Section 3.2 does allow for non-constant diffusion matrices $D : \mathbb{R}^d \to \mathbb{R}^{d \times d}, x \mapsto D(x)$, as does [CS18]. However, when constructing a scheme one needs to account for the non-constant diffusion by altering the transport problem (see [Lis09]) to

$$W_{D_h}^2(\mu, \nu) := \inf \Big\{ \int_{\mathbb{R}^{2d}} \mathbf{d}^2(x, y) d\gamma(x, y) \ : \ \gamma \in \Pi(\mu, \nu) \Big\},$$

where

$$\mathbf{d}(x, y) := \inf \Big\{ \int_0^1 \sqrt{\langle D_h^{-1}(\rho(t)) \dot{\rho}(t), \dot{\rho}(t) \rangle} dt \ : \ \rho(0) = x, \ \rho(1) = y, \ \rho \in AC([0, 1]; \mathbb{R}^d) \Big\},$$

with $AC([0, 1]; \mathbb{R}^d)$ the space of absolutely continuous curves parameterized in the interval $[0, 1]$. This generalisation is something we plan to do in the future.

3.2.2 Main result

We state the main result of this chapter: the interpolations of our discrete scheme converge to the weak solution of our evolution equation. First we give a precise definition of a weak solution.

Definition 3.2.3 (Weak solution)**.** A curve $\rho : [0, T] \to \mathcal{P}_2^r(\mathbb{R}^d)$, is called a weak solution to the general evolution equation (3.2.2) if for all $\varphi \in C_c^\infty([0, T] \times \mathbb{R}^d)$ we have

$$\int_0^T \int_{\mathbb{R}^d} \rho(t, x) \Big(\partial_t \varphi(t, x) + b(x) \cdot \nabla \varphi(t, x) + \operatorname{div}\big(D \nabla \varphi(t, x)\big) \Big) dx dt + \int_{\mathbb{R}^d} \rho^0(x) \varphi(0, x) dx = 0. \tag{3.2.15}$$

The following theorem gives the existence of weak solutions of the evolution equation (3.2.2).

Theorem 3.2.4. Let $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ satisfy $H(\rho_0|\rho_\infty) < \infty$. Let $h > 0$, $N \in \mathbb{N}$ with $hN = T$, and let $\rho_h, \tilde{\rho}_h$ and $\rho_h^\dagger$ be defined as above. Suppose that Assumption 3.2.1 holds. Then

(i) for each $t \in [0, T]$ as $h \to 0$ ($N \to \infty$ abiding by $hN = T$) we have

$$\rho_h(t, \cdot), \tilde{\rho}_h(t, \cdot), \rho_h^\dagger(t, \cdot) \underset{h \to 0}{\longrightarrow} \rho(t) \quad \text{weakly in} \quad L^1\big(\mathbb{R}^d\big). \tag{3.2.16}$$

(ii) Moreover, there exists a map $[0,T] \ni t \mapsto \rho(t,\cdot)$ in $\mathcal{P}_2^r(\mathbb{R}^d)$ such that for all $1 \le p < 2$

$$\lim_{h\to 0} \sup_{t\in[0,T]} \max\left\{W_p(\rho_h(t,\cdot),\rho(t,\cdot)), W_p(\tilde{\rho}_h(t,\cdot),\rho(t,\cdot)), W_p(\rho_h^\dagger(t,\cdot),\rho(t,\cdot))\right\} = 0. \tag{3.2.17}$$

The maps ρ appearing in the above limits are weak solutions of (3.2.2) in the sense of Definition 3.2.3. Again, the convergence $h \to 0$ is to be understood as up to a subsequence.

3.3 Example: the hypocoercive Ornstein-Uhlenbeck process

Here we apply our results to the hypocoercive Ornstein-Uhlenbeck diffusion process

$$dZ_t = -\Theta Z_t dt + \sqrt{2}\sigma dW_t, \tag{3.3.1}$$

where Θ, σ are constant matrices in $\mathbb{R}^{d\times d}$. Define the diffusion matrix $D := \sigma\sigma^T$. The associated Fokker-Planck equation is

$$\partial_t \rho = \mathscr{L}'\rho = \operatorname{div}(D\nabla\rho + \Theta x\rho). \tag{3.3.2}$$

Throughout we make the following assumption.

Assumption 3.3.1 (Assumption on the coeficients matrices)**.** We assume that

(i) there is no non-trivial Θ^T-invariant subspace of $\ker D$,

(ii) the matrix Θ is positively stable, i.e. all eigenvalues of Θ have real part greater than zero.

In the above assumption, (i) is a hypoellipticity condition for the differential operator $\partial_t - \mathscr{L}'$, i.e. ρ will be smooth in every open set that $\partial_t\rho - \mathscr{L}'\rho$ is smooth. In particular, it ensures smoothness of solutions to (3.3.2), see [Hör67, page 148]. The condition (ii) means that the map $\mathbb{R}^d \ni x \mapsto \langle \Theta x, x\rangle$ acts as a confining potential. In-fact [AE14, Theorems 3.1 and 4.9] shows that Assumption 3.3.1 is sufficient and necessary for the existence of a unique invariant distribution for (3.3.1), and exponential convergence of solutions to (3.3.2) towards that distribution. In that sense the operator $\mathscr{L}'$ is hypocoercive, and Assumption 3.3.1 can be read as hypoellipticity (condition (i)) plus a confining potential (condition (ii)) is equal to hypocoercivity for the system (3.3.1). [AE14, page 5] also provides a heuristic explanation of the Assumption 3.3.1: it implies that the solution cannot stay in the kernel of the dissipative part of $\mathscr{L}'$, therefore the evolution acts dissipative in all directions. The unique invariant distribution of (3.3.2) is given by

$$\rho_\infty(x) = \frac{1}{(4\pi)^{d/2}(\det K)^{\frac{1}{2}}} e^{-\frac{\langle K^{-1}x,x\rangle}{2}}, \tag{3.3.3}$$

where K is the unique positive definite, invertible, solution to the Lyapunov equation

$$2D = \Theta K + K\Theta^T.$$

There are algorithms for solving the Lyapunov equation, for instance in Matlab by the function *lyap*. Now note, Assumption 3.2.1 holds with: ρ_∞ given in (3.3.3), and b, b_∞ given by

$$b(x) := -\Theta x, \quad b_\infty(x) := (DK^{-1} - \Theta)x.$$

It is easily verified that the operator driving the conservative part of the dynamics $B'\rho = \operatorname{div}(\rho(DK^{-1} - \Theta)x)$ is antisymmetric in both $L^2(\mathbb{R}^d)$ and $L^2_{\rho_\infty}(\mathbb{R}^d)$: indeed

$$\begin{aligned}\langle B'\rho, g\rangle_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^d} \operatorname{div}((DK^{-1}-\Theta)x\rho) g dx &= \int_{\mathbb{R}^d} \operatorname{Trace}(DK^{-1}-\Theta)\rho + (DK^{-1}-\Theta)x\cdot\nabla\rho\big)g dx \\ &= \int_{\mathbb{R}^d} -\operatorname{div}(DK^{-1}-\Theta xg)\rho dx = \langle \rho, -B'g\rangle_{L^2(\mathbb{R}^d)},\end{aligned}$$

using that $\mathrm{Trace}(DK^{-1} - \Theta) = 0$, since $DK^{-1} - \Theta = RK^{-1}$ where $R =: \frac{1}{2}(K\Theta^T - \Theta K)$ is antisymmetric and K^{-1} is symmetric. The antisymmetry in $L^2_{\rho_\infty}(\mathbb{R}^d)$ is similar.

Taking all of this into account, we can apply Theorem 3.2.4, giving the convergence of any of the three interpolations (3.2.11)-(3.2.13), whereby the conservative part of the dynamics can be solved exactly as

$$\tilde{\rho}_h^{n+1} = X(h,\cdot)_{\#}\rho_h^n, \quad \text{for } X(h,x) = e^{h(DK^{-1}-\Theta)}x.$$

To the best of our knowledge, this is the first variational scheme for (3.3.1) which leverages the Wasserstein pre-GENERIC/hypocoercive splitting structure, combining the conservative part of the dynamics (for which the exact solution is explicit) with a JKO scheme. The reason that the hypocoercive Ornstein-Uhlenbeck has remained intractable in the JKO variational framework is due to the degeneracy of D, and that it is a conservative-dissipative system for which its splitting structure is not immediately obvious. Although this example does fit into the class of equations we studied in Chapter 2, the correct splitting structure could only be identified once (3.3.1) was viewed through the Wasserstein pre-GENERIC lens of the current chapter. This highlights the main strength of the framework in Sections 3.1 and 3.2: they reveal the physically relevant splitting structure for a general evolution (3.3.2). This splitting of (3.3.2) is not novel, it has been studied by various authors e.g. [KAT05, equation (5)][6], where it is used after a linearisation is made to the force near a critical point. In particular, it is just an example of the non-isotropic diffusion studied by [CS18] as discussed in Section 3.1.

3.4 Proof of the main result

The reader is warned that the procedure for proving the main result is not very enlightening, since many of the results are a repetition of the previous chapter. However, the ease at which the results manifest as a consequence of the $L^2_{\rho_\infty}(\mathbb{R}^d)$ antisymmetry of $\mathcal{W}$ should be noted. Again, the results hold under the assumptions of Theorem 3.2.4, and for all $0 < h < 1$ small enough, note that we are ultimately interested in the case where $h \to 0$.

3.4.1 Preliminary results on the conservative dynamics

Since our assumption on the conservative part of the dynamics is the same as Chapter 2, the proof of the following results are immediate from there. The only detail added here is that the full free energy functional (the relative entropy) is conserved.

Lemma 3.4.1. Let $\rho_h^n \in \mathcal{P}_2^r(\mathbb{R}^d)$. Then the following results hold for any $n \in \{0, \dots, N-1\}$.

(i) There exists a unique $X : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}^d$, such that for a.e. $x \in \mathbb{R}^d$ the map $t \mapsto X(t,x)$ solves (3.2.6),

$$X(t,x) = x + \int_0^t b_\infty \circ X(s,x)ds.$$

Moreover, $\mathbb{R}^d \ni x \mapsto X(\cdot,x) \in L^1_{\mathrm{loc}}(\mathbb{R}^d; C(\mathbb{R}))$, and for a.e. $x \in \mathbb{R}^d$ the map $\mathbb{R}_+ \ni t \mapsto X(t,x) \in C^1(\mathbb{R})$. In particular, X satisfies the properties of a flow, i.e. $X(0,\cdot) = \mathrm{id}$ and $X(t+s,x) = X(t, X(s,x))$, and hence X is a bijection.

(ii) For $t \in [t_n, t_{n+1})$, $\rho_h^\dagger(t,\cdot)$ solves the continuity equation (3.2.14) over the interval $[0,h)$.

(iii) For any $t \in \mathbb{R}_+$, the map $X(t,\cdot)$ preserves ρ_∞ i.e. $X(t,\cdot)_{\#}\rho_\infty = \rho_\infty$. Moreover, we have the following entropy preservation identities

$$H\big(\rho_h^\dagger(t,\cdot)|\rho_\infty\big) = H(\rho_h^n|\rho_\infty) \;\; \forall t \in [t_n, t_{n+1}), \qquad H(\tilde{\rho}_h^{n+1}|\rho_\infty) = H(\rho_h^n|\rho_\infty). \tag{3.4.1}$$

Proof. In regard to (iii), note that since $\mathcal{W}^* = -\mathcal{W}$, we have that $\mathrm{div}(b_\infty \rho_\infty) = 0$ (see for example [Vil09, Proposition 3]). Now, again by [DL89, Theorem III.1], $X(t,\cdot)_{\#}\rho_\infty$ is the unique weak solution of the continuity equation

[6] In their work U corresponds to K^{-1} and Q corresponds to $\Theta K - D$

$$\partial_t \mu + \operatorname{div}(b_\infty \mu) = 0, \quad \mu(0) = \rho_\infty. \tag{3.4.2}$$

Moreover, $\mu(t) = \rho_\infty$ is a strong solution of (3.4.2) since $\operatorname{div}(b_\infty \rho_\infty) = 0$, and hence $X(t,\cdot)_\# \rho_\infty = \rho_\infty$, i.e. $X(t,\cdot)$ preserves ρ_∞. Now for the preservation of the relative entropy, note that for $t \in [t_n, t_{n+1})$ we have

$$\begin{aligned} H(\rho_h^\dagger(t,\cdot)|\rho_\infty) &= H(X(t,\cdot)_\# \rho_h^n|\rho_\infty) && (3.4.3)\\ &= H(X(t,\cdot)_\# \rho_h^n | X(t,\cdot)_\# \rho_\infty) && (3.4.4)\\ &= H(\rho_h^n|\rho_\infty). && (3.4.5) \end{aligned}$$

(3.4.3) is the definition of $\rho_h^\dagger$, (3.4.4) is the preservation of ρ_∞, and (3.4.5) is since the relative entropy is preserved under one-to-one transformations, see Lemma 3.A.1. □

Lemma 3.4.2. The following result holds for any $n \in \{0,\dots,N-1\}$. Let $\rho_h^n \in \mathcal{P}_2^r(\mathbb{R}^d)$. Let μ be the solution of (3.2.14) over the interval $[0,h]$. Then the following hold.

(i) Let $0 \le s_1 \le s_2 \le h$ then

$$W_2^2(\mu(s_1,\cdot),\mu(s_2,\cdot)) \le Ch \int_{s_1}^{s_2} \big(1 + M(\mu(s,\cdot))\big) ds. \tag{3.4.6}$$

(ii) For any $t \in [t_n, t_{n+1})$, $M(\rho_h^\dagger(t,\cdot)), M(\tilde\rho_h(t,\cdot)) < C\big(M(\rho_h^n) + 1\big)$.

3.4.2 Discrete Euler-Lagrange equation

The Euler-Lagrange equations are the same as the previous chapter, the only difference being that we calculate the variation of the relative entropy.

Lemma 3.4.3 (First Variation of the Relative Entropy)**.** Let $\rho \in \mathcal{P}_2^r(\mathbb{R}^d)$, and $\eta \in C_c^\infty(\mathbb{R}^d;\mathbb{R}^d)$ with flow $Y : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}^d$

$$\partial_s Y_s = \eta \circ (Y_s), \; Y_0 = \mathrm{id}.$$

The first variation of $H(\cdot|\rho_\infty)$ at ρ along η, and denoted by $\delta_\eta H(\rho|\rho_\infty)$, is

$$\delta_\eta H(\rho|\rho_\infty) := \frac{d}{ds} H((Y_s)_\# \rho|\rho_\infty)\Big|_{s=0} = -\int_{\mathbb{R}^d} \Big(\operatorname{div}(\eta(x)) + \nabla \log \rho_\infty(x)\cdot \eta(x)\Big)\rho(x)dx. \tag{3.4.7}$$

Proof. Just note by definition of the push-forward

$$\begin{aligned} \delta_\eta H(\rho|\rho_\infty) =& \delta_\eta H(\rho) - \delta_\eta \Big(\int \log \rho_\infty(y) d(Y_s)_\# \rho\Big)\\ =& -\int \rho \operatorname{div}(\eta)dx - \lim_{s\to 0} \int_{\mathbb{R}^d} \frac{\log(\rho_\infty \circ Y_s) - \log(\rho_\infty)}{s} \rho dx, \end{aligned}$$

where the first variation of the entropy H was well known (e.g [JKO98, page 10 and 11]). The result now follows when one can see the limit under the integral in the last expression is $\lim_{s\to 0} \frac{\log(\rho_\infty\circ Y_s) - \log(\rho_\infty)}{s} = \nabla \log \rho_\infty \cdot \partial_s Y_s|_{s=0} = \nabla \log\rho_\infty \cdot \eta$. □

Lemma 3.4.4 (Euler-Lagrange equation)**.** Let $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$, and h small enough. Let ν be the optimum in (3.2.10), and let γ be the corresponding optimal plan in $W_{c_h}(\mu,\nu)$. Then, for any $\eta \in C_c^\infty(\mathbb{R}^d;\mathbb{R}^d)$ we have

$$0 = \frac{1}{2h} \int_{\mathbb{R}^{2d}} \Big\langle \eta(y), \nabla_y c_h(x,y)\Big\rangle d\gamma(x,y) + \delta_\eta H(\nu|\rho_\infty).$$

In particular, for any $\varphi \in C_c^\infty(\mathbb{R}^d)$, by choosing $\eta(x) = D_h \nabla\varphi(x)$, and $\tilde\gamma_h^{n+1,c}$ defined in Section 3.2.1, we have

$$0 = \frac{1}{h} \int_{\mathbb{R}^{2d}} \Big\langle y - x, \nabla\varphi(x)\Big\rangle d\tilde\gamma_h^{n+1,c}(x,y) + \delta_{D_h\nabla\varphi} H(\rho_h^{n+1}|\rho_\infty). \tag{3.4.8}$$

3.4.3 A priori estimates

In this section we establish estimates that will provide enough compactness to conclude the convergence of our scheme. To not make the notation over cumburdson we drop the dependence on h of our iterates $\rho^n, \tilde{\rho}^{n+1}$ in the proofs.

Lemma 3.4.5. Let $n \in \{0, 1, \ldots, N-1\}$. If there exists a constant $C_1 > 0$, independent of h and n, such that $M(\rho_h^n), H(\rho_h^n|\rho_\infty) < C_1$, then $\tilde{\rho}_h^{n+1}$ obtained from (3.2.5) satisfies

$$M(\tilde{\rho}_h^{n+1}), H(\rho_h^{n+1}|\rho_\infty) < C.$$

As usual, the constant C appearing is also independent of h and n, but will depend on C_1.

Proof. This is a consequence of point (iii) from Lemma 3.4.1 and point (ii) from Lemma 3.4.2. □

The following lemma controls the sum of the optimal transport costs of the JKO steps, by using $\tilde{\rho}_h^{n+1}$ as a competitor to ρ_h^{n+1} in (3.2.7). Notice the ease to which this result is obtained in comparison to Lemma 2.3.8.

Lemma 3.4.6. For any $n \in \{1, \ldots, N-1\}$ it holds that

$$\sum_{i=0}^{n-1} W_{c_h}(\tilde{\rho}_h^{i+1}, \rho_h^{i+1}) \leq ChH(\rho^0|\rho_\infty). \tag{3.4.9}$$

Proof. Let $i \in \{0, 1, \ldots, N-1\}$. Since ρ^{i+1} attains the infimum in (3.2.7) we can compare it against $\tilde{\rho}^{i+1}$. This gives

$$\frac{1}{2h} W_{c_h}(\tilde{\rho}^{i+1}, \rho^{i+1}) \leq H(\tilde{\rho}^{i+1}|\rho_\infty) - H(\rho^{i+1}|\rho_\infty).$$

Using that relative entropy is conserved, proven in Lemma 3.4.1, the above is equivalent to

$$\frac{1}{2h} W_{c_h}(\tilde{\rho}^{i+1}, \rho^{i+1}) \leq H(\rho^{i}|\rho_\infty) - H(\rho^{i+1}|\rho_\infty).$$

Summing the above expression we get

$$\frac{1}{2h} \sum_{i=0}^{n-1} W_{c_h}(\tilde{\rho}^{i+1}, \rho^{i+1}) \leq H(\rho^0|\rho_\infty) - H(\rho^n|\rho_\infty), \tag{3.4.10}$$

and noting that the relative entropy is non-negative gives the result. □

Note that the previous Lemma allows us to easily obtain uniform bounds on the relative entropy, that is, we can rearrange (3.4.10), and noting that the optimal transport problem is non-negative gives the uniform bound $H(\rho_h^n|\rho_\infty) \leq H(\rho^0|\rho_\infty)$ for all $n \in \{1, \ldots, N\}$. We note again this bound was easier to obtain than the uniform bounds on the free energy in Chapter 2. The following Lemma provides uniform bounds for the moments and positive parts of the entropy, the proof can be made by an almost identical argument to Lemma 2.3.9, other than the uniform bounds for the relative entropy, which we have just obtained.

Lemma 3.4.7 (Boundedness of the relative entropy, 2nd moments and the positive part of the entropy functionals)**.** For all $n \in \{0, 1, \ldots, N\}$, we have

$$M(\rho_h^n), H(\rho_h^n|\rho_\infty), H_+(\rho_h^n) \leq C, \qquad \text{and} \qquad M(\tilde{\rho}_h^n), H(\tilde{\rho}_h^n|\rho_\infty), H_+(\tilde{\rho}_h^n) \leq C.$$

At this point we can follow exactly steps in Section 2.3.3, yielding the same results but now with respect to the sequences $\{\rho_h^n\}, \{\tilde{\rho}_h^n\}$ obtained from (3.2.5)-(3.2.7). These results are collected into a single lemma to be used in the following section.

Lemma 3.4.8. For all $t \in [0,T]$, we have the following uniform bounds for the interpolations

$$M(\rho_h(t,\cdot)), M(\tilde{\rho}_h(t,\cdot)), M(\rho_h^\dagger(t,\cdot)) \le C, \qquad H(\rho_h(t,\cdot),|\rho_\infty), H(\tilde{\rho}_h(t,\cdot)|\rho_\infty), H(\rho_h^\dagger(t,\cdot)|\rho_\infty) \le C,$$
$$\text{and} \qquad H_+(\rho_h(t,\cdot)), H_+(\tilde{\rho}_h(t,\cdot)), H_+(\rho_h^\dagger(t,\cdot)) \le C.$$

We also have

$$\sum_{n=0}^{N-1} W_{c_h}(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}), \ \sum_{n=0}^{N-1} W_2^2(\tilde{\rho}_h^{n+1}, \rho_h^{n+1}), \ \sum_{n=0}^{N-1} W_2^2(\rho_h^n, \tilde{\rho}_h^{n+1}) \le Ch. \tag{3.4.11}$$

3.4.4 Convergence of the scheme

In this section, we first show the convergence of the interpolations $\rho_h(t,\cdot), \tilde{\rho}_h(t,\cdot), \rho_h^\dagger(t,\cdot)$ in W_p $(1 \le p < 2)$ as well as the weak convergence of their respective densities in $L^1(\mathbb{R}^d)$. We then identify the limit curve ρ as the weak solution of (3.2.2), we skip over much of the details.

Lemma 3.4.9. [Convergence of the time-interpolations in W_p] There exists a curve $[0,T] \ni t \mapsto \rho(t,\cdot) \in \mathcal{P}_2^r(\mathbb{R}^d)$, such that for all $1 \le p < 2$

$$\lim_{h\to 0} \sup_{t\in[0,T]} \max\Big\{ W_p(\rho_h(t,\cdot), \rho(t,\cdot)), W_p(\tilde{\rho}_h(t,\cdot), \rho(t,\cdot)), W_p(\rho_h^\dagger(t,\cdot), \rho(t,\cdot)) \Big\} = 0, \tag{3.4.12}$$

where the convergence $h \to 0$ is done taking subsequences if necessary.

Proof. We provide the first part of the argument for $\rho_h^\dagger$ only, the remaining part is made identically to Lemma 2.3.13. Let $n \in \{1, \ldots, N-1\}$. Fix any $s, t \in [0,T]$, define the path $\nu_h : [0,T] \to \mathcal{P}_2(\mathbb{R}^d)$ by concatenating $\tilde{\rho}_h^n$ and $\tilde{\rho}_h^{n+1}$ on $[t_{n-1}, t_n]$ by a constant speed geodesic. Then for $t \in [t_{n-1}, t_n)$

$$\begin{aligned} W_2(\rho_h^\dagger(t), \nu_h(t)) \le W_2(\rho_h^\dagger(t), \tilde{\rho}_h^n) + W_2(\tilde{\rho}_h^n, \nu_h(t)) =& W_2(\rho_h^\dagger(t), \tilde{\rho}_h^n) + W_2(\nu_h(t_{n-1}), \nu_h(t)) \\ \le& Ch + W_2(\tilde{\rho}_h^n, \tilde{\rho}_h^{n+1})(t - t_{n-1}) \qquad (3.4.13) \\ \le& Ch, \qquad (3.4.14) \end{aligned}$$

where the bound (3.4.13) was obtained by using (3.4.6) and the bounded moments of Lemma 3.4.7 for the first term, and the definition of a geodesic for the second term. From here we can show, in an identical fashion to Lemma 2.3.13, the convergence of this concatenation (via Arzela-Ascoli), from which we induce the desired convergence for the original path $\rho_h^\dagger$. ☐

As in the previous chapter an argument by equi-continuity gives the weak $L^1(\mathbb{R}^d)$ convergence of $\rho_h(t,\cdot)$, $\tilde{\rho}_h(t,\cdot)$, and $\rho_h^\dagger(t,\cdot)$ to $\rho(t,\cdot)$ for each $t \in [0,T]$. Recall this implies weak $L^1((0,T)\times\mathbb{R}^d)$ convergence, which we will use throughout the following proof to conclude the main result of this chapter.

Proof of Theorem 3.2.4. Following the exact line of argument as in Section 2.3.4, i.e. summing over the Euler-Lagrange equations (3.4.8), and mimicking the steps in Lemma 2.3.14 just replacing b by b_∞, one arrives at

$$\int_0^T \int_{\mathbb{R}^d} \rho_h^\dagger(t,x)\Big(\partial_t\varphi + b_\infty \cdot \nabla\varphi\Big)(t,x)dxdt + \int_{\mathbb{R}^d} \rho^0(x)\varphi(0,x)dx = O(h) + h\sum_{n=0}^{N-1} \delta_{D_h\nabla\varphi(t_{n+1},\cdot)} H(\rho_h^{n+1}|\rho_\infty). \tag{3.4.15}$$

for any $\varphi \in C_c^\infty([0,T)\times\mathbb{R}^d)$.

Plugging the value of b_∞ and the first variation of the relative entropy (3.4.7) into (3.4.15) and rewriting the multiplication by h as an integral we get

$$\begin{aligned}
&R(h) + Q(h) = O(h), &(3.4.16)\\
&R(h) := \int_0^T \int_{\mathbb{R}^d} \rho_h^\dagger(t,x)\Big(\partial_t\varphi - (D\nabla\log\rho_\infty - b)\cdot\nabla\varphi\Big)(t,x)dxdt + \int_{\mathbb{R}^d}\rho^0(x)\varphi(0,x)dx,\\
&Q(h) := \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_{\mathbb{R}^d}\Big(\operatorname{div}(D_h\nabla\varphi(t_{n+1},x)) + \nabla\log\rho_\infty(x)\cdot D_h\nabla\varphi(t_{n+1},x)\Big)\rho_h(t,x)dxdt.
\end{aligned}$$

We now take the limit $h\to 0$ in the above expression (taking subsequences if necessary). Note $\partial_t\varphi - (D\nabla\log\rho_\infty - b)\cdot\nabla\varphi \in L^\infty((0,T)\times\mathbb{R}^d)$ since $\varphi\in C_c^\infty([0,T)\times\mathbb{R}^d)$. Therefore, the convergence of $R(h)$ is straightforward. So we are left to evaluate the limit of $Q(h)$. Consider the first term in $Q(h)$,

$$\begin{aligned}
&\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_{\mathbb{R}^d}\rho_h(t,x)\operatorname{div}(D_h\nabla\varphi(t_{n+1},x))dxdt\\
&\qquad = \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_{\mathbb{R}^d}\rho_h(t,x)\Big(\operatorname{div}\big(D\nabla\varphi(t_{n+1},x)\big) + \operatorname{div}\big((D_h - D)\nabla\varphi(t_{n+1},x)\big)\Big)dxdt,
\end{aligned}$$

the second term here tends to zero since $|\operatorname{div}\big((D_h - D)\nabla\varphi(t_{n+1},x)| \le h\sup_{x,t}|\operatorname{Trace}(\nabla^2\varphi(t,x))| \le Ch$. Adding and subtracting $\rho_h(t,x)\operatorname{div}\big(D\nabla\varphi(t,x)\big)$ from the first term we have

$$\begin{aligned}
&\sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\int_{\mathbb{R}^d}\rho_h(t,x)\operatorname{div}\big(D\nabla\varphi(t_{n+1},x)\big)dxdt\\
&\quad = \int_0^T\int_{\mathbb{R}^d}\rho_h(t,x)\operatorname{div}\big(D\nabla\varphi(t,x)\big)dxdt + \sum_{n=0}^{N-1}\int_{t_n}^{t_{n+1}}\rho_h(t,x)\Big(\operatorname{div}\big(D\big(\nabla\varphi(t_{n+1},x) - \nabla\varphi(t,x)\big)\big)dxdt,
\end{aligned}$$

which tends to $\int_0^T\int_{\mathbb{R}^d}\rho(t,x)\operatorname{div}\big(D\nabla\varphi(t,x)\big)dxdt$, since

$$\operatorname{div}\big(D\big(\nabla\varphi(t_{n+1},x) - \nabla\varphi(t,x)\big)\big) \le |D|_{\max}\sup_{[u_h,r_h]\subset[0,T),|u_h-r_h|\le h}\ \sup_{s\in[u_h,r_h],x\in\mathbb{R}^d}|\operatorname{Trace}(\nabla^2\varphi(u_h,x) - \nabla^2\varphi(s,x))|$$

and $\nabla^2\varphi$ is uniformly continuous, (it is a compactly supported continuous function). This concludes the convergence of the first term in $Q(h)$. The second term in $Q(h)$ can be dealt with in a very similar manner, giving that

$$\lim_{h\to 0}Q(h) = \int_0^T\int_{\mathbb{R}^d}\Big(\operatorname{div}(D\nabla\varphi(t,x)) + D\nabla\log\rho_\infty(x)\cdot\nabla\varphi(t,x)\Big)\rho(x)dxdt.$$

This concludes the proof of Theorem 3.2.4. $\square$

Appendix

3.A Supplementary results

The next result states that relative entropy is preserved under coordinate transformations.

Lemma 3.A.1. Let $\mu, \nu \in \mathcal{P}(\mathbb{R}^d)$, with $\mu \ll \nu$. Let $X : \mathbb{R}^d \to \mathbb{R}^d$ be a measurable bijective mapping. Then $H(\mu|\nu) = H(X_\#\mu|X_\#\nu)$.

Proof. Note that since X is invertible, we have for any measurable set $A \subset \mathbb{R}^d$

$$X_\#\mu(A) = \mu(X^{-1}(A)) = \int_{X^{-1}(A)} \frac{d\mu}{d\nu} d\nu = \int_A \frac{d\mu}{d\nu} \circ X^{-1} dX_\#\nu,$$

i.e. $\frac{dX_\#\mu}{dX_\#\nu}(x) = \frac{d\mu}{d\nu} \circ X^{-1}(x)$, using this

$$\begin{aligned} H(X_\#\mu|X_\#\nu) = \int_{\mathbb{R}^d} \log\Big(\frac{dX_\#\mu}{dX_\#\nu}\Big) dX_\#\mu &= \int_{\mathbb{R}^d} \log\Big(\frac{dX_\#\mu}{dX_\#\nu} \circ X\Big) d\mu \\ &= \int_{\mathbb{R}^d} \log\Big(\frac{d\mu}{d\nu}\Big) d\mu = H(\mu|\nu). \end{aligned}$$

□

The following proof is very similar to the proof of Proposition 2.3.4, we include it for completeness.

Proof of Proposition 3.2.2. Fix $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$ with $H(\mu|\rho_\infty) < \infty$, and let $h > 0$ be small enough. First we will show that the functional $\mathcal{P}_2^r(\mathbb{R}^d) \ni \nu \mapsto J_{c_h}(\mu, \nu) := \frac{1}{2h} W_{c_h}(\mu, \nu) + H(\nu|\rho_\infty)$ is bounded from below and deduce the existence of a minimising sequence. Note that for any $\nu \in \mathcal{P}_2^r(\mathbb{R}^d)$, $J_{c_h}(\mu, \nu) \geq 0$ by the non-negativity of $W_{c_h}(\cdot, \cdot)$ and $H(\cdot|\cdot)$. Moreover there exists a ν such that $J_{c_h}(\nu, \mu)$ is finite, indeed take $\nu = \mu$, giving $J_{c_h}(\mu, \mu) = H(\mu|\rho_\infty) < \infty$. Hence we can consider a minimising sequence $\{\nu_k\}$ of $J_{c_h}(\cdot, \mu)$. Next we show that we can abstract a sub-sequence $\{\nu_{k_l}\}$ such that $\{M(\nu_k)\}$,$\{H(\nu_k)\}$ are uniformly bounded, and it weakly converges to some $\nu^* \in \mathcal{P}_2^r(\mathbb{R}^d)$. Note that, since our sequence is minimising we can have that

$$J_{c_h}(\nu_{k-1}, \mu) \geq J_{c_h}(\nu_k, \mu) \geq W_{c_h}(\mu, \nu_k) \pm M(\mu) + H(\nu_k|\rho_\infty) \geq \frac{1}{C} M(\nu_k) + H(\nu_k) + C(\rho_\infty),$$

for a constant $C(\rho_\infty)$ that we stress only depends on ρ_∞, in the above we have used (3.2.9) and that ρ_∞ is bounded above (see Assumption 3.2.1). Therefore $\{M(\nu_k)\}$ and $\{H(\nu_k)\}$ are uniformly bounded. Since $\{M(\nu_k)\}$ is uniformly bounded we have that $\{\nu_k\}$ is tight, hence there exists a weakly converging sub-sequence $\{\nu_{k_l}\}$, $\nu_{k_l} \rightharpoonup \nu^* \in \mathcal{P}(\mathbb{R}^d)$. Moreover, $\nu^* \in \mathcal{P}_2(\mathbb{R}^d)$ since uniform bounded 2nd moments and weak convergence implies the limit has a bounded 2nd moment. Furthermore, $\nu^* \in \mathcal{P}_2^r(\mathbb{R}^d)$ by the weak lower semi-continuity of entropy under bounded 2nd moments (2.2.2). Lastly we argue that the limit ν^* is in-fact a minimiser, and it is unique. ν^* is a minimiser of $J_{c_h}(\mu, \cdot)$ by the lower semi-continuity of $W_{c_h}(\cdot, \mu)$ (see Lemma 2.A.3) in combination with the lower semi-continuity of $H(\cdot|\rho_\infty)$ (classical result). Finally, over the convex set $\mathcal{P}_2^r(\mathbb{R}^d)$, $W_{c_h}(\mu, \cdot)$ is convex and $H(\cdot|\rho_\infty)$ is strictly convex, hence ν^* is unique. □

Chapter 4

An Entropic Variational One-step Scheme

The work contained here is taken from our paper [DAdR22].

4.1 Introduction

In this chapter we develop entropy regularised one-step schemes for a general class of non-gradient systems and apply the abstract framework to several concrete examples.

An abstract framework. We focus on systems where the operator $\mathscr{L}'$ has a general non-linear drift-diffusion form

$$\partial_t \rho = \mathscr{L}' \rho = \operatorname{div}\big(b\rho\big) + \operatorname{div}\Big(\rho D \nabla \frac{\delta \mathcal{F}}{\delta \rho}\Big), \qquad \rho|_{t=0} = \rho_0. \tag{4.1.1}$$

where $b\colon \mathbb{R}^d \to \mathbb{R}^d$ is a given vector field, D is a symmetric (possibly degenerate) matrix in $\mathbb{R}^{d\times d}$ and $\mathcal{F}\colon \mathcal{P}(\mathbb{R}^d) \to \mathbb{R}$ is the free energy functional which is the sum of an internal energy and an external energy, see Section 4.2 for a precise formulation. When $b = 0$ and D is non-singular, (4.1.1) is a (weighted) Wasserstein gradient flow [Lis09]. However, in general (4.1.1) is a non-reversible dynamics due to the fact that the drift b is not necessarily a gradient [ADPZ13]. This class covers non-gradient systems such as the non-linear kinetic Fokker-Planck equation and a non-linear degenerate diffusion equation of Kolmogorov type, which will be discussed in detail in Section 4.3 as concrete applications.

Entropic regularisation for non-gradient systems.
In this chapter, we develop an entropy regularised variational approximation scheme for the evolution equation (4.1.1). The scheme is as follows: given a small parameter (which is the strength of the regularisation) $\epsilon > 0$ and a time-step $h > 0$, define $\rho^0_{h,\epsilon} = \rho_0$, then $\rho^n_{h,\epsilon}$ is iteratively (over $n = 1, \ldots, N$ with h such that $hN = T$) determined as the unique minimiser of the following minimisation problem

$$\min_{\rho} \frac{1}{2h} W_{c_h,\epsilon}(\rho^{n-1}_{h,\epsilon}, \rho) + \mathcal{F}(\rho), \tag{4.1.2}$$

over the space $\mathcal{P}_2^r(\mathbb{R}^d)$ of absolutely continuous probability measures with finite 2nd moment. Here $W_{c_h,\epsilon}$ is an appropriate regularised Monge-Kantorovich optimal transport cost functional

$$W_{c_h,\epsilon}(\mu,\nu) := \inf_{\gamma \in \Pi(\mu,\nu)} \Big\{ \int_{\mathbb{R}^{2d}} c_h(x,y)\gamma(dx,dy) + \epsilon H(\gamma) \Big\}, \tag{4.1.3}$$

where the infimum is taken over the couplings between μ and ν. In (4.1.3), the function $c_h : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, which depends on the time-step h, should be thought of as the cost of displacing mass from point x to y in a time-step h. The regularisation term, $H(\gamma)$, is the entropy of γ. We note that no specific form for the cost c_h is prescribed, instead, it is assumed to satisfy the conditions in Assumption 4.2.5 (see below) which in turn means that c_h is not necessarily a metric. To the best of our knowledge we are unaware of any general algorithm yielding c_h given the generator $\mathscr{L}$, nonetheless, in our examples Section 4.3 below we provide concrete methods to identify c_h. The minimisation problem (which is (4.1.2) for a single step),

$$\operatorname{argmin}_{\nu\in\mathcal{P}_2^r(\mathbb{R}^d)}\Big\{\frac{1}{2h}W_{c_h,\epsilon}\big(\mu,\nu\big)+\mathcal{F}(\nu)\Big\}, \tag{4.1.4}$$

will play an essential role in this work. The contribution of the present chapter includes:

1. Proposition 4.5.1 proves the well-posedness of the optimal transport minimisation problem (4.1.4).

2. *An abstract framework.* Theorem 4.2.13 establishes, under certain conditions on the drift vector b, the diffusion matrix D and the cost function c_h (see Section 4.2 for precise statements), the convergence of the regularised scheme (4.1.2) to a weak solution of (4.1.1).

3. *Concrete applications.* We illustrate the generality of our work in Section 4.3 by providing three examples to which our work is applicable: a non-linear diffusion equation with a general (constant, possibly singular) diffusion matrix, the non-linear kinetic Fokker-Planck (Kramers) equation, and a non-linear degenerate diffusion equation of Kolmogorov type. The drift vector field b is not present in the first example but plays an important role in the last two cases.

4. *Numerics.* In Section 4.4 a numerical implementation of our scheme, via a matrix scaling algorithm, is shown to solve Kramers equation.

As with previous chapters the proof of Proposition 4.5.1 follows the direct method of calculus of variations. We now provide further discussion concerning the points 2, 3 4.

Comparison with the existing literature. The general framework we detail in Section 4.2 provides a sufficient condition to guarantee the convergence of the regularised variational iterative scheme (4.1.2) to a weak solution of (4.1.1). We emphasise that the three distinguishing features of the PDE class we handle and which makes this an involved task are: the drift b is not assumed to be of gradient type, D can be singular and the operator $\mathscr{L}'$ can be non-linear. We have not found other works which deal with these features simultaneously (with or without regularisation). The proof of the main abstract theorem follows the now well-established procedure introduced originally in [JKO98]. However, due to the incorporation of the mentioned features, several technical improvements are performed, in particular the introduction/construction of change of variable maps to deal with the non-metric essence of the cost function c_h (see Assumption 4.2.8). Our framework generalises several specific cases that have been studied previously in the literature.

A regularised variational scheme for the non-linear diffusion equation, without the drift b and with the diffusion matrix D the identity matrix, has been studied in [CDPS17]. This paper actually inspires our work and we slightly extend it to the case when D is a general (possibly singular) matrix. This provides an entropy regularised scheme for weighted-Wasserstein gradient flows [Lis09]. More importantly, as mentioned above, our framework accommodates singular diffusion coefficients. In this vein, our work generalises, by allowing non-linear diffusions and including regularisation, previous works that develop unregularised JKO-type variational approximation schemes for the linear kinetic Fokker-Planck (Kramers) equation [DPZ14, Hua00] and a degenerate diffusion equation of Kolmogorov type [DT18]. In addition, several papers numerically investigate and implement regularised schemes for these equations but do not rigorously prove the convergence of the schemes as the regularisation strength tends to zero [CH21, CH19]. Thus our present work provides a rigorous foundation for these works. We emphasise that our proof of convergence also holds true without regularisation. By introducing regularisation, our proposed schemes are also computationally tractable and useful for numerical purposes (see Section 4.4 for discussion on the numerical implementation and illustrations).

Comparison with two-step schemes. There are merits to studying both one-step and two-step schemes, building the two theories in parallel is one of the objectives of this research. The distinguished feature of two-step schemes is that they immediately reveal an explicit cost function, whereas for the one-step schemes there is no fool-proof procedure for identifying it. Therefore, two-step schemes might be more suitable for building a unified theory for systems with mixed dynamics since they can directly utilise the structure of GENERIC. On the other hand, purely variational (one-step) schemes circumvent the error introduced by splitting. In particular, it will be beneficial to further investigate the non-metric, non-homogeneous[1] cost functions, and their relationship to the large deviation rate function of the underlying microscopic particle systems.

In comparison to classical numerical PDE methods, both variational schemes we study do not provide benefits in efficiency. However, both schemes possess the favourable property that they are structure preserving. The biggest drawback of our schemes is that they are liable to numerical underflow. By comparing the dependence of one and two-step schemes on the time-step h, it is clear that two-step schemes are less prone to numerical underflow (see Section 4.4.2), this allows for a smaller choice of time-step during implementation. It should be noted that, in contrast to two-step schemes, one-step schemes do not require (a potentially costly) computation of the flow ODE. Of course in some cases, like the Hypocoercive Ornstein-Uhlenbeck process (Section 3.3) the flow is explicitly given. The two methods differ drastically when it comes to domain discretization. For one-step schemes it is standard to use a predefined uniform grid which immediately provides the multiplying mass factor (λ in Section 4.4). Such a grid is fixed during simulation. Implementing the two-step scheme will require the use of mesh-free methods, this is beyond the scope of this thesis and is left for future work. In particular, the points at which the distribution is evaluated evolves according to the conservative dynamics, this is due to the conservative (push forward) step in the splitting scheme. I conjecture that the mass factor λ can remain constant since the Lebesgue measure is invariant under the conservative dynamics.

Outlook for future work. As discussed in detail in Chapter 3, many of the examples we consider belong to the GENERIC class. The appearance of the concepts of energy and entropy in the formulation of GENERIC suggests a strong variational connection. However, establishing a variational formulation (even unregularised) akin to the JKO-minimising movement scheme (1.2.5), in particular identifying a suitable cost function for GENERIC systems is still open, although, encouraging attempts have been made recently for several systems as discussed above. Another interesting problem for future work is to develop and establish the convergence of JKO-type minimising movement schemes for (non-linear, non-gradient) non-diffusive systems. For these systems, a proof following the seminal procedure in [JKO98], which is employed in this chapter, cannot be directly applied because the corresponding objective functional is not superlinear due to the absence of the entropy term. Thus, a delicate analysis needs to be introduced to obtain necessary compactness properties for the sequence of the discrete minimisers. Such analysis has been carried out for the transport equation [KT06] and its linear kinetic counterpart [DL19]; however, for more complicated systems such as the kinetic equation of granular media [Agu16] it is still an open question. Finally, the convergence analysis of (fully discretised) regularised schemes which possess a time-step dependent, non-homogeneous, non-metric cost function such as the ones in this chapter has not been explored.

Organisation of the chapter. In Section 4.2 we present the framework and the main abstract result of this chapter, Theorem 4.2.13. Section 4.3 outlines some explicit examples of where our work is applicable, their verification is left to the appendix. A numerical implementation of our scheme applied to Kramers equation is carried out and analysed in Section 4.4. Section 4.5 contains the well-posedness of the scheme, and in Section 4.6 we prove the main result. In the Appendix we recall some technical lemmas from the literature, and provide verification of the examples.

4.2 The abstract framework and the main result

In this section we present the working assumptions of our abstract framework, namely, the assumptions placed on the operator $\mathscr{L}'$ (4.1.1), and transport cost c_h, which are assumed to hold throughout. We also state the main abstract result of this chapter, Theorem 4.2.13, which says that, under these assumptions, the regularised scheme (4.1.2) can be shown to be well-posed and to converge to the weak solution of the evolution equation (4.1.1).

[1]A cost function c is said to be $r-$homogeneous if $c(ax, ay) = a^r c(x, y)$.

Assumption 4.2.1 (Free energy)**.** We assume there is a fixed constant $C > 0$ such that the following holds. The free energy functional $\mathcal{F} : \mathcal{P}_2^r(\mathbb{R}^d) \to \mathbb{R}$ is the sum of a potential energy and an internal energy functional

$$\mathcal{F}(\rho) = F(\rho) + U(\rho), \tag{4.2.1}$$

with

$$F(\rho) = \int f(x)\rho(x)dx, \quad \text{and} \quad U(\rho) = \int u(\rho(x))\,dx.$$

The internal energy function $u : [0,\infty) \to \mathbb{R}$ is twice differentiable $u \in C^2((0,\infty);\mathbb{R})$, convex, $u(0) = 0$, superlinear

$$\lim_{s\to\infty} \frac{u(s)}{s} = \infty,$$

and there exists $\frac{d}{d+2} < \alpha < 1$ such that

$$u(s) \geq -Cs^{\alpha}. \tag{4.2.2}$$

Moreover, for any $s \in [0,\infty)$ we call $p(s) := u'(s)s - u(s)$ the pressure associated to U, and assume there exists some $m \in \mathbb{N}$ such that

$$p(s) \leq Cs^m, \quad \text{and} \quad p'(s) \geq \frac{s^{m-1}}{C}, \tag{4.2.3}$$

and

$$\frac{1}{C}\int_{\mathbb{R}^d} (\rho(x))^m dx \leq CM(\rho) + U(\rho), \quad \forall \rho \in \mathcal{P}_2^r(\mathbb{R}^d). \tag{4.2.4}$$

The potential energy $f \in C(\mathbb{R}^d)$ is assumed to be non-negative $f(x) \geq 0$, and Lipschitz

$$|f(x) - f(y)| \leq C\|x - y\|, \qquad \forall x, y \in \mathbb{R}^d. \tag{4.2.5}$$

Using the formula of the free energy, (4.1.1) can be written explicitly in terms of the drift b, the diffusion matrix D, the potential f and the pressure p as follows

$$\partial_t \rho = \mathscr{L}'\rho = \operatorname{div}\big(b\rho\big) + \operatorname{div}\Big[D\Big(\nabla p(\rho) + \rho\nabla f\Big)\Big].$$

Remark 4.2.2*.* To comment on the scope of Assumption 4.2.1, note that the convexity and superlinear growth at infinity of u ensure that the functional U is lower semi-continuous with respect to the weak convergence of measures, see Lemma 4.A.2. (4.2.2) implies that the negative part of $u(\rho)$ is in $L^1(\mathbb{R}^d)$ (for $\rho \in \mathcal{P}_2(\mathbb{R}^d)$). The infinitesimal pressure is modelled by p and is clearly non-negative and increasing, we refer to [Vil08, Chapter 15] for a further discussion. (4.2.3) allows for a large class of internal energy functionals U, capturing in particular the cases of the Boltzmann entropy and power functions.

It is natural for the potential f to be assumed bounded from below, this ensures the lower semi-continuity of F with respect to weak convergence. Also, a Lipschitz f means that $\frac{f(x)}{\|x\|+1} < C$ and hence F will be finite. The aforementioned lower semi-continuity, as well as the linearity of F and convexity of U is the standard framework to obtain the well-posedness of the scheme.

Assumption 4.2.3. [On b and D] The constant matrix $D \in \mathbb{R}^{d\times d}$ is symmetric. The vector field $b \in C(\mathbb{R}^d;\mathbb{R}^d)$ is Lipschitz.

Remark 4.2.4*.* Most notably, we allow for the matrix D to be singular and the vector field b to not necessarily have gradient form. This permits us to study a wider class of PDEs, see Section 4.3. When Equation (4.1.1) is the Kolmogorov forward equation of the associated SDE, D takes the form of the product of a diffusion matrix with its transpose, hence assuming its symmetry is natural.

Next, we detail the relationship between D, b and the cost c_h.

Assumption 4.2.5 (The cost c_h)**.** There exists an $h_0 > 0$ such that for all $0 < h < h_0$ the cost map $c_h : \mathbb{R}^{2d} \to \mathbb{R}$ is continuous and satisfies the following assumptions.

(i) Fix any $x \in \mathbb{R}^d$, the map $y \mapsto c_h(x,y)$ is differentiable.

(ii) There exists a real valued $d \times d$-matrix B_h of order $O(h)$ such that

$$\big\langle \nabla_y c_h(x,y), \tilde{\eta} \big\rangle - \big\langle 2(y-x) - 2hb(y), \eta \big\rangle = O(h^2)(1 + \|\eta\|)(\|x\|^2 + \|y\|^2 + 1) + O(1) c_h(x,y), \quad (4.2.6)$$

for all $\eta, x, y \in \mathbb{R}^d$, where $\tilde{\eta} := (D + B_h)\eta$.

(iii) There exists a constant $C(h) > 0$, possibly depending on h, such that

$$\|\nabla_y c_h(x,y)\| \leq C(h)\big(\|x\|^2 + \|y\|^2 + 1\big), \qquad \forall x, y \in \mathbb{R}^d. \quad (4.2.7)$$

(iv) There exists $C > 0$ for all $x, y \in \mathbb{R}^d$ such that

$$\|x - y\|^2 \leq C\big(c_h(x,y) + h^2(\|x\|^2 + \|y\|^2)\big), \quad (4.2.8)$$

and, for some constant $C(h) > 0$, possibly depending on h,

$$c_h(x,y) \leq C(h)\big(\|x\|^2 + \|y\|^2\big), \quad (4.2.9)$$

and

$$0 \leq c_h(x,y). \quad (4.2.10)$$

Before proceeding, a thorough review of this assumption is in order and we do so via the following sequence of remarks.

Remark 4.2.6.

1. It is the main step of the JKO procedure that motivates (4.2.6). That is, (4.2.6) provides the essential link between the discrete Euler-Lagrange equations of our scheme ((4.6.3) below) and the weak solution of (4.1.1) (given by (4.2.14) below). Equation (4.2.6) lets us replace the cost term by the drift b in the discrete Euler-Lagrange equation. The RHS of (4.2.6) then guarantees that the error we make when doing this operation is still of the correct order, see Lemma 4.6.2.

2. Conditions (4.2.8) and (4.2.9) allow us to estimate the optimal transport cost functional $W_{c_h,\epsilon}$, which is generally not a distance, in terms of the traditional Wasserstein distance. Both (4.2.9) and (4.2.10) are natural conditions to guarantee that $W_{c_h,\epsilon}(\cdot,\cdot)$ is well defined on $\mathcal{P}_2^r(\mathbb{R}^d) \times \mathcal{P}_2^r(\mathbb{R}^d)$. The condition (4.2.10) also provides weak lower semi-continuity of $\gamma \mapsto (c_h, \gamma)$ which is essential, see the proof of Proposition 4.5.1, for the well-posedness of the minimisation problem (4.1.4). Again, the constant $C(h)$ may blow up as $h \to 0$.

3. Condition (4.2.7) will be used to obtain a strong convergence for the (non-linear) pressure term when establishing the convergence of the scheme by passing to the limit $h \to 0$. Specifically, for each fixed $h > 0$ (4.2.7) guarantees integrability of $\|\nabla_y c_h\|$ against measures in $\mathcal{P}_2(\mathbb{R}^{2d})$.

We now remark on the generality of the cost map c_h.

Remark 4.2.7 (The generality of the cost c_h and concrete Examples). Notably, the cost is *not* restricted to those of the form $c_h(x,y) = c_h(x-y)$ with $c_h(x,x) = 0$, indeed such costs are usually associated to gradient flows [Agu05, JKO98, Lis09]. It is clear that Assumption 4.2.5 is verifiable in the case of $b = 0$, D symmetric non-singular, and $c_h(x,y) = \langle D^{-1}(x-y), x-y \rangle$ the weighted Euclidean. Indeed in (4.2.6) one can pick $B_h = 0$, and obtain the exact equation

$$\Big\langle \nabla_y c_h(x,y), D\eta \Big\rangle = \Big\langle 2(y-x), \eta \Big\rangle.$$

We claim that many fundamental non-linear PDEs will fit the structure of Assumption 4.2.5, and refer the reader to Section 4.3 for illustrative examples.

Assumption 4.2.8 (The regularisation change of variables)**.** For each $h > 0$ there exists a function $\mathcal{T}_h : \mathbb{R}^d \to \mathbb{R}^d$, called henceforth a 'change of variable', such that for some $\beta > 0$ and any $\sigma > 0$, $z, x \in \mathbb{R}^d$

$$c_h(x, \mathcal{T}_h(x) + \sigma z) \leq C\Big(\frac{\sigma}{h^\beta}\big(\|z\|^2 + 1\big) + h^2\big(\|x\|^2 + 1\big)\Big), \tag{4.2.11}$$

and

$$\big|f(\mathcal{T}_h(x) + \sigma z) - f(x)\big| \leq C\Big(\frac{\sigma}{h^\beta}\big(\|z\|^2 + 1\big) + h\big(\|x\|^2 + 1\big)\Big), \tag{4.2.12}$$

and the partial derivatives of $\mathcal{T}_h$ are assumed continuous.

Remark 4.2.9. The above change of variables is used in Lemma 4.6.3 to construct an admissible plan in the entropy regularised minimisation problem, allowing one to obtain a priori estimates which are crucial in establishing the convergence of the scheme. Although the above assumption may seem burdensome to check, in practice it is not. In the classical case $c_h(x, y) = \|x - y\|^2$ one simply takes $\mathcal{T}_h(x) = x$. Other examples of $\mathcal{T}_h$ are given in Section 4.3, where its clear that (4.2.12) will be straightforward since f is assumed Lipschitz.

Assumption 4.2.10 (The regularisation's scaling parameters)**.** Take three sequences $\{N_k\}_{k\in\mathbb{N}} \subset \mathbb{N}$, $\{\epsilon_k\}_{k\in\mathbb{N}} \subset \mathbb{R}_+$, and $\{h_k\}_{k\in\mathbb{N}} \subset \mathbb{R}_+$, which, for any $k \in \mathbb{N}$, abide by the following scaling

$$h_k N_k = T, \quad \text{and} \quad 0 < \epsilon_k \leq \epsilon_k |\log \epsilon_k| \leq C h_k^2, \tag{4.2.13}$$

and are such that $h_k, \epsilon_k \to 0$ and $N_k \to \infty$ as $k \to \infty$.

Remark 4.2.11. The scaling (4.2.13) is a theoretical constraint introduced in [CDPS17] for the convergence of the JKO procedure. It ensures that the entropic regularisation is sufficiently small such that the error made by its introduction in the optimal transport problem is lost in the limit $k \to \infty$.

In this work, we are interested in weak solutions to (4.1.1) as defined next.

Definition 4.2.12 (Weak solutions)**.** A function $\rho \in L^1(\mathbb{R}_+ \times \mathbb{R}^d)$, with $p(\rho) \in L^1(\mathbb{R}_+ \times \mathbb{R}^d)$, is called a weak solution of Equation (4.1.1) with initial datum $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ if it satisfies the following weak formulation

$$\int_0^T \int_{\mathbb{R}^d} \partial_t \varphi \rho dx\, dt + \int_0^T \int_{\mathbb{R}^d} (\mathscr{L}\varphi)\rho dx\, dt = -\int_{\mathbb{R}^d} \varphi(x)\rho_0 dx, \quad \text{for all} \quad \varphi \in C_c^\infty(\mathbb{R} \times \mathbb{R}^d), \tag{4.2.14}$$

concretely, using the form of $\mathscr{L}$ (4.1.1),

$$\begin{aligned}\int_0^T \int_{\mathbb{R}^d} \partial_t \varphi \rho(dx)\, dt = &-\int_{\mathbb{R}^d} \varphi(x)\rho_0(dx) + \int_0^T \int_{\mathbb{R}^d} \rho(t,x)\Big(\Big\langle D\nabla f(x), \nabla\varphi(t,x)\Big\rangle - \Big\langle b(x), \nabla\varphi(t,x)\Big\rangle\Big) dxdt \\ &- \int_0^T \int_{\mathbb{R}^d} p(\rho(t,x))\mathrm{div}\Big(D\nabla\varphi(t,x)\Big) dxdt, \quad \text{for all} \quad \varphi \in C_c^\infty(\mathbb{R} \times \mathbb{R}^d).\end{aligned}$$

The main (abstract) result of the chapter is the following theorem which holds under all the above assumptions.

Theorem 4.2.13. [Convergence of the entropic regularisation scheme] Let $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ satisfy $\mathcal{F}(\rho_0) < \infty$. Let $k \in \mathbb{N}$ and take $\{\rho^n_{\epsilon_k,h_k}\}_{n=0}^{N_k}$ to be the solution of the entropic regularisation scheme (4.1.2). Define the piecewise constant interpolation $\rho_{\epsilon_k,h_k} : (0,\infty) \times \mathbb{R}^d \to [0,\infty)$ by

$$\rho_{\epsilon_k,h_k}(t) := \rho^{n+1}_{\epsilon_k,h_k} \quad \text{when} \quad t \in [nh_k, (n+1)h_k). \tag{4.2.15}$$

Suppose that Assumptions 4.2.1, 4.2.3, 4.2.5, 4.2.8, and 4.2.10 hold. Then, as $k \to \infty$, we have the following convergence up to a subsequence

$$\rho_{\epsilon_k,h_k} \to \rho \quad \text{in} \quad L^m((0,T) \times \mathbb{R}^d),$$

where ρ is a weak solution of the evolution equation (4.1.1) in the sense of Definition 4.2.12.

The proof of this theorem is given in Section 4.6.4. In the next section we provide immediately several examples of interest as an illustration of our main results.

Remark 4.2.14. We do not prove uniqueness of the weak solution (4.2.14) in the general setting, however if uniqueness holds then Theorem 4.2.13 ensures that there is full convergence of the sequence. In some cases the uniqueness has already been proved, for instance, if D is the identity $b = 0$ and $\mathcal{F}$ is λ-displacement convex [AGS08], or in the case of the Kinetic FPE [Hua00].

4.3 Concrete problems

Theorem 4.2.13 gives a general framework in which one can check if the evolution equation (4.1.1) can be approximated by the regularised JKO-type variational scheme (4.1.2). Our setup does not immediately provide the cost or the change of variables, this has to be done on a case by case basis. In this section we present a number of examples showcasing the scope of Theorem 4.2.13. In each case an explicit cost c_h, approximation matrix B_h, and change of variables $\mathcal{T}_h$ are provided, these are then shown to satisfy Assumptions 4.2.5 and 4.2.8. In the following examples it is clear that the challenging part is identifying c_h and B_h, whereas the change of variables usually comes for free. In Section 4.3.2 the identification of c_h comes from the large deviation rate function, and in Section 4.3.3 we take c_h to be minus the log of the fundamental solution, inspired by the fact that the Euclidean distance squared is minus the log of the fundamental solution for Brownian motion[2].

The examples below make ample use of Theorem 4.2.13, and thus the proofs of the statements for each example are by verification of the several assumptions of the main theorem. Thus we provide the example and results, and postpone the (sometimes tedious) verification to the corresponding Appendix.

4.3.1 Non-linear diffusion equations: an illustrative toy example

In the case that $b=0$ (4.1.1) becomes the non-linear diffusion equation

$$\partial_t \rho = \operatorname{div}\Big(\rho D\big(\frac{\nabla p(\rho)}{\rho} + \nabla f\big)\Big). \tag{4.3.1}$$

A prototypical example of (4.3.1) is the Porous Medium Equation $\partial_t \rho = \Delta \rho^m$, corresponding to $f = 0$, $p(\rho) = \frac{\rho^m}{m-1}$ and D is the identity matrix. Equation (4.3.1) models non-linear diffusion with drift in homogeneous anisotropic material. In [Lis09] the author proved the convergence of a weighted-Wasserstein variational approximation scheme for (4.3.1) when D is symmetric non-singular, non-constant, and elliptic. In [CDPS17] the authors proved the convergence of an entropic regularised scheme for (4.3.1) when D is the identity matrix, in this respect, the following Proposition 4.3.1 extends their work. Therefore we only use this as an illustrative toy example of Theorem 4.2.13 in action. However, note that we allow the diffusion matrix D to be possibly singular, this means that (4.3.1) can be degenerate in (at least) one direction. Our strategy is to proceed via the same perturbation of D as in the previous chapters, one might call this a viscosity approach.

Proposition 4.3.1. Let D be symmetric and positive semi-definite, let $b=0$. Define the free energy $\mathcal{F}$ by (4.2.1) and let f, p satisfy Assumption 4.2.1. Let $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ satisfy $\mathcal{F}(\rho_0) < \infty$.

Define the cost $c_h : \mathbb{R}^{2d} \to \mathbb{R}$ as

$$c_h(x,y) := \langle (D+hI)^{-1}(x-y), x-y\rangle. \tag{4.3.2}$$

Let $k \in \mathbb{N}$ and take $\{\rho^n_{\epsilon_k,h_k}\}_{n=0}^{N_k}$ to be the solution of the entropy regularised scheme (4.1.2) with c_h and $\mathcal{F}$ as defined above. Define the associated piecewise constant interpolation $\rho_{\epsilon_k,h_k} : (0,\infty)\times\mathbb{R}^d \to [0,\infty)$ as in (4.2.15).

Then, taking subsequences if necessary, as $k\to\infty$, with N_k, h_k, ϵ_k abiding by Assumption 4.2.13, we have

$$\rho_{\epsilon_k,h_k} \to \rho \quad \text{in} \quad L^m((0,T)\times\mathbb{R}^d), \tag{4.3.3}$$

where ρ is a weak solution of the evolution equation (4.3.1), with initial datum ρ_0,

$$\begin{aligned}\int_0^T\int_{\mathbb{R}^d} \partial_t\varphi(t,x)\rho(t,x)dx\,dt = &-\int_{\mathbb{R}^d}\varphi(0,x)\rho_0(x)dx + \int_0^T\int_{\mathbb{R}^d}\rho(t,x)\Big(\Big\langle D\nabla f(x), \nabla\varphi(t,x)\Big\rangle dxdt \\ &+ \int_0^T\int_{\mathbb{R}^d}\Big\langle D\nabla p(\rho(t,x)), \nabla\varphi(t,x)\Big\rangle dxdt, \quad \text{for all} \quad \varphi\in C_c^\infty(\mathbb{R}\times\mathbb{R}^d).\end{aligned} \tag{4.3.4}$$

The proof of the proposition is given in Appendix 4.B.1.

[2]We haven't yet found a way to rigorously justify this choice.

4.3.2 The non-linear kinetic Fokker-Planck (Kramers) equation

Let the dimension $d = 2\tilde{d}$, and let

$$b(x,v) = \begin{pmatrix} -v \\ \nabla_x g(x) \end{pmatrix}, \qquad f(x,v) = f(v), \qquad D = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}, \tag{4.3.5}$$

for some $g : \mathbb{R}^{\tilde{d}} \to \mathbb{R}$, and where, in the matrix D, I is the $\tilde{d} \times \tilde{d}$-dimensional identity matrix and 0 stands for a $\tilde{d} \times \tilde{d}$-matrix of zeros. Substituting the above into (4.1.1) one obtains the non-linear Kinetic FPE,

$$\partial_t \rho = -\mathrm{div}_x\Big(\rho v\Big) + \mathrm{div}_v\Big(\rho \nabla_x g(x)\Big) + \mathrm{div}_v\Big(\rho \nabla_v f(v)\Big) + \Delta_v p\big(\rho\big). \tag{4.3.6}$$

If $p(\cdot)$ is the identity map, (4.3.6) reduces to the classical Kinetic FPE equation

$$\partial_t \rho = -\mathrm{div}_x\Big(\rho v\Big) + \mathrm{div}_v\Big(\rho \nabla_x g(x)\Big) + \mathrm{div}_v\Big(\rho \nabla_v f(v)\Big) + \Delta_v \rho, \tag{4.3.7}$$

where ρ describes the density of a Brownian particle with inertia

$$\begin{aligned} dX(t) &= V(t)dt, \\ dV(t) &= -\nabla g(X(t))dt - \nabla f(V(t))dt + \sqrt{2}dW(t). \end{aligned} \tag{4.3.8}$$

Recall the discussion we made on the conservative-dissipative forces in the kinetic Fokker-Planck equation in Section 1.3.1, it is not a gradient flow and contains degenerate diffusion. For a discussion on the applications of (4.3.7) see [Ris89], one of these applications being a simplified model of chemical reactions, which is the context in which Kramer [Kra40] originally introduced it. In this chapter, we will be interested in (4.3.6) for a non-linear pressure p, this can be derived via generalised thermodynamical theory [Cha03], motivated by the non-universality of the Boltzmann distribution. It has found applications in a wide variety of fields: physics, astrophysics, biology, [Cha06, CLL04]. Unregularised (one-step) variational approximation schemes for the linear kinetic FPE (4.3.7) have been developed in [DPZ14, Hua00]. A similar approach for the Vlasov–Poisson–Fokker–Planck systems was conducted in [HJ00]. In addition, operator-splitting schemes, which consist of a transport (Hamiltonian flow) step and a steepest descent step, for (4.3.7) have also been developed [DPZ14, MS20a], see also similar results for the non-linear non-local Fokker-Planck equation [CL17] and the Boltzmann equation [CG04].

Since the pressure is incorporated into the free energy, using Theorem 4.2.13 one can develop a variational scheme for (4.3.6) using the cost functions derived in [DPZ14]. Our extension of [DPZ14] is twofold, firstly the scheme has been regularised, and secondly we allow for a non-linear pressure term p. Including regularisation and a non-linear pressure would make the calculations in [DPZ14] more delicate, this added difficulty is incorporated via Theorem 4.2.13.

Assumption 4.3.2. Assume that $g \in C^3(\mathbb{R}^{\tilde{d}})$ is bounded from below and there exists a constant $C > 0$ for all $x_1, x_2 \in \mathbb{R}^{\tilde{d}}$,

$$\frac{1}{C}\|x_1 - x_2\|^2 \leq \Big\langle x_1 - x_2, \nabla g(x_1) - \nabla g(x_2)\Big\rangle, \tag{4.3.9}$$

$$\|\nabla g(x_1) - \nabla g(x_2)\| \leq C\|x_1 - x_2\|, \tag{4.3.10}$$

$$\|\nabla^2 g(x_1)\|, \|\nabla^3 g(x_1)\| \leq C. \tag{4.3.11}$$

We note that (4.3.10)-(4.3.11) implies that g has quadratic growth at infinity. Without loss of generality we assume that $g \geq 0$ and $g(0) = 0$, which implies that for any $x \in \mathbb{R}^{\tilde{d}}$

$$\|\nabla g(x)\| \leq C\|x\|.$$

We begin by proving the convergence of the entropy regularised scheme with the cost function [DPZ14, Eq. (13)]. As argued in [DPZ14], this cost function, which is derived from large deviation theory, naturally captures the conservative-dissipative coupling of the kinetic Fokker-Planck equation. The proof of the following proposition is given in Appendix 4.B.2.

Proposition 4.3.3. Let D, b and f be given by (4.3.5), with g satisfying Assumption 4.3.2. Define the free energy $\mathcal{F}$ by (4.2.1) and let f, p satisfy Assumption 4.2.1. Let $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ satisfy $\mathcal{F}(\rho_0) < \infty$.

Define the cost function $c_h : \mathbb{R}^{2d} \to \mathbb{R}$ ([DPZ14, Eq. (13)])

$$c_h(x, v; x', v') \\ := h \inf \Big\{ \int_0^h \|\ddot{\xi}(t) + \nabla g(\xi(t))\|^2 dt \ : \ \xi \in C^2([0,h]; \mathbb{R}^d), \ (\xi, \dot{\xi})(0) = (x, v), \ (\xi, \dot{\xi})(h) = (x', v') \Big\}. \quad (4.3.12)$$

Let $k \in \mathbb{N}$ and take $\{\rho^n_{\epsilon_k, h_k}\}_{n=0}^{N_k}$ to be the solution of the entropy regularised scheme (4.1.2) with c_h and $\mathcal{F}$ defined above. Define the piecewise constant interpolation $\rho_{\epsilon_k, h_k} : (0, \infty) \times \mathbb{R}^d \to [0, \infty)$ as in (4.2.15). Then, as $k \to \infty$, with N_k, h_k, ϵ_k abiding by Assumption 4.2.13, we have

$$\rho_{\epsilon_k, h_k} \to \rho \quad \text{in} \quad L^m((0,T) \times \mathbb{R}^d),$$

where ρ is a weak solution of the evolution equation (4.3.6) with initial datum ρ_0, that is

$$\int_0^T \int_{\mathbb{R}^d} \partial_t \varphi \rho dx dv dt = \int_0^T \int_{\mathbb{R}^d} \Big(\langle \nabla_x g + \nabla_v f, \nabla_v \varphi \rangle - \langle v, \nabla_x \varphi \rangle + \langle \nabla_v p(\rho), \nabla_v \varphi \rangle \Big) \rho dx dv dt \\ - \int_{\mathbb{R}^d} \varphi(0, x, v) \rho_0 dx dv, \quad \text{for all} \quad \varphi \in C_c^\infty(\mathbb{R} \times \mathbb{R}^d). \quad (4.3.13)$$

From a modelling perspective (4.3.12) is the most natural choice for a cost since it is derived directly from the large deviation principle, however it has no explicit expression and is therefore inconvenient for practical purposes. It has been shown that the explicit cost [DPZ14, Eq. (15)], which is an approximation of (4.3.12), can be implemented numerically [CH19]. We now argue that we can employ Theorem 4.2.13 to get the convergence of the entropy regularised scheme constructed with this cost too. The proof of the following proposition is given in Appendix 4.B.2.

Proposition 4.3.4. Let D, b and f be given by (4.3.5), with g satisfying Assumption 4.3.2. Define the free energy $\mathcal{F}$ by (4.2.1) and let f, p satisfy Assumption 4.2.1. Let $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ satisfy $\mathcal{F}(\rho_0) < \infty$.

Define the cost function $c_h : \mathbb{R}^{2d} \to \mathbb{R}$ by [DPZ14, Eq. (15)] that is

$$c_h(x, v; x', v') := \|v' - v + h \nabla g(x)\|^2 + 12 \Big\| \frac{x' - x}{h} - \frac{v' + v}{2} \Big\|^2. \quad (4.3.14)$$

Let $k \in \mathbb{N}$ and take $\{\rho^n_{\epsilon_k, h_k}\}_{n=0}^{N_k}$ to be the solution of the entropy regularised scheme (4.1.2) with c_h and $\mathcal{F}$ defined above. Define the piecewise constant interpolation $\rho_{\epsilon_k, h_k} : (0, \infty) \times \mathbb{R}^d \to [0, \infty)$ as in (4.2.15).

Then, as $k \to \infty$, with N_k, h_k, ϵ_k abiding by Assumption 4.2.13, we have

$$\rho_{\epsilon_k, h_k} \to \rho \quad \text{in} \quad L^m((0,T) \times \mathbb{R}^d),$$

where ρ is a weak solution of the evolution equation (4.3.6) with initial datum ρ_0, that is (4.3.13) also holds true.

4.3.3 A degenerate diffusion equation of Kolmogorov-type

Let $\tilde{d}, n \in \mathbb{N}$, and denote $\mathbf{x} = \big(x_1, x_2, \ldots, x_{n-1}, x_n\big)^T$, where $x_i \in \mathbb{R}^{\tilde{d}}$. Set $d = \tilde{d} n$, and

$$b(\mathbf{x}) = -(x_2, x_3, \ldots, x_n, 0)^T, \qquad D = \begin{pmatrix} 0 & 0 \\ 0 & I \end{pmatrix}, \qquad f(\mathbf{x}) = f(x_n), \quad (4.3.15)$$

where, in the matrix D, I is the $\tilde{d} \times \tilde{d}$-dimensional identity matrix and 0 stands for a $\tilde{d}(n-1) \times \tilde{d}(n-1)$-matrix of zeros. Then (4.1.1) reduces to the following non-linear degenerate diffusion equation of Kolmogorov type

$$\partial_t \rho(t, x_1, \ldots, x_n) = -\sum_{i=2}^n \mathrm{div}_{x_{i-1}}(x_i \rho) + \mathrm{div}_{x_n}(\nabla f(x_n) \rho) + \Delta_{x_n} p(\rho), \quad (4.3.16)$$

for which, using Theorem 4.2.13, a weak solution will be shown to exist as the limit of a regularised variational scheme.

To gain insight into choosing an appropriate cost function we consider the linear case where $p(\cdot)$ is the identity. In this case (4.3.16) becomes

$$\partial_t \rho(t, x_1, \ldots, x_n) = -\sum_{i=2}^{n} \mathrm{div}_{x_{i-1}}(x_i \rho) + \mathrm{div}_{x_n}(\nabla f(x_n)\rho) + \Delta_{x_n} \rho, \tag{4.3.17}$$

which is the forward Kolmogorov equation of the associated stochastic differential equations

$$\begin{aligned} d\xi_1 &= \xi_2\, dt \\ d\xi_2 &= \xi_3\, dt \\ &\vdots \\ d\xi_{n-1} &= \xi_n\, dt \\ d\xi_n &= -\nabla f(\xi_n)\, dt + \sqrt{2}\, dW(t), \end{aligned} \tag{4.3.18}$$

where $W(t)$ is a $\tilde{d}$-dimensional Wiener process. The above system describes a system of n coupled oscillators, each of them moving vertically and being connected to their nearest neighbours, the last oscillator being forced by a friction and a random noise. Of course the simplest cases of $n = 1, n = 2$ correspond to the heat equation and Kramers equation (with no background potential) respectively. When $n > 2$ these type of equations arise as models of simplified finite Markovian approximations of generalised Langevin dynamics [OP11], or harmonic oscillator chains [BL08, DM10].

Recently [DT18] showed that the fundamental solution to (4.3.17) is determined by the following minimisation problem

$$c_h(\mathbf{x}, \mathbf{y}) := h \inf_{\xi} \int_0^h \|\xi^{(n)}(s)\|^2\, ds, \tag{4.3.19}$$

where $\mathbf{x} = (x_1, \ldots, x_n) \in \mathbb{R}^{\tilde{d}n}$, $\mathbf{y} = (y_1, \ldots, y_n) \in \mathbb{R}^{\tilde{d}n}$ and the infimum is taken over all curves $\xi \in C^n([0,T]; \mathbb{R}^d)$ that satisfy the boundary conditions

$$(\xi, \dot{\xi}, \ldots, \xi^{(n-1)})(0) = (x_1, x_2, \ldots, x_n) \quad \text{and} \quad (\xi, \dot{\xi}, \ldots, \xi^{(n-1)})(h) = (y_1, y_2, \ldots, y_n). \tag{4.3.20}$$

The optimal value $c_h(\mathbf{x}, \mathbf{y})$ is called the *mean squared derivative cost function* and has been found to be useful in the modelling and design of various real-world systems such as motor control, biometrics, online-signatures and robotics, see [DT17] for further discussion.

Theorem [DT17, Theorem 1.2] states that the mean square derivative cost function $c_h(\mathbf{x}, \mathbf{y})$ can be written in the explicit form,

$$c_h(\mathbf{x}, \mathbf{y}) = h^{2-2n} \left[\mathbf{b}(h, \mathbf{x}, \mathbf{y})\right]^T \mathcal{M} \mathbf{b}(h, \mathbf{x}, \mathbf{y}), \tag{4.3.21}$$

where $\mathbf{b} : \mathbb{R}_+ \times \mathbb{R}^{2\tilde{d}n} \to \mathbb{R}^{\tilde{n}d}$ and $\mathcal{M} \in \mathbb{R}^{2\tilde{d}n}$ are explicitly given by (4.B.1). Using this explicit form of the cost function, [DT18, Theorem 1.4] proved the convergence of an unregularised variational scheme to the weak solution of (4.3.17).

In the following proposition we use the cost (4.3.21) to construct a variational scheme for the highly degenerate non-linear PDE (4.3.16), the proof of which is in Appendix 4.B.3. Our contributions are again twofold, firstly we allow for a non-linear p, and secondly our scheme is regularised.

Proposition 4.3.5. Let D, f, and b be given by (4.3.15), with f satisfying Assumption 4.2.1. Define $\mathcal{F}$ by (4.2.1). Let $\rho_0 \in \mathcal{P}_2^r(\mathbb{R}^d)$ satisfy $\mathcal{F}(\rho_0) < \infty$. Define the cost function c_h by (4.3.21).

Let $k \in \mathbb{N}$ and take $\{\rho^n_{\epsilon_k, h_k}\}_{n=0}^{N_k}$ to be the solution of the entropy regularised scheme (4.1.2) with c_h and $\mathcal{F}$ defined above. Define the piecewise constant interpolation $\rho_{\epsilon_k, h_k} : (0, \infty) \times \mathbb{R}^d \to [0, \infty)$ as in (4.2.15).

Then, as $k \to \infty$, with N_k, h_k, ϵ_k abiding by Assumption 4.2.13, we have

$$\rho_{\epsilon_k, h_k} \to \rho \quad \text{in} \quad L^m((0,T) \times \mathbb{R}^d),$$

where ρ is a weak solution of the evolution equation (4.3.16), with initial datum ρ_0,

$$\int_0^T \int_{\mathbb{R}^d} \partial_t \varphi \rho d\mathbf{x} dt = \int_0^T \int_{\mathbb{R}^d} \Big(-\sum_{i=2}^n \langle x_i, \nabla_{x_{i-1}} \varphi \rangle + \langle \nabla_{x_n} f(x_n), \nabla_{x_n} \varphi \rangle + \langle \nabla_{x_n} p(\rho), \nabla_{x_n} \varphi \rangle \Big) \rho d\mathbf{x} dt$$
$$- \int_{\mathbb{R}^d} \varphi(0, \mathbf{x}) \rho_0 d\mathbf{x}, \quad \text{for all} \quad \varphi \in C_c^\infty(\mathbb{R} \times \mathbb{R}^d).$$

Remark 4.3.6. The above examples can be cast into the GENERIC framework which describes evolution equations containing both reversible dynamics and irreversible dynamics [DO21, DPZ13, KLMP20] (see Chapter 3). Due to the splitting structure, a possible alternative approach to address GENERIC systems is to construct operator-splitting schemes. This is a challenging problem, which we have made initial attempts at in Chapters 2 and 3, as have the works [CG04, CL17, DPZ14, MS20a].

4.4 An illustrative numerical experiment

We illustrate our findings with a numerical implementation of our algorithm applied to the Kramers equation of Section 4.3.2. The matrix scaling algorithm that we use is inspired by the work [Cut13, Pey15, CDPS17], which are based on entropic regularisation. Our simulations (and their quality) are on par with other results found in the literature, for example [CH19].

4.4.1 Discretisation and the matrix scaling algorithm

We first carry out a discretisation and rewriting of our general scheme (4.1.2) into a form which lends itself amenable to a numerical implementation. For a chosen $M \in \mathbb{N}$ we consider some discrete points $\{x_i\}_{i=1}^M \subset \mathbb{R}^d$, which are assumed to form a uniform grid in $\mathbb{R}^d$, with each grid tile having volume $\lambda > 0$.

We consider discrete probability measures ρ on $\mathbb{R}^d$ fully supported on this grid, which are identified by their one-to-one correspondence with the probability simplex

$$\Sigma^M := \left\{ \rho \in \mathbb{R}_+^M : \sum_{i=1}^M \rho_i = 1 \right\}.$$

Note the small abuse of notation where the symbol ρ denotes the discrete probability measure and its corresponding element in Σ^M. The density approximation of a discrete measure ρ is then taken with respect to the discrete Lebesgue measure $\Lambda := \lambda \sum_{i=1}^M \delta_{x_i}$, and is given by the vector $\frac{1}{\lambda}\rho$.

The discrete approximation of the regularised optimal transport problem (4.1.3) is then defined as, for any $\mu, \nu \in \Sigma^M$,

$$\overline{W}_{c_h,\epsilon}(\mu, \nu) := \inf_{\pi \in \mathbb{R}_+^{M \times M}} \left\{ \sum_{i,j=1}^M (c_h)_{i,j} \pi_{i,j} + \epsilon \pi_{i,j} \log\left(\frac{\pi_{i,j}}{\lambda^2}\right) \; : \; \pi \mathbb{1} = \mu, \pi^T \mathbb{1} = \nu \right\}, \tag{4.4.1}$$

where, of course, $(c_h)_{i,j} = c_h(x_i, x_j)$ and $\mathbb{1} = (1, \dots, 1)^T \in \mathbb{R}^M$. With this in hand, our discrete approximation to the JKO scheme (4.1.2) becomes: given $\epsilon, h > 0$, and some $\rho_{h,\epsilon}^0 \in \Sigma^M$, then, for $n = 1, \dots, N$ with h such that $hN = T$, $\rho_{h,\epsilon}^n$ determined iteratively as the unique minimiser of the following (discrete version of (4.1.2))

$$\min_{\rho \in \Sigma^M} \frac{1}{2h} \overline{W}_{c_h,\epsilon}(\rho_{h,\epsilon}^{n-1}, \rho) + \overline{\mathcal{F}}(\rho), \tag{4.4.2}$$

where $\overline{\mathcal{F}}(\rho) := \sum_{i=1}^M f(x_i)\rho_i + \lambda u\big(\rho_i/\lambda\big)$, since u acts on the density of ρ with respect to discrete Lebesgue measure. Define the Gibbs Kernel $K \in \mathbb{R}^{M \times M}$ by $K_{i,j} = \exp(-\frac{c_h(x_i,x_j)}{\epsilon})$. Next, due to the entropic regularisation, we can make the well-known and celebrated observation [Pey15] that (4.4.2) can be reformulated by taking $\rho_{h,\epsilon}^n = \pi^T \mathbb{1}$, where π minimises

$$\min_{\pi \in \mathbb{R}_+^{M \times M}} \mathrm{KL}(\pi || K) + \mathcal{G}_n(\pi \mathbb{1}) + \frac{2h}{\epsilon} \overline{\mathcal{F}}(\pi^T \mathbb{1}), \tag{4.4.3}$$

where $\mathrm{KL}(\pi||K) := \sum_{i,j}^{M} \pi_{i,j} \log\left(\frac{\pi_{i,j}}{K_{i,j}}\right) - \pi_{i,j} + K_{i,j}$ stands for the Kullback-Leibler divergence (KL divergence), and

$$\mathcal{G}_n(\rho) := \begin{cases} 0 & \text{if } \rho = \rho_{h,\epsilon}^{n-1} \\ \infty & \text{otherwise.} \end{cases}$$

Problems taking the form (4.4.3) can be tackled by highly parallelizable matrix scaling algorithms [CPSV18, Algorithm 1]; these are a generalisation of the Sinkhorn algorithm. Moreover, for the energy functional $\mathcal{F}$ that we consider, there exist relatively simple formulas for the computation of the projections that appear in [CPSV18, Algorithm 1]. It should be noted that [CPSV18] considers general measure spaces, where the product measure is taken as a reference in the KL divergence. Since we consider a uniform grid, for us, the discrete KL divergence with respect to the product discrete Lebesgue measure is the appropriate approximation to the continuous KL divergence. Hence, the reference measures $d\mathbf{x}, d\mathbf{y}$ in [CPSV18] can be ignored in our case as our Gibbs kernel already has the mass factors multiplying it.

4.4.2 Numerical simulation of Kramers equation

We now provide the results of our simulations for Kramers equation using a form of [CPSV18, Algorithm 1] re-cast to solve minimisation problems of the type of (4.4.3). Note that in comparison with [CH19, Section V] we consider a different model, and employ a different spatial discretisation for which we use a uniform grid while they use grid-points as given by the forward simulated paths (a random space grid). We study this particular equation as we have access to its explicit solution and hence we are able to quantify the scheme's error. We point out that until our work (Proposition 4.3.4), the scheme used in [CH19, Section V] was not theoretically justified.

The dynamics is studied in dimension 2 and without an external potential, i.e., we consider (4.3.6) with p the identity, $g = 0$, and $f(v) = \frac{v^2}{2}$. That is we solve

$$\partial_t \rho(t,x,v) = -v\partial_x \rho(t,x,v) + \partial_v\big(\rho(t,x,v)v\big) + \partial_v^2 \rho(t,x,v). \tag{4.4.4}$$

If we consider the sharp initial condition $\rho(0,x,v) = \delta(x-x_0)\delta(v-v_0)$ for some $x_0, v_0 \in \mathbb{R}$, then, defining

$$\begin{aligned} &S_1(t) = (1-e^{-2t}),\ S_2(t) = (1-e^{-t})^2, \\ &S_3(t) = 2t - 3 + 4e^{-t} - e^{-2t}, \\ &\delta_1(x,t) = x - \big(x_0 + v_0(1-e^{-t})\big),\ \delta_2(v,t) = v - v_0 e^{-t}, \end{aligned}$$

the fundamental of (4.4.4) is (see [Bal08])

$$\rho_{\text{exact}}(t,x,v) = \frac{1}{2\pi\sqrt{S_1 S_3 - S_2^2}} \exp\Big\{ -\frac{S_1\delta_1^2 - 2S_2\delta_1\delta_2 + S_3\delta_2^2}{2(t - 2 + 4e^{-t} - (t+2)e^{-2t})} \Big\}. \tag{4.4.5}$$

To avoid the Dirac singularity at $t = 0$ we offset the initial time, i.e., we equip (4.4.4) with the initial condition $\rho(0) = \rho_{\text{exact}}(t_0)$ for some $t_0 > 0$. We simulate the entropy regularised scheme with initial condition $\rho_{\text{exact}}(t_0)$. The simulations are run on a fixed discretised grid of $[-0.5, 0.5] \times [-2.4, 2.4]$, using 200×130 points equidistant apart, using the discretised scheme described in Section 4.4.1 across three different choices of regularisation parameter $\epsilon = 0.5, 0.09, 0.05$. The approximation at time t is compared to the exact solution $\rho_{\text{exact}}(t+t_0)$ via the $L^1(\Lambda)$-norm (we compare integral of the absolute value of the difference of joint densities with respect to the discrete Lebesgue measure Λ, for $\lambda = \frac{4.8}{26000}$).

Figure 4.4.1 shows the evolution of the position and velocity marginals. The well-known effect of blurring on the optimal transport problem stemming from regularisation [PC19] is also clear from these figures: as the regularisation increases the mass is forced to spread out. Moreover, there is a roughness, especially in the velocity marginal, which disappears as the regularisation is increased (this smooths the kink) and/or the number of grid points are increased (this reduces numerical underflow and increases overall precision, see below). The latter suggests why the kink is more apparent in the velocity marginal - it is supported on a larger domain and hence requires a finer grid spacing. However, this has to be balanced against the (high) computational effort induced by performing optimal transport in higher dimensions. For our algorithm, we are forced to have a fine grid spacing in the position component to counterbalance the h appearing in the cost function (and to capture the speed of diffusion). Matching this grid spacing also in the velocity component is computationally prohibitive (with our implementation).

Figure 4.4.2 gives a quantitative analysis of the error between our scheme and the exact solution ρ_{exact} (the joint density) as a function of time. As anticipated the error reduces as the entropic blurring is decreased, and the error increases with time.

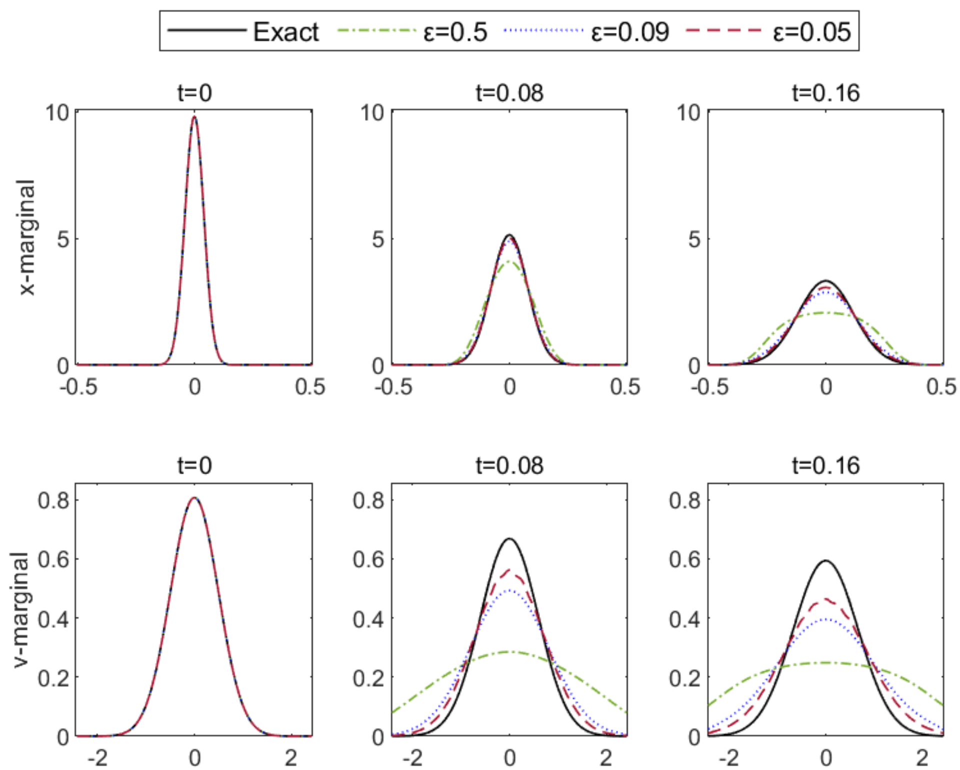

Figure 4.4.1: Comparison between the exact solution (black line) and our entropy regularised scheme for the position x-marginal and velocity v-marginal, across three time-slices $t = 0, 0.08, 0.16$ and three regularisation choices $\epsilon = 0.5, 0.09, 0.05$. Simulation over the position-velocity domain $[-0.5, 0.5] \times [-2.5, 2.5]$. All cases are ran with a step-size of $h = 0.02$.

We now discuss some of the drawbacks of the numerical implementation of this JKO scheme. As pointed out already, regularisation introduces blurring into the system giving less sharp results. To circumvent this, one takes a small value for the regularisation parameter, however this causes numerical underflow due to the exponential form of the Gibbs Kernel K (defined just above (4.4.3)). For the vanilla Sinkhorn algorithm this is discussed in [PC19, Remark 4.7], and for more general scaling algorithms see [CPSV18, Sch19]. This issue can be partly minimised by carrying out the computations in the log-domain [PC19, Section 4.4]. Critically, the log-domain strategy is very costly due to many additional operations introduced, the algorithm is no longer just a matrix scaling algorithm. This issue is mitigated to a certain extent by the absorbing algorithm [Sch19, Algorithm 2.].

There is a further added difficulty for schemes with a time-step dependent cost function, such as the ones introduced in our manuscript. Namely, for a fixed spatial discretization, as the time-step tends to zero the cost function "blows up", which stems from a $O(1/h^2)$-order term appearing in the cost function (4.3.14). This (in addition to the $1/\epsilon$ appearing in the Gibbs Kernel K and discussed above) requires careful tuning, otherwise it will lead to numerical underflow. This suggests an operator-splitting scheme as in the previous chapters, may be more favourable in simulating Kramers equation, since the cost function appearing there

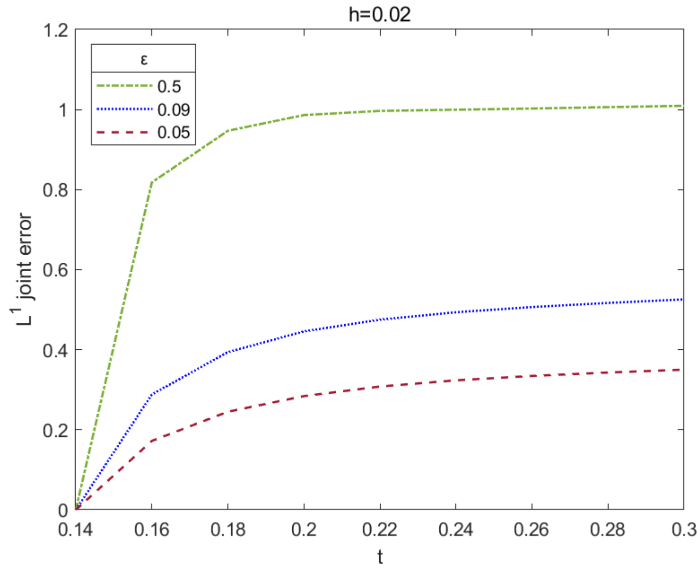

Figure 4.4.2: $L^1(\Lambda)$-norm joint error of the regularised scheme as a map of time over $[0.14, 0.3]$ for multiple regularisation parameters $\epsilon = 0.5, 0.09, 0.05$. Simulation over the position-velocity domain $[-0.5, 0.5] \times [-2.5, 2.5]$. All cases are ran with a step-size of $h = 0.02$.

is only of order $1/h$ (instead of the order $1/h^2$ appearing in our cost term).

Lastly, we note that in full rigour one should show the convergence of the fully discretised scheme (4.4.2) to its continuous version as the volume λ of each grid tile tends to zero. Such analysis has been done for many Wasserstein-type gradient flows [BCMS20, JMO17, MO14, MS20b], however it is still an open question for the systems we consider here. As in the mentioned papers, we expect that some conditions, such as Courant–Friedrichs–Lewy (CFL) type condition, need to be imposed on the temporal and spatial meshes to guarantee the convergence of the fully discretised schemes. Revealing such conditions for non-gradient systems is nontrivial and we leave this question for future work.

4.5 Well-posedness of the regularised JKO scheme

The main result of this section is Proposition 4.5.1, stating the existence of a unique minimiser to the optimisation problem (4.1.4). It is natural to achieve well-posedness of the scheme through finiteness, lower semi-continuity, and convexity of the functionals which appear in it. There exist $h_0, \epsilon_0 > 0$ depending only on the constants in our assumptions, such that all the following results hold for all h, ϵ such that $h_0 > h > 0$ $\epsilon_0 > \epsilon > 0$. Note that we are ultimately interested in the case where $h, \epsilon \to 0$. We now give the main result of this section, the well-posedness of the optimal transport optimisation problem (4.1.4).

Proposition 4.5.1. Take $h, > 0$ small enough with $\frac{\epsilon}{h} \leq 1$ and $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$ with $\mathcal{F}(\mu) < \infty$. Then, there exists a unique $\nu^* \in \mathcal{P}_2^r(\mathbb{R}^d)$ such that

$$\nu^* = \underset{\nu \in \mathcal{P}_2^r(\mathbb{R}^d)}{\operatorname{argmin}} \left\{ \frac{1}{2h} W_{c_h,\epsilon}(\mu, \nu) + \mathcal{F}(\nu) \right\}.$$

The proof is provided at the end of the section after stating and proving a sequence of auxiliary results.

4.5.1 Proofs and auxiliary results

From (4.2.8) in Assumption 4.2.5 we immediately have the following result.

Lemma 4.5.2. For any $h > 0$ small enough, and any μ and ν in $\mathcal{P}_2(\mathbb{R}^d)$ with γ the associated optimal plan in (4.1.3), it holds that

$$M(\nu) \leq C\Big((c_h, \gamma) + M(\mu)\Big),$$

where the constant $C > 0$ is independent of h, ϵ.

Proof. Let γ be optimal plan in (4.1.3) with first marginal μ and second marginal ν. Since for all $x, y \in \mathbb{R}^d$ $\|y\|^2 \leq 2(\|x\|^2 + \|x-y\|^2)$, we have

$$\begin{aligned} M(\nu) = \int_{\mathbb{R}^{2d}} \|y\|^2 d\gamma(x,y) \leq & 2\int_{\mathbb{R}^{2d}} \|x\|^2 + \|x-y\|^2 d\gamma(x,y) \\ \leq & 2\int_{\mathbb{R}^{2d}} \|x\|^2 + C\big(c_h(x,y) + h^2(\|x\|^2 + \|y\|^2)\big) d\gamma(x,y), \end{aligned} \tag{4.5.1}$$

where in (4.5.1) we have used (4.2.8). Hence for some $C > 0$

$$M(\nu) \leq C\Big((c_h, \gamma) + (1+h^2)M(\mu) + h^2 M(\nu)\Big),$$

which implies that for small enough h,

$$M(\nu) \leq C\Big((c_h, \gamma) + M(\mu)\Big).$$

□

Of course if $\rho^n_{h,\epsilon}, \rho^{n-1}_{h,\epsilon}$ are built from the scheme (4.1.2) with associated plan $\gamma^n_{h,\epsilon}$, then Lemma 4.5.2 says that for small enough h

$$M(\rho^n_{h,\epsilon}) \leq C\Big((c_h, \gamma^n_{h,\epsilon}) + M(\rho^{n-1}_{h,\epsilon})\Big). \tag{4.5.2}$$

Lemma 4.5.3 (Weak lower semi-continuity of $\gamma \mapsto (c_h, \gamma)$)**.** Let $h > 0$. Let $\{\gamma_k\}_{k\in\mathbb{N}} \subset \mathcal{P}(\mathbb{R}^{2d})$, $\gamma \in \mathcal{P}(\mathbb{R}^{2d})$, with $\gamma_k \rightharpoonup \gamma$. Then

$$(c_h, \gamma) \leq \liminf_{k\to\infty} (c_h, \gamma_k).$$

Proof. The map $c_h : \mathbb{R}^{2d} \to \mathbb{R}$ is continuous and non-negative by Assumption 4.2.5, hence the result is given by [Vil08, Lemma 4.3]. □

Lemma 4.5.4 (Weak lower semi-continuity of entropy under bounded 2nd moments)**.** Let $\{\gamma_k\}_{k\in\mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^{2d})$, $\gamma \in \mathcal{P}_2(\mathbb{R}^{2d})$ with $\gamma_k \rightharpoonup \gamma$. Further assume that there exists a $C > 0$, such that for all $k \in \mathbb{N}$, $M(\gamma_k), M(\gamma) < C$, then

$$H(\gamma) \leq \liminf_{k\to\infty} H(\gamma_k).$$

Proof. This follows immediately by Lemma 4.A.2 taking $u(a) = a\log(a)$. □

Lemma 4.5.5 (Existence of minimising couplings in the optimal transport problem)**.** Given $\mu, \nu \in \mathcal{P}_2^r(\mathbb{R}^d)$ with finite entropy $H(\mu), H(\nu) < \infty$. Then, there exists a $\gamma \in \Pi(\mu,\nu)$ with $H(\gamma) < \infty$ which attains the infimum in $W_{c_h,\epsilon}(\mu,\nu)$.

Proof. By [Vil08, Lemma 4.4] $\Pi(\mu,\nu)$ is tight, and hence by Prokhorov's Theorem it is also relatively compact. Let $\gamma_k \in \Pi(\mu,\nu)$, $k \in \mathbb{N}$, be a minimising sequence of $W_{c_h,\epsilon}(\mu,\nu)$.

Now, using that $\Pi(\mu,\nu)$ is relatively compact, we can say (extracting a sub-sequence and relabelling) that $\gamma_k \rightharpoonup \gamma^* \in \Pi(\mu,\nu)$ (since $\Pi(\mu,\nu)$ is weakly closed). Lemmas 4.5.3, 4.5.4 proved lower semi-continuity of $\gamma \mapsto (c_h, \gamma)$, $\gamma \mapsto H(\gamma)$ respectively, which implies the limit, γ^*, is a minimiser.

It remains only to show that γ^* has a density. Using (4.2.9) (and that there exists an admissible plan, e.g., the product measure $\mu \otimes \nu$) we see that $W_{c_h,\epsilon}(\mu,\nu) < \infty$. Since $W_{c_h,\epsilon}(\mu,\nu) < \infty$ and $(c_h, \gamma^*) \geq 0$ we deduce that $H(\gamma^*) < \infty$. □

So far we have shown that there exists an absolutely continuous transport plan with finite entropy that solves the optimal transport problem (4.1.3) between any two measures in $\mathcal{P}_2^r(\mathbb{R}^d)$. Next, we explore some properties of the Kantorovich optimal transport cost functional $W_{c_h,\epsilon}$ defined by (4.1.3).

Lemma 4.5.6 (Strict Convexity of $\nu \mapsto W_{c_h,\epsilon}(\mu,\nu)$)**.** For a fixed $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$,

$$\mathcal{P}_2^r(\mathbb{R}^d) \ni \nu \mapsto W_{c_h,\epsilon}(\mu,\nu),$$

is strictly convex.

Proof. This follows as in [CDPS17, Lemma 2.5] by linearity of $\gamma \mapsto (c_h,\gamma)$ and strict convexity of H. □

Lemma 4.5.7 (Lower semi-continuity of $\nu \mapsto W_{c_h,\epsilon}(\mu,\nu)$ restricted to $\mathcal{P}_2^r(\mathbb{R}^d)$ and uniform moment bounds)**.** Let $\{\nu_k\}_{k\in\mathbb{N}} \subset \mathcal{P}_2^r(\mathbb{R}^d)$, $\mu,\nu \in \mathcal{P}_2^r(\mathbb{R}^d)$, with $\nu_k \rightharpoonup \nu$. Moreover, assume for all $k \in \mathbb{N}$ the probability measures ν_k,μ,ν have uniformly bounded entropy and 2nd moments. Then

$$W_{c_h,\epsilon}(\mu,\nu) \le \liminf_{k\to\infty} W_{c_h,\epsilon}(\mu,\nu_k).$$

Proof. Let $\{\nu_k\},\mu,\nu$ be as assumed above, and $\{\gamma_k\}$ be the associated optimal plans in $W_{c_h,\epsilon}(\mu,\nu_k)$. Note $\{\gamma_k\} \subset \Pi(\mu,\{\nu_k\})$ (see notation, Section 1.4). Since $\{\nu_k\}$ is weakly convergent it is tight, and [Vil08, Lemma 4.4] implies that $\Pi(\mu,\{\nu_k\})$ is too, hence extracting (and relabelling) a sub-sequence $\{\gamma_k\}$, we know that $\gamma_k \rightharpoonup \gamma \in \mathcal{P}(\mathbb{R}^{2d})$. In fact $\gamma \in \Pi(\mu,\nu)$ since weak convergence of γ_k implies weak convergence of its marginals (and we know $\nu_k \rightharpoonup \nu$). Now, the lower semi-continuity established in Lemmas 4.5.3 and 4.5.4 implies that

$$\begin{aligned}\liminf_{k\to\infty} W_{c_h,\epsilon}(\mu,\nu_k) = \liminf_{k\to\infty} \frac{1}{2h}(c_h,\gamma_k) + \epsilon H(\gamma_k) &\ge \frac{1}{2h}(c_h,\gamma) + \epsilon H(\gamma)\\ &\ge W_{c_h,\epsilon}(\mu,\nu).\end{aligned}$$

□

Lemma 4.5.8. [Lower-semi continuity of $\mathcal{F}$ under uniformly bounded moments] Let $\{\mu_k\}_{k\in\mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^d)$, $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ with $\mu_k \rightharpoonup \mu$. Assume $\sup_k M(\mu_k) < \infty$, then

$$\mathcal{F}(\mu) \le \liminf_{k\to\infty} \mathcal{F}(\mu_k). \tag{4.5.3}$$

Proof. The lower semi-continuity of U follows from the uniform bounded moments, Assumption 4.2.1 and Lemma 4.A.2. The lower semi-continuity of F follows from [AFP00, Theorem 2.38], since $(x,y) : \mathbb{R}^d \times \mathbb{R} \to \mathbb{R}$, $(x,y) \mapsto f(x)y$ is clearly 1-homogeneous and convex in y for fixed x (as f is non-negative). □

We are now in a position to prove the main result of this section.

Proof of proposition 4.5.1. Denote $J_{c_h,\epsilon}(\mu,\nu) := \frac{1}{2h}W_{c_h,\epsilon}(\mu,\nu)+\mathcal{F}(\nu)$, and γ the optimal coupling in $W_{c_h,\epsilon}(\mu,\nu)$. Note that since $f \ge 0$ and by Lemma 4.A.1 we have, for some fixed $C > 0$ and $0 < \alpha < 1$,

$$J_{c_h,\epsilon}(\mu,\nu) \ge \frac{1}{2h}W_{c_h,\epsilon}(\mu,\nu) - C(1+M(\nu))^\alpha. \tag{4.5.4}$$

Furthermore, since the sum of infima is less than the infima of the sum, and by the property of the entropy and marginals $H(\gamma) \ge H(\mu) + H(\nu)$, we have

$$\frac{1}{2h}W_{c_h,\epsilon}(\mu,\nu) \ge \frac{1}{2h}(c_h,\gamma) + \frac{\epsilon}{2h}\big(H(\mu)+H(\nu)\big).$$

Moreover, using Lemma 4.5.2 we have, for $h,\epsilon > 0$ small enough

$$\begin{aligned}\frac{1}{2h}W_{c_h,\epsilon}(\mu,\nu) \ge& \frac{1}{2h}(c_h,\gamma) + M(\mu) - M(\mu) + \frac{\epsilon}{2h}\big(H(\mu)+H(\nu)\big)\\ \ge& C_1 M(\nu) + C_{\mu,\epsilon,h} + \frac{\epsilon}{2h}H(\nu),\end{aligned}$$

with fixed constants $C_1 > 0$, and $C_{\mu,\epsilon,h}$ depending only on μ, ϵ, h. Consequently by Lemma 4.A.1 we arrive at

$$\frac{1}{2h} W_{c_h,\epsilon}(\mu,\nu) \geq C_1 M(\nu) + C_{\mu,\epsilon,h} - \frac{\epsilon}{2h} C(1+M(\nu))^{\alpha}. \tag{4.5.5}$$

Combining (4.5.5) with (4.5.4), and choosing h, ϵ small enough we get that

$$J_{c_h,\epsilon}(\mu,\nu) \geq C_1 M(\nu) + C_{\mu,\epsilon,h} - C_1(1+M(\nu))^{\alpha}. \tag{4.5.6}$$

Since $\alpha \in (0,1)$, one can see that (4.5.6) implies that the functional $\nu \mapsto J_{c_h,\epsilon}(\mu,\nu)$ is bounded from below. Note that there exists a $\nu \in \mathcal{P}_2^r(\mathbb{R}^d)$ such that $J_{c_h,\epsilon}(\mu,\nu) < \infty$, for example, take $\nu = \mu$ (and the product plan). Let $\{\nu_k\}$ be a minimising sequence of $\nu \mapsto J_{c_h,\epsilon}(\mu,\nu)$. Note $M(\nu_k), H(\nu_k)$ are uniformly bounded. Since $M(\nu_k)$ is uniformly bounded, the set $\{\nu_k\}$ is tight, hence extracting a subsequence (not relabelled) we obtain $\nu_k \rightharpoonup \nu \in \mathcal{P}(\mathbb{R}^d)$. Moreover, $\nu \in \mathcal{P}_2(\mathbb{R}^d)$ since uniform bounded 2nd moments and weak convergence implies the limit has a bounded 2nd moment. The lower semi-continuity proved in Lemmas 4.5.7 and 4.5.8 ensures that the limit ν is a minimiser. That $\nu \in \mathcal{P}_2^r(\mathbb{R}^d)$ follows since lower semi-continuity of $\mapsto H(\nu)$ under uniformly bounded 2nd moments (see Lemma 4.A.2), which implies $H(\nu)$ is finite. Finally the uniqueness of ν follows from the linearity of F, convexity of U, and that $W_{c_h,\epsilon}$ is strictly convex by Lemma 4.5.6. □

4.6 Proof of the main result

This section presents the proof of the main result, Theorem 4.2.13. We first establish discrete Euler-Lagrange equations for the minimisers of the regularised scheme 4.1.2, then we derive necessary a priori estimates, and finally we prove the convergence (up to a subsequence) of the scheme.

4.6.1 Discrete Euler-Lagrange equations

In this section we study the minimisers of the optimisation problem (4.1.4). This is done by studying the functional $\frac{1}{2h} W_{c_h,\epsilon}\big(\mu,\cdot\big) + \mathcal{F}(\cdot)$ (for a fixed $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$) at small perturbations around its minimiser. Recall that Proposition 4.5.1 ensured well-posedness of (4.1.4) for small enough $h, \epsilon > 0$, and thus the associated Euler-Lagrange equations will also hold for such h, ϵ small enough.

When (4.1.1) is describing a Wasserstein gradient flow its solution can be viewed as the minimiser of a large deviation rate functional [ADPZ13]. With this perspective one can view the Euler-Lagrange equations, established below in Lemma 4.6.2, as the discrete analogue of (4.2.14).

Throughout this section, for a given vector field $\eta \in C_c^\infty(\mathbb{R}^d;\mathbb{R}^d)$ we call $\Phi : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}^d$ the flow through η with dynamics

$$\partial_s \Phi_s = \eta(\Phi_s), \;\; \Phi_0 = \mathrm{id}. \tag{4.6.1}$$

The following result is well established (for instance see [CDPS17, Proposition 3.5]).

Lemma 4.6.1. Let $\nu \in \mathcal{P}_2^r(\mathbb{R}^d)$, and $\eta \in C_c^\infty(\mathbb{R}^d;\mathbb{R}^d)$ with flow Φ_s defined in (4.6.1). The first variation of the free energy $\mathcal{F}$ at ν along η, and denoted by $\delta\mathcal{F}(\nu,\eta)$, is

$$\delta\mathcal{F}(\nu,\eta) := \frac{d}{ds}\mathcal{F}\big((\Phi_s)_{\#}\nu\big)\Big|_{s=0} = \int_{\mathbb{R}^d} \nu(y)\Big\langle \eta(y), \nabla f(y)\Big\rangle dy - \int_{\mathbb{R}^d} p(\nu(y))\mathrm{div}(\eta(y))dy. \tag{4.6.2}$$

Lemma 4.6.2 (Euler-Lagrange equation)**.** Let $\mu \in \mathcal{P}_2^r(\mathbb{R}^d)$, and h, ϵ be small enough. Let ν be the optimum in (4.1.4), and let γ be the corresponding optimal plan in $W_{c_h,\epsilon}(\mu,\nu)$. Then, for any $\eta \in C_c^\infty(\mathbb{R}^d;\mathbb{R}^d)$ we have

$$0 = \frac{1}{2h}\int_{\mathbb{R}^{2d}} \Big\langle \eta(y), \nabla_y c_h(x,y)\Big\rangle d\gamma(x,y) - \frac{\epsilon}{2h}\int_{\mathbb{R}^d} \nu(y)\mathrm{div}(\eta(y))dy + \delta\mathcal{F}(\nu,\eta). \tag{4.6.3}$$

In particular, by (4.2.6), we have for any function $\varphi \in C_c^\infty(\mathbb{R}^d)$

$$\begin{aligned}\frac{1}{h}\int_{\mathbb{R}^{2d}} \Big\langle (y-x), \nabla\varphi(y)\Big\rangle d\gamma(x,y) \\ = \int_{\mathbb{R}^d} \nu(y)\Big\langle b(y), \nabla\varphi(y)\Big\rangle dy + \frac{\epsilon}{2h}\int_{\mathbb{R}^d} \nu(y)\mathrm{div}\big((D+B_h)\nabla\varphi(y)\big)dy \\ - \delta\mathcal{F}(\nu, (D+B_h)\nabla\varphi) + O(h)(1+\|\nabla\varphi\|_\infty)\Big(M(\mu)+M(\nu)+1\Big) + O\big(\frac{1}{h}\big)(c_h,\gamma)\end{aligned} \tag{4.6.4}$$

Proof. Let Φ be defined as in (4.6.1). Since ν is optimal for the minimisation problem (4.1.4) we have

$$\frac{1}{2h}W_{c_h,\epsilon}(\mu,\nu) + \mathcal{F}(\nu) \le \frac{1}{2h}W_{c_h,\epsilon}(\mu,(\Phi_s)_\#\nu) + \mathcal{F}((\Phi_s)_\#\nu),$$

which implies,

$$0 \le \limsup_{s\to 0} \frac{1}{2hs}\Big(W_{c_h,\epsilon}(\mu,(\Phi_s)_\#\nu) - W_{c_h,\epsilon}(\mu,\nu)\Big) + \delta\mathcal{F}(\nu,\eta). \tag{4.6.5}$$

Let γ be the optimal coupling in (4.1.4). Then, for $\tilde\Phi_s := (\mathrm{id}, \Phi_s)$, we know $(\tilde\Phi_s)_\#\gamma \in \Pi(\mu, (\Phi_s)_\#\nu)$ with $H((\tilde\Phi_s)_\#\gamma) < \infty$ so we have

$$\begin{aligned}\limsup_{s\to 0} \frac{1}{2hs}\Big(W_{c_h,\epsilon}(\mu,(\Phi_s)_\#\nu) - W_{c_h,\epsilon}(\mu,\nu)\Big) \\ \le \limsup_{s\to 0}\frac{1}{2hs}\Big((c_h,(\tilde\Phi_s)_\#\gamma) - (c_h,\gamma) + \epsilon\Big(H((\tilde\Phi_s)_\#\gamma) - H(\gamma)\Big)\Big).\end{aligned}$$

By Fatou's Lemma we have

$$\limsup_{s\to 0}\frac{(c_h,(\tilde\Phi_s)_\#\gamma) - (c_h,\gamma)}{2hs} \le \frac{1}{2h}\int_{\mathbb{R}^{2d}} \Big\langle \eta(y), \nabla_y c_h(x,y)\Big\rangle d\gamma(x,y),$$

and also

$$\begin{aligned}\limsup_{s\to 0}\frac{\epsilon\Big(H((\tilde\Phi_s)_\#\gamma) - H(\gamma)\Big)}{2hs} &\le \limsup_{s\to 0}\frac{-\epsilon}{2hs}\Big(\int_{\mathbb{R}^d} \log(|\mathrm{det} J\Phi_s(y)|) - \log(|\mathrm{det} J\Phi_0(y)|)d\nu(y)\Big) \\ &= -\frac{\epsilon}{2h}\int_{\mathbb{R}^{2d}} \nu(y)\mathrm{div}\big(\eta(y)\big)dy.\end{aligned}$$

Injecting this result into (4.6.5) and substituting η for $-\eta$ gives the result. □

4.6.2 A priori estimates

In this section we provide a number of a priori estimates which will help to establish the compactness arguments of Section 4.6.3. Throughout this section the results hold for each fixed $k \in \mathbb{N}$, that is, for each h_k, ϵ_k, N_k of the sequences satisfying (4.2.13), and the sequence $\{\rho^n_{h_k,\epsilon_k}\}_{n=0}^{N_k-1}$ built from the scheme (4.1.2) with the associated sequence of optimal couplings $\{\gamma^n_{h_k,\epsilon_k}\}_{n=1}^{N_k}$. For notational convenience we omit the dependence on k and simply write $h, \epsilon, N, \{\rho^n\}_{n=0}^{N-1}, \{\gamma^n\}_{n=1}^{N}$.

Lemma 4.6.3. For all $n \in \{1, \dots, N\}$, we have

$$(c_h, \gamma^n) \le Ch^2\Big(M(\rho^{n-1}) + 1\Big) - \epsilon H(\rho^n) + 2h\Big(\mathcal{F}(\rho^{n-1}) - \mathcal{F}(\rho^n)\Big), \tag{4.6.6}$$

for $C > 0$ a constant depending only on ρ_0 and the constants in the assumptions.

In the well established JKO procedure [JKO98, Eqs. (42)-(45)] one compares $\frac{1}{2h}W_2^2(\rho^{n-1},\rho^n) + \mathcal{F}(\rho^n)$ against $\frac{1}{2h}W_2^2(\rho^{n-1},\rho^{n-1}) + \mathcal{F}(\rho^{n-1})$. The term $W_2^2(\rho^{n-1},\rho^{n-1})$ is zero, and hence one would end up with a control of $W_2(\rho^{n-1},\rho^n)$ in terms of the free energy. However, in the present work, since $W_{c_h,\epsilon}$ is not a metric, we need to pick a new distribution to compare the performance of ρ^n against. We judiciously choose such a distribution as to make the cost c_h of transporting mass free.

Proof. This proof has two steps. First, is the choice of the distribution ρ_σ against which to compare ρ^n. The second part is carrying out the said comparison.

Step 1: the candidate distribution ρ_σ and its properties. Let $G \in C_c^\infty(\mathbb{R}^d)$ be a probability density, such that $M(G) = 1$, $H(G) < \infty$. For a scaling parameter $\sigma > 0$, to be chosen later, define $G_\sigma(\cdot) := \sigma^{-d} G(\frac{\cdot}{\sigma})$. For $\mathcal{T}_h$ defined in Assumption 4.2.8 define

$$\gamma_\sigma(x, y) := \rho^{n-1}(x) G_\sigma\big(y - \mathcal{T}_h(x)\big),$$

as a joint distribution with first marginal ρ^{n-1}, and second marginal

$$\rho_\sigma(y) := \int \gamma_\sigma(x, y) dx.$$

Then, the change of variables $y = \mathcal{T}_h(x) + \sigma z$ and leaving x unchanged, has Jacobian

$$J(x, z) := \begin{pmatrix} D\mathcal{T}_h(x) & \sigma \\ 1 & 0 \end{pmatrix}, \tag{4.6.7}$$

with determinant $\big|\det J(x, z)\big| = \sigma^d$. Where the entries $\sigma, 1, 0$ are $d \times d$-dimensional matrices of that entry multiplied by the identity matrix. Applying the change of variable and calculating we have

$$\begin{aligned} (c_h, \gamma_\sigma) &= \int_{\mathbb{R}^d} c_h(x, y) \rho^{n-1}(x) G_\sigma(y - \mathcal{T}_h(x)) dx dy \\ &= \int_{\mathbb{R}^d} c_h(x, \mathcal{T}_h(x) + \sigma z) \rho^{n-1}(x) G(z) dx dz. \end{aligned} \tag{4.6.8}$$

Hence by Assumption 4.2.8, it follows

$$\begin{aligned} (c_h, \gamma_\sigma) \leq & C \int_{\mathbb{R}^{2d}} \Big(\frac{\sigma}{h^\beta} \Big(\|z\|^2 + 1 \Big) + h^2 \Big(\|x\|^2 + 1 \Big) \Big) \rho^{n-1}(x) G(z) dx dz \\ = & C \Big(\frac{\sigma}{h^\beta} \Big(\int_{\mathbb{R}^d} \|z\|^2 G(z) dz + 1 \Big) + h^2 \Big(\int_{\mathbb{R}^{2d}} \|x\|^2 \rho^{n-1}(x) dx + 1 \Big) \Big) \\ = & C \Big(\frac{\sigma}{h^\beta} + h^2 \big(M(\rho^{n-1}) + 1 \big) \Big). \end{aligned} \tag{4.6.9}$$

Moreover, a straightforward calculation gives

$$H(\gamma_\sigma) = H(\rho^{n-1}) - d \log \sigma + H(G). \tag{4.6.10}$$

Again by Assumption 4.2.8 and the change of variables above we have the following estimate for the potential energy

$$\begin{aligned} F(\rho_\sigma) &= \int_{\mathbb{R}^d} f(y) \rho_\sigma(y) dy \\ &\leq \int_{\mathbb{R}^{2d}} \Big(|f(y) - f(x)| + f(x) \Big) \rho^{n-1}(x) G_\sigma(y - \mathcal{T}_h(x)) dx dy \\ &= \int_{\mathbb{R}^{2d}} \Big(|f(\mathcal{T}_h(x) + \sigma z) - f(x)| \Big) \rho^{n-1}(x) G(z) dx dy + \int_{\mathbb{R}^{2d}} f(x) \rho^{n-1}(x) G(z) dx dz \\ &\leq C \int_{\mathbb{R}^{2d}} \Big(\frac{\sigma}{h^\beta} \Big(\|z\|^2 + 1 \Big) + h \Big(\|x\|^2 + 1 \Big) \Big) \rho^{n-1}(x) G(z) dx dz + F(\rho^{n-1}) \\ &\leq C \Big(\frac{\sigma}{h^\beta} + h \Big(M(\rho^{n-1}) + 1 \Big) \Big) + F(\rho^{n-1}). \end{aligned} \tag{4.6.11}$$

Jensen's inequality implies (by the convexity of u) that for the internal energy

$$U(\rho_\sigma) = \int_{\mathbb{R}^d} u \Big(\int_{\mathbb{R}^d} \gamma_\sigma(x, y) dx \Big) dy \leq \int_{\mathbb{R}^{2d}} u(\rho^{n-1}) G_\sigma(y - \mathcal{T}_h(x)) dx dy = U(\rho^{n-1}). \tag{4.6.12}$$

Therefore, (4.6.11) and (4.6.12) together yields

$$\begin{aligned}\mathcal{F}(\rho_\sigma) &\leq C\Big(\frac{\sigma}{h^\beta} + h\Big(M(\rho^{n-1}) + 1\Big)\Big) + F(\rho^{n-1}) + U(\rho^{n-1}) \\ &= C\Big(\frac{\sigma}{h^\beta} + h\Big(M(\rho^{n-1}) + 1\Big)\Big) + \mathcal{F}(\rho^{n-1}). \end{aligned} \tag{4.6.13}$$

Step 2: comparing ρ_σ and ρ^n. Since the $\{\rho^n\}$ are built from the scheme (4.1.2), and γ_σ is a coupling of ρ^{n-1} and ρ_σ, we have

$$\frac{1}{2h}\Big((c_h, \gamma^n) + \epsilon H(\gamma^n)\Big) + \mathcal{F}(\rho^n) \leq \frac{1}{2h} W_{c_h,\epsilon}(\rho^{n-1}, \rho_\sigma) + \mathcal{F}(\rho_\sigma) \leq \frac{1}{2h}\Big((c_h, \gamma_\sigma) + \epsilon H(\gamma_\sigma)\Big) + \mathcal{F}(\rho_\sigma). \tag{4.6.14}$$

Substituting the above calculations (4.6.9), (4.6.10) and (4.6.13) into (4.6.14) we get

$$\begin{aligned}\frac{1}{2h}\Big((c_h, \gamma^n) + \epsilon H(\gamma^n)\Big) + \mathcal{F}(\rho^n) \leq &\frac{1}{2h}\Big(C\Big(\frac{\sigma}{h^\beta} + h^2\Big(M(\rho^{n-1}) + 1\Big)\Big) + \epsilon\Big(H(\rho^{n-1}) - d\log\sigma + H(G)\Big)\Big) \\ &+ C\Big(\frac{\sigma}{h^\beta} + h\Big(M(\rho^{n-1}) + 1\Big)\Big) + \mathcal{F}(\rho^{n-1}). \end{aligned} \tag{4.6.15}$$

Rearranging the terms and using that $H(\gamma^n) \geq H(\rho^n) + H(\rho^{n-1})$ we obtain

$$\begin{aligned}(c_h, \gamma^n) \leq &C\Big(\frac{\sigma}{h^\beta} + h^2\Big(M(\rho^{n-1}) + 1\Big)\Big) + \epsilon\Big(- H(\rho^n) - d\log\sigma + H(G)\Big) \\ &+ 2hC\Big(\frac{\sigma}{h^\beta} + h\Big(M(\rho^{n-1}) + 1\Big)\Big) + 2h\Big(\mathcal{F}(\rho^{n-1}) - \mathcal{F}(\rho^n)\Big). \end{aligned} \tag{4.6.16}$$

Now we are free to choose $\sigma = \epsilon^{1+\frac{\beta}{2}}$. Recall that the scaling (4.2.13) implies $\frac{\sigma}{h^\beta} \leq Ch^2$ and $-\epsilon d \log\sigma \leq (1 + \frac{\beta}{2})\epsilon d \log|\epsilon|$, we thus have

$$(c_h, \gamma^n) \leq Ch^2\Big(M(\rho^{n-1}) + 1\Big) - \epsilon H(\rho^n) + 2h\Big(\mathcal{F}(\rho^{n-1}) - \mathcal{F}(\rho^n)\Big).$$

□

From Lemma 4.6.3 we are able to establish uniform boundedness of the 2nd moment, energy and entropy, of the solutions to the variational scheme (4.1.2). This is the result we present next. One should note that in the following bounds the constant C depends on the dimension d, the constants of our assumptions, the initial data ρ^0, but importantly is independent of k. We mention that the following proof differs from classical a priori bounds for a JKO scheme since c_h is not assumed to be a metric. We follow a similar strategy to that found in [DPZ14, Hua00], first obtaining bounds locally and then extending them over the full time interval.

Lemma 4.6.4 (Bounded Moments, Energy, and Entropy)**.** For small enough $h, \epsilon > 0$, we have for all $n \in \{1, \ldots, N\}$

$$M(\rho^n), |\mathcal{F}(\rho^n)|, -H(\rho^n) < C. \tag{4.6.17}$$

Proof. We begin by finding an $N_0 \in \mathbb{N}$ and $h_0 \in \mathbb{R}$ independent of the initial data, and a $\bar{C}$ depending only on $M(\rho^0), \mathcal{F}(\rho^0)$ such that

$$M(\rho^n), \mathcal{F}(\rho^n). \tag{4.6.18}$$

holds for all $n \leq N_0$ with $h \leq h_0$. Now for any $i \in \{1, \ldots, N\}$

$$M(\rho^i)^{\frac{1}{2}} \leq M(\rho^{i-1})^{\frac{1}{2}} + W_2(\rho^{i-1}, \rho^i) \tag{4.6.19}$$

$$\leq M(\rho^{i-1})^{\frac{1}{2}} + C\Big((c_h, \gamma^i) + h^2(M(\rho^{i-1}) + M(\rho^i)\Big)^{\frac{1}{2}} \tag{4.6.20}$$

$$\leq M(\rho^{i-1})^{\frac{1}{2}} + C\Big((c_h, \gamma^i)^{\frac{1}{2}} + h(M(\rho^{i-1})^{\frac{1}{2}} + M(\rho^i)^{\frac{1}{2}})\Big),$$

where in (4.6.19) we have used the Minkowski integral inequality, and in (4.6.20) we have used Lemma 4.5.2. Summing over $i = 1, \dots, n$, we get

$$M(\rho^n)^{\frac{1}{2}} \leq C\Big(M(\rho^0)^{\frac{1}{2}} + \sum_{i=1}^{n}(c_h, \gamma^i)^{\frac{1}{2}} + h\sum_{i=1}^{n} M(\rho^i)^{\frac{1}{2}}\Big). \tag{4.6.21}$$

Squaring (4.6.21), and then using Cauchy–Schwarz inequality we get

$$\begin{aligned} M(\rho^n) \leq & C\Big(M(\rho^0) + \big(\sum_{i=1}^{n}(c_h, \gamma^i)^{\frac{1}{2}}\big)^2 + h^2\big(\sum_{i=1}^{n} M(\rho^i)^{\frac{1}{2}}\big)^2\Big) \\ \leq & C\Big(M(\rho^0) + n\sum_{i=1}^{n}(c_h, \gamma^i) + h^2 n\sum_{i=1}^{n} M(\rho^i)\Big). \end{aligned}$$

Now applying Lemma (4.6.3), and recalling $Nh = T$, we have

$$M(\rho^n) \leq C\Big(M(\rho^0) - n\epsilon\sum_{i=1}^{n} H(\rho^i) + 2hn\Big(\mathcal{F}(\rho^0) - \mathcal{F}(\rho^n)\Big) + h\sum_{i=1}^{n} M(\rho^i)\Big),$$

Next recalling that f is positive, and using Lemma 4.A.1 twice, we can deduce

$$M(\rho^n) \leq C\Big(M(\rho^0) + \mathcal{F}(\rho^0) + \epsilon n\sum_{i=1}^{n}(1 + M(\rho^i))^\alpha + (1 + M(\rho^n))^\alpha + h\sum_{i=1}^{n} M(\rho^i)\Big). \tag{4.6.22}$$

The scaling 4.2.10 and (4.6.22) implies that for some fixed constant $C(\rho^0) > 0$ depending only on $M(\rho^0), \mathcal{F}(\rho^0)$, and a fixed the constant $C_0 > 0$ independent of the initial condition we have

$$M(\rho^n) \leq C_0\Big(C(\rho^0) + h\sum_{i=1}^{n}(1 + M(\rho^n))^\alpha + h\sum_{i=1}^{n} M(\rho^i)\Big). \tag{4.6.23}$$

Now since C_0 is fixed and independent of the initial condition we can find an $N_0 \in \mathbb{N}$ $h_0 \in \mathbb{R}$ such that for all $h \leq h_0$ we have $N_0 h C_0 \leq \frac{1}{2}$. Define $M_{N_0} := \max_{i=1,\dots,N_0} M(\rho^n)$. Then (4.6.23) implies

$$M_{N_0} \leq C_0\Big(C(\rho^0) + hN_0(1 + M_{N_0})^\alpha + hN_0 M_{N_0}\Big)$$

rearranging gives

$$\frac{1}{2}M_{N_0} \leq C_0\Big(C(\rho^0) + hN_0(1 + M_{N_0})^\alpha\Big). \tag{4.6.24}$$

Using (4.6.24) we can directly conclude the uniform bounded moments $M(\rho^n)$ for all $h \leq h_0$ and $n = 1, \dots, N_0$. Now we obtain a similar bound for $\mathcal{F}(\rho^n)$. Rearranging (4.6.6), and using the non-negativity of c_h, we see that for any $i \in \{1, \dots, N_0\}$

$$h\big(\mathcal{F}(\rho^i) - \mathcal{F}(\rho^{i-1})\big) \leq Ch^2\big(1 + M(\rho^i)\big) - \epsilon H(\rho^i). \tag{4.6.25}$$

Employing (4.A.2) for $-H(\rho^i)$, dividing through by h, and using the bounded moments gives

$$\mathcal{F}(\rho^i) - \mathcal{F}(\rho^{i-1}) \leq \bar{C}h$$

For some $\bar{C}$ depending only on $M(\rho^0), \mathcal{F}(\rho^0)$. Summing the above inequality over $i = 1, \dots, n \leq N_0$, and using that $hN \leq T$, yields

$$\mathcal{F}(\rho^n) \leq \bar{C} \tag{4.6.26}$$

for a new constant $\bar{C}$ depending only on $M(\rho^0), \mathcal{F}(\rho^0)$. Hence for all $h \leq h_0$ and $n \in \{1, \dots, N_0\}$,

$$M(\rho^n), \mathcal{F}(\rho^n), \tag{4.6.27}$$

for some constant $\bar{C}$ depending only on $M(\rho^0)$ and $\mathcal{F}(\rho^0)$. Since the N_0 and h_0 we have chosen are independent of the initial data we can extend the bound (4.6.27) to all $n \in \{1, \dots, N\}$ similarly as has been done in [Hua00, Lemma 5.3], see also [DPZ14]. Indeed : generate a sequence $\tilde{\rho}^n$ corresponding to the initial data $\rho^0 = \rho^{N_0}$, then, as before, we have that for all $1 \leq n \leq N_0$

$$M(\rho^{N_0+n}) = M(\tilde{\rho}^n) \leq C(\rho^{N_0}), \quad \mathcal{F}(\rho^{N_0+n}) = \mathcal{F}(\tilde{\rho}^n) \leq C(\rho^{N_0}),$$

where $C(\rho^{N_0}) > 0$ is a fixed constant depending only on $M(\rho^{N_0}), \mathcal{F}(\rho^{N_0})$, which by (4.6.27) we know are bounded by a constant only depending on $M(\rho^0), \mathcal{F}(\rho^0)$. Therefore, $C(\rho^{N_0})$ ultimately only depends on $M(\rho^0), \mathcal{F}(\rho^0)$. Repeating this argument enough times we find that for all $n \in \{1, \dots N\}$ we have that $M(\rho^n), \mathcal{F}(\rho^n) \leq C$. Note from the uniform bounded moments we can also deduce the uniform bounds $-H(\rho^n) < C$ by (4.A.2), and $-\mathcal{F}(\rho^n)$ by (4.A.1) for U and the fact that f is Lipschitz for F. This gives the result. □

Corollary 4.6.5 (The total sum of the costs)**.** Let h be sufficiently small, then we have

$$\sum_{i=1}^{N} (c_h, \gamma^n) \leq Ch.$$

Proof. Summing (4.6.6) over n, using the bounds of Lemma 4.6.4, and the scaling Assumption 4.2.10 yields the result. □

4.6.3 The limiting procedure

Let $\{\rho^n_{h_k,\epsilon_k}\}_{n=0}^{N_k}$ be the solution of our scheme (4.1.2) with associated optimal plans $\{\gamma^n_{h_k,\epsilon_k}\}_{n=1}^{N_k}$, and interpolation ρ_k defined in (4.2.15). For notational convenience throughout this section we write $\rho^n_{h_k,\epsilon_k} = \rho^n_k$, $\gamma^n_{h_k,\epsilon_k} = \gamma^n_k$. As is common in the JKO procedure, the a priori estimates give us enough compactness to pass, at least along a subsequence, to the limit of ρ_k to some ρ in $L^1((0,T) \times \mathbb{R}^d)$. We show that ρ is in fact a weak solution of (4.1.1).

Lemma 4.6.6. The sequence of interpolations $\rho_k : [0,T] \times \mathbb{R}^d \to \mathbb{R}$ constructed from (4.2.15) satisfies, for any $\varphi \in C_c^\infty((0,T) \times \mathbb{R}^d)$,

$$\int_0^T \int_{\mathbb{R}^d} \rho_k(t,x)\Big(\frac{\varphi(t+h_k,x) - \varphi(t,x)}{h_k}\Big) dxdt = -\int_0^{h_k} \int_{\mathbb{R}^d} \rho^0(x) \frac{\varphi(t,x)}{h_k} dxdt + Q_k + R_k + O(h_k), \tag{4.6.28}$$

where

$$\begin{aligned} Q_k = &\int_0^T \int_{\mathbb{R}^d} \rho_k(t,y)\Big(\Big\langle \nabla f(y), \Big(D + B_{h_k}\Big)\nabla\varphi(t,y)\Big\rangle - \Big\langle b(y), \nabla\varphi(t,y)\Big\rangle\Big) dydt \\ &- \frac{\epsilon_k}{2h_k}\int_0^T \int_{\mathbb{R}^d} \rho_k(t,y)\mathrm{div}\Big(\Big(D + B_{h_k}\Big)\nabla\varphi(t,y)\Big)\Big) dydt, \end{aligned} \tag{4.6.29}$$

$$R_k = -\int_0^T \int_{\mathbb{R}^d} p(\rho_k(t,y))\mathrm{div}\Big(\Big(D + B_{h_k}\Big)\nabla\varphi(t,y)\Big) dydt. \tag{4.6.30}$$

Proof. Again, for notational convenience, we write $h_k = h, \epsilon_k = \epsilon, N_k = N$ omitting the dependence on k but leave the dependence explicit in γ_k and ρ_k. Let $t \in [0,T]$, the Taylor expansion yields

$$\begin{aligned} \int_{\mathbb{R}^d} \Big(\rho^n_k(x) - \rho^{n-1}_k(x)\Big)\varphi(t,x)dx &= \int_{\mathbb{R}^{2d}} \Big(\varphi(t,y) - \varphi(t,x)\Big) d\gamma^n_k(x,y) \\ &= \int_{\mathbb{R}^{2d}} \Big\langle y - x, \nabla\varphi(t,y)\Big\rangle d\gamma^n_k(x,y) + \kappa_n(t), \end{aligned} \tag{4.6.31}$$

where the remainder κ_n is bounded using (4.2.8) and Lemma 4.6.4, namely,

$$\begin{aligned}|\kappa_n(t)| \leq \frac{1}{2}\|\nabla^2\varphi\|_\infty \int_{\mathbb{R}^{2d}} \|x-y\|^2 d\gamma_k^n(x,y) &\leq C\int_{\mathbb{R}^{2d}} \Big(c_h(x,y) + h^2\Big(\|x\|^2 + \|y\|^2\Big)\Big) d\gamma_k^n(x,y) \\ &= C\Big((c_h,\gamma_k^n) + h^2\Big(M(\rho_k^{n-1}) + M(\rho_k^n)\Big)\Big) \\ &\leq C\Big((c_h,\gamma_k^n) + h^2\Big). \end{aligned} \tag{4.6.32}$$

From (4.6.31) and using (4.6.4), whose $O(\cdot)$ terms absorb (4.6.32), we have

$$\begin{aligned}\int_{\mathbb{R}^d} \Big(\frac{\rho_k^n(x)-\rho_k^{n-1}(x)}{h}\Big)\varphi(t,x)dx = &\int_{\mathbb{R}^{2d}} \Big\langle b(y), \nabla\varphi(t,y)\Big\rangle d\gamma_k^n(x,y) \\ &+ \int_{\mathbb{R}^d} \Big(p(\rho_k^n(y)) + \frac{\epsilon}{2h}\rho_k^n(y)\Big)\mathrm{div}\Big(\Big(D+B_h\Big)\nabla\varphi(t,y)\Big)dy \\ &- \int_{\mathbb{R}^d} \rho_k^n(y)\Big\langle \nabla f(y), \Big(D+B_h\Big)\nabla\varphi(t,y)\Big\rangle dy \\ &+O(h)(1+\|\nabla\varphi\|_\infty)\Big(M(\rho_k^{n-1}) + M(\rho_k^n) + 1\Big) + O\Big(\frac{1}{h}\Big)(c_h,\gamma_k^n). \end{aligned} \tag{4.6.33}$$

Integrating over the interval (t_{n-1}, t_n), and summing over n leads to

$$\begin{aligned}&\sum_{n=1}^{N}\int_{t_{n-1}}^{t_n}\int_{\mathbb{R}^d} \Big(\frac{\rho_k^n(x)-\rho_k^{n-1}(x)}{h}\Big)\varphi(t,x)dxdt \\ &= \int_0^T\int_{\mathbb{R}^d} \rho_k(t,y)\Big\langle b(y), \nabla\varphi(t,y)\Big\rangle dydt + \int_0^T\int_{\mathbb{R}^d} \Big(p(\rho_k(t,y)) + \frac{\epsilon}{2h}\rho_k(t,y)\Big)\mathrm{div}\Big(\Big(D+B_h\Big)\nabla\varphi(t,y)\Big)dydt \\ &\qquad - \int_0^T\int_{\mathbb{R}^d} \rho_k(t,y)\Big\langle \nabla f(y), \Big(D+B_h\Big)\nabla\varphi(t,y)\Big\rangle dydt + O(h), \qquad (4.6.34) \\ &= -Q_k - R_k + O(h),\end{aligned}$$

where Q_k and R_k given are by (4.6.29) and (4.6.30). To establish the first equality we used the bounded moments result in Lemma 4.6.4, Corollary 4.6.5 on the sum of the costs to control for the very last term in (4.6.33) after being summed up over n, and have used that $Nh = T$. By summation by parts, the LHS is equal

$$\begin{aligned}&\sum_{n=1}^{N_k}\int_{t_{n-1}}^{t_n}\int_{\mathbb{R}^d} \Big(\frac{\rho_k^n(x)-\rho_k^{n-1}(x)}{h}\Big)\varphi(t,x)dxdt \\ &\qquad = -\int_0^h\int_{\mathbb{R}^d} \rho^0(x)\frac{\varphi(t,x)}{h}dxdt + \int_0^T\int_{\mathbb{R}^d} \rho_k(t,x)\Big(\frac{\varphi(t,x)-\varphi(t+h,x)}{h}\Big)dxdt.\end{aligned} \tag{4.6.35}$$

Joining (4.6.34) and (4.6.35), and re-arranging gives the result (4.6.28). □

Inline with the classical strategy developed in [JKO98] we are left to take limits in (4.6.28). The convergence of the additional terms involving $b, \frac{\epsilon}{h}$ is easy since they are linear in ρ_k and we have the scaling (4.2.13). The convergence of the non-linear term is dealt with in the following section, after which we conclude the proof of Theorem 4.2.13.

Strong Convergence of the pressure of ρ_k. We emphasise the weak convergence of ρ_k is not enough to deal with convergence of the non-linear term

$$\int_0^T\int_{\mathbb{R}^d} p(\rho_k(t,y))\mathrm{div}\Big(\Big(D+B_h\Big)\nabla\varphi(t,y)\Big)dydt.$$

Instead, the convergence of $\rho_k \to \rho$ in $L^m([0,T],\mathbb{R}^d)$ is obtained via the compactness argument [RS03, Theorem 2] similar to that done in [CDPS17, CL17]. Then, (4.2.3) implies p is continuous from $L^m([0,T],\mathbb{R}^d)$ to $L^1([0,T],\mathbb{R}^d)$ and hence $p(\rho_k) \to p(\rho)$ in $L^1([0,T],\mathbb{R}^d)$.

Lemma 4.6.7. Consider the sequence of interpolations $\rho_k : [0,T] \times \mathbb{R}^d \to \mathbb{R}$ constructed from (4.2.15), and $m \in \mathbb{N}$ introduced in Assumption 4.2.1. For k large enough we have that

$$\int_0^T \int_{\mathbb{R}^d} \big((\rho_k(t,y))^m + \|\nabla(\rho_k(t,y))^m\|\big) dydt \le C, \tag{4.6.36}$$

where $C > 0$ independent of k.

Proof. The estimate of Lemma 4.6.4 and (4.2.4) yield directly

$$\int_0^T \int_{\mathbb{R}^d} (\rho_k(t,y))^m dydt \le C.$$

It remains to show

$$\int_0^T \int_{\mathbb{R}^d} \|\nabla(\rho_k(t,y))^m\| dydt \le C. \tag{4.6.37}$$

Omit the dependence on k from $\rho_k^n = \rho^n$ and $\gamma_k^n = \gamma^n$ for this proof. Set $\mu^n := \frac{\epsilon}{2h}\rho^n + p(\rho^n)$ and notice that $\mu^n \in L^1(\mathbb{R}^d)$ by (4.2.4) and Lemma 4.6.4. From the Euler-Lagrange equation Lemma 4.6.2

$$\int_{\mathbb{R}^d} \mu^n(y)\mathrm{div}(\eta(y))dy = \frac{1}{2h}\int_{\mathbb{R}^{2d}} \Big\langle \nabla_y c_h(x,y), \eta(y)\Big\rangle d\gamma^n(x,y) + \int_{\mathbb{R}^d} \Big\langle \rho^n(y)\nabla f(y), \eta(y)\Big\rangle dy. \tag{4.6.38}$$

Since $\gamma^n \in \Pi(\rho^{n-1}, \rho^n)$ with $H(\gamma^n) < \infty$, by the disintegration of measures [AFP00, Theorem 2.28] there exists a measure valued map $y \to \gamma_y^n$ such that $\gamma^n = \gamma_y^n \times \rho^n$, so that one can write

$$\int_{\mathbb{R}^{2d}} \Big\langle \nabla_y c_h(x,y), \eta(y)\Big\rangle d\gamma^n(x,y) = \int_{\mathbb{R}^d} \Big\langle \eta(y), \Big(\rho^n(y)\int_{\mathbb{R}^d} \nabla_y c_h(x,y)\gamma_y^n(x)dx\Big)\Big\rangle dy.$$

Note that, for each fixed $h > 0$, $y \mapsto \big(\rho^n(y)\int_{\mathbb{R}^d} \nabla_y c_h(x,y)\gamma_y^n(x)dx\big) \in L^1(\mathbb{R}^d)$, since by (4.2.7) and Lemma 4.6.4,

$$\begin{aligned}\int_{\mathbb{R}^d} \Big|\rho^n(y)\int_{\mathbb{R}^d} \nabla_y c_h(x,y)\gamma_y^n(x)dx\Big| dy \le& \int_{\mathbb{R}^{2d}} \|\nabla_y c_h(x,y)\|\gamma^n(x,y)dxdy\\ \le& C(h)\Big(M(\rho^n) + M(\rho^{n-1}) + 1\Big) < \infty.\end{aligned}$$

Moreover, since f is differentiable and Lipschitz it is clear that $y \mapsto \rho^n(y)\nabla f(y) \in L^1(\mathbb{R}^d)$. Hence μ^n has a weak derivative $\nabla\mu^n \in L^1(\mathbb{R}^d)$. Moreover, we prove next that $\mu^n \in \mathrm{BV}(\mathbb{R}^d)$, concretely,

$$\begin{aligned}\Big|\int_{\mathbb{R}^d} \mu^n(y)\mathrm{div}(\eta(y))dy\Big| \le& \Big|\frac{1}{2h}\int_{\mathbb{R}^{2d}} \Big\langle \nabla_y c_h(x,y), \eta(y)\Big\rangle d\gamma^n(x,y)dxdy\Big| + C\|\eta\|_\infty \qquad (4.6.39)\\ =& \Big|\frac{1}{h}\int_{\mathbb{R}^{2d}} \Big\langle \Big((y-x) - hb(y)\Big), (D+B_h)\eta(y)\Big\rangle d\gamma^n(x,y)\Big| \qquad (4.6.40)\\ &+ \Big|O(h)(1+\|\eta\|_\infty)(M(\rho^{n-1}) + M(\rho^n) + 1) + O\Big(\frac{1}{h}\Big)(c_h, \gamma^n)\Big| + C\|\eta\|_\infty,\end{aligned}$$

where (4.6.39) follows using that f is differentiable and Lipschitz, and (4.6.40) follows by (4.2.6). Notice now that the moments in (4.6.40) are finite because of Lemma 4.6.4 and the $O(h)$ terms are dominated by a constant C. Therefore,

$$\begin{aligned}(4.6.40) \le& \Big|\frac{1}{h}\int_{\mathbb{R}^{2d}} \Big\langle \Big((y-x) - hb(y)\Big), (D+B_h)\eta(y)\Big\rangle d\gamma^n(x,y)\Big|\\ &+ O\Big(\frac{1}{h}\Big)(c_h, \gamma^n) + C\Big(1 + \|\eta\|_\infty\Big).\end{aligned} \tag{4.6.41}$$

Consider the first term in (4.6.41)

$$\Big|\frac{1}{h}\int_{\mathbb{R}^{2d}}\Big\langle\Big((y-x)-hb(y)\Big),(D+B_h)\eta(y)\Big\rangle d\gamma^n(x,y)\Big|$$

$$\leq O(1)\|\eta\|_\infty\Big(\frac{1}{h}\int_{\mathbb{R}^{2d}}\|x-y\|d\gamma^n(x,y)+\int_{\mathbb{R}^d}\|b(y)\|\rho^n(y)dy\Big) \tag{4.6.42}$$

$$\leq O(1)\|\eta\|_\infty\Big(\frac{1}{h}\Big(\int_{\mathbb{R}^{2d}}\|x-y\|^2d\gamma^n(x,y)\Big)^{1/2}+1+\int_{\mathbb{R}^d}\|y\|^2\rho^n(y)dy\Big) \tag{4.6.43}$$

$$\leq O(1)\|\eta\|_\infty\frac{1}{h}\Big((c_h,\gamma^n)+O(h^2)\Big)^{1/2}+C\|\eta\|_\infty, \tag{4.6.44}$$

where: (4.6.42) is because of Cauchy-Schwarz inequality and that $\|(D+B_h)\eta\|_\infty \leq O(1)\|\eta\|_\infty$ when $h<1$. (4.6.43) follows by Jensen's inequality and Assumption 4.2.3. (4.6.44) follows by (4.2.8) and Lemma 4.6.4, the constant C depends only on the moment bound and the vector field b. We thus have, using the bound (4.6.44) in conjunction with (4.6.41),

$$\Big|\int_{\mathbb{R}^d}\mu^n(y)\mathrm{div}(\eta(y))dy\Big| \leq \|\eta\|_\infty O\Big(\frac{1}{h}\Big)\Big((c_h,\gamma^n)+O(h^2)\Big)^{1/2} \tag{4.6.45}$$

$$+O\Big(\frac{1}{h}\Big)(c_h,\gamma^n)+C\Big(1+\|\eta\|_\infty\Big). \tag{4.6.46}$$

Since μ^n has weak derivative $\nabla\mu^n \in L^1(\mathbb{R}^d)$ we have that

$$\|\nabla\mu^n\|_{L^1(\mathbb{R}^d)} = \sup_{\{\eta\in C_c^\infty(\mathbb{R}^d;\mathbb{R}^d)\,:\,\sup\|\eta\|\leq 1\}}\int_{\mathbb{R}^d}\mu^n(y)\mathrm{div}(\eta(y))dy \tag{4.6.47}$$

$$\leq C\Big(\frac{1}{h}\Big((c_h,\gamma^n)+O(h^2)\Big)^{1/2}+\frac{1}{h}(c_h,\gamma^n)+1\Big), \tag{4.6.48}$$

for some $C>0$. Therefore, by Cauchy-Schwarz inequality, Corollary 4.6.5, and the scaling Assumption 4.2.10, we have

$$\begin{aligned} h\sum_{n=1}^N\|\nabla\mu^n\|_{L^1(\mathbb{R}^d)} \leq& C\sum_{i=1}^N\Big((c_h,\gamma^n)+O(h^2)\Big)^{1/2}+\sum_{n=1}^N(c_h,\gamma^n)+TC \\ \leq& C\sqrt{N}\Big(\sum_{i=1}^N(c_h,\gamma^n)+O(h^2)\Big)^{1/2}+C \leq C\sqrt{Nh}+C\leq C, \end{aligned} \tag{4.6.49}$$

for a constant C independent of k. To finish the proof we provide a sketch of the argument and refer the reader to [CDPS17, Proposition 3.13] for the full details. One can show that $\|(\rho^n)^{m-1}\nabla\rho^n\| \leq C\|\nabla\mu^n\|$, so that $(\rho^n)^m \in W^{1,1}(\mathbb{R}^d)$, with

$$\|\nabla(\rho^n)^m\| \leq C\|\nabla\mu^n\|.$$

Therefore, using (4.6.49)

$$\int_0^T\int_{\mathbb{R}^d}\|\nabla(\rho_k)^m\|dxdt \leq h\sum_{n=1}^N\int_{\mathbb{R}^d}\|\nabla(\rho^n)^m\|dx \leq Ch\sum_{n=1}^N\int_{\mathbb{R}^d}\|\nabla(\mu^n)^m\|dx \leq C. \tag{4.6.50}$$

□

By Lemma 4.6.7 we can use the compactness results in [RS03, Theorem 2]. That is, following identically [CDPS17, Proposition 3.14, Lemma 3.15] we have the following strong convergence (we omit the proof).

Lemma 4.6.8. As $k\to\infty$, up to a suitable subsequence if necessary, we have $\rho_k\to\rho$ in $L^m([0,T],\mathbb{R}^d)$ and $p(\rho_k)\to p(\rho)$ in $L^1([0,T],\mathbb{R}^d)$.

4.6.4 Proof of the main result

We are finally in a position to prove the main result.

Proof of Theorem 4.2.13. Taking the limit, up to a subsequence if necessary, $k \to \infty$ ($h, \epsilon \to 0$, $N \to \infty$) in (4.6.28) and using the convergence of Lemma 4.6.8 we can argue the convergence of Q_k and R_k in (4.6.28) as follows. For Q_k of (4.6.29) we have

$$\lim_{k\to\infty} Q_k = \int_0^T \int_{\mathbb{R}^d} \rho(t,y)\Big(\Big\langle \nabla f(y), D\nabla\varphi(t,y)\Big\rangle - \Big\langle b(y), \nabla\varphi(t,y)\Big\rangle\Big) dydt,$$

since b is continuous (Assumption 4.2.3), and $\|\nabla f\|$ is uniformly bounded, and we have used the scaling (4.2.13), namely, $\epsilon_k/h_k \to 0$.

For R_k of (4.6.30) it is clear that

$$\lim_{k\to\infty} R_k = -\int_0^T \int_{\mathbb{R}^d} p(\rho(t,y))\mathrm{div}\Big(D\nabla\varphi(t,y)\Big) dydt$$

We see that the limit ρ satisfies (4.2.14). $\square$

Appendix

4.A Properties of the internal energy

The following are well established properties of the entropy functional first used in [JKO98, Proposition 4.1], and extended to general internal energies in [CDPS17].

Lemma 4.A.1. [CDPS17, Remark 3.2] There exists a $C > 0$ and $0 < \alpha < 1$ such that if U is defined as in Assumption 4.2.1 then

$$U(\mu) \geq -C(M(\mu)+1)^{\alpha}, \quad \forall \mu \in \mathcal{P}_2^r(\mathbb{R}^d). \tag{4.A.1}$$

In particular

$$H(\mu) \geq -C(M(\mu)+1)^{\alpha}, \quad \forall \mu \in \mathcal{P}_2^r(\mathbb{R}^d). \tag{4.A.2}$$

Note C is chosen large enough so that (4.A.2) and (4.A.1) hold simultaneously.

The next result provides lower semi-continuity for the internal energy under uniformly bounded moments, note it is an extension of the result we have already seen (2.2.2) for the entropy functional.

Lemma 4.A.2. [CDPS17, Corollary A.4] Let u satisfy the Assumption 4.2.1, and U be defined as

$$U(\mu) = \begin{cases} \int_{\mathbb{R}^d} u(\mu(x))dx & \text{if } \mu \in \mathcal{P}^r(\mathbb{R}^d) \\ \infty & \text{otherwise} \end{cases}.$$

Then U is weakly lower semi-continuous under uniformly bounded moments, i.e if $\{\mu_k\}_{k\in\mathbb{N}} \subset \mathcal{P}_2(\mathbb{R}^d)$, $\mu \in \mathcal{P}_2(\mathbb{R}^d)$ with $\mu_k \rightharpoonup \mu$, and there exists $C > 0$ such that $M(\mu_k), M(\mu) < C$ for all $k \in \mathbb{N}$, then

$$U(\mu) \leq \liminf_{k\to\infty} U(\mu_k). \tag{4.A.3}$$

4.B Verification for the examples

4.B.1 Non-linear diffusion equations

Proof of proposition 4.3.1. By Theorem 4.2.13 one only needs to check that Assumptions 4.2.1, 4.2.3, 4.2.5 and 4.2.10 hold. The Assumptions 4.2.1, 4.2.3 and 4.2.10 follow directly from the statement of the proposition and hence their verification is omitted.

We now check Assumption 4.2.5 on the cost function. Clearly (4.2.7) and (4.2.9) and (4.2.10) hold. Let us now verify (4.2.8). Let $\lambda_1, \lambda_2, \ldots$ with $0 < \lambda_1 = h \leq \lambda_2 \leq \ldots$ be the eigenvalues of $D + hI$. Note for all $i = 1, \ldots, d$, $\lambda_i = C_i + h$ for some $C_i \geq 0$. Hence $D + hI$ is invertible, with an inverse $(D + hI)^{-1}$ that is symmetric with eigenvalues $\frac{1}{\lambda_1}, \frac{1}{\lambda_2}, \ldots$. Since it is symmetric it is diagonalizable and therefore its normalised eigenvectors form an orthonormal basis. Let $v_1, \ldots, v_d$ be the normalised eigenvectors of $(D + hI)^{-1}$. For any $x \in \mathbb{R}^d$ we can write $x = \sum_{i=1}^d x_i v_i$, where $x_i := \langle x, v_i \rangle$. Now since $\|x\|^2 = \sum_{i=1}^d x_i^2$, we have

$$\left\langle (D + hI)^{-1}x, x \right\rangle = \sum_{i=1}^d \frac{1}{\lambda_i} x_i^2 \geq \frac{1}{\lambda_d} \|x\|^2 \geq \frac{1}{C+2} \|x\|^2,$$

for $h < 1$ and some $C > 0$, verifying (4.2.8). Lastly (4.2.6) holds by the symmetry of $D + hI$, where we have taken $B_h = hI$ in (4.2.6). To complete the proof it remains only to check the change of variable Assumption 4.2.8. For this take $\mathcal{T}_h(x) = x$, so that (4.2.11) holds trivially since $c_h(x, x + \sigma z) \le \sigma \|(D + hI)^{-1}\| \|z\|^2 = \sigma O(h^{-\beta}) \|z\|^2$ for some $\beta > 0$. Lastly, (4.2.12) holds with this $\mathcal{T}_h$ as f is Lipschitz. □

4.B.2 The non-linear kinetic Fokker-Planck (Kramers) equation

Proof of Proposition 4.3.3. By Theorem 4.2.13 one only needs to check that Assumptions 4.2.1, 4.2.3, 4.2.5, 4.2.8, and 4.2.10 hold. The Assumptions 4.2.1, 4.2.3, and 4.2.10 follow directly from the statement of the proposition and hence their verification is omitted. We now check Assumption 4.2.5 on the cost function. Clearly (4.2.10) holds. The inequality (4.2.9) follows by substituting the estimates [DPZ14, Eq. (46),(47)][3] into c_h, giving $c_h(x, v; x', v') \le O(h^{-3})(\|x\|^2 + \|v\|^2 + \|x'\|^2 + \|v'\|^2)$. The inequality (4.2.7) is verified by the estimates [DPZ14, Eqs. (40a),(40b),(41)] in conjunction with (4.2.9) just obtained. For (4.2.8) see [DPZ14, Eqs. (39b),(39c)]. For (4.2.6) we take inspiration from [DPZ14], defining, for any $h > 0$,

$$B_h := \begin{pmatrix} -\frac{h^2}{6} & \frac{h}{2} \\ -\frac{h}{2} & 0 \end{pmatrix},$$

where, in the matrix B_h, each entry is a $\tilde{d} \times \tilde{d}$-dimensional matrix of that entry multiplied by the identity matrix. Then for

$$\tilde{\eta} = (D + B_h)\eta,$$

set η^1 (resp η^2) as the first $\tilde{d}$ components of η (resp last $\tilde{d}$ components), and similarly for $\tilde{\eta}$. Then the estimate [DPZ14, page 2531]

$$\begin{aligned}
\Big\langle \nabla_{x'} c_h(x, v; x', v'), \tilde{\eta}^1 \Big\rangle &+ \Big\langle \nabla_{v'} c_h(x, v; x', v'), \tilde{\eta}^2 \Big\rangle \\
&= 2\Big(\Big\langle x' - x, \eta^1 \Big\rangle + \Big\langle v' - v, \eta^2 \Big\rangle - h \Big\langle v', \eta^1 \Big\rangle \Big) \\
&\quad + 2\Big\langle h \nabla g(x') + \frac{1}{2} \tau_h(x, v; x', v'), -\frac{h}{2}\eta^1 + \eta^2 \Big\rangle \\
&\quad + 2\Big\langle -h \nabla^2 g(x') v' + \frac{1}{2} \sigma_h(x, v; x', v'), -\frac{h^2}{6}\eta^1 + \frac{h}{2}\eta^2 \Big\rangle,
\end{aligned}$$

where [DPZ14, Eq. (41)] gives bounds on τ_h, σ_h, ensures that (4.2.6) holds.

We now verify Assumption 4.2.8 with the change of variables $\mathcal{T}_h(x, v) = (x + hv, v)$, consider the admissible, in the sense of (4.3.12), cubic

$$\bar{\xi}(t) = x + vt + \Big(\frac{3}{h^2}(x' - x - vh) - \frac{v' - v}{h} \Big) t^2 + \Big(\frac{v' + v}{h^2} - \frac{2}{h^3}(x' - x) \Big) t^3,$$

starting at (x, v) and ending at (x', v'). Using Assumption 4.3.2 we have

$$c_h(x, v; x', v') \le 2Ch \Big(\int_0^h \|\ddot{\bar{\xi}}(t)\|^2 dt + \int_0^h \|\bar{\xi}(t)\|^2 dt \Big).$$

Note that

$$\begin{aligned}
h \int_0^h \|\ddot{\bar{\xi}}(t)\|^2 dt &\le h^2 \sup_{t \in [0,h} \|\ddot{\bar{\xi}}(t)\|^2 \\
&\le C\Big(h^2 \Big\| \frac{3}{h^2}\Big(x' - x - vh\Big) - \frac{v' - v}{h} \Big\|^2 + h^4 \Big\| \frac{v' + v}{h^2} - \frac{2}{h^3}\Big(x' - x\Big) \Big\|^2 \Big),
\end{aligned}$$

and

$$\begin{aligned}
h \int_0^h \|\bar{\xi}(t)\|^2 dt \le & h^2 \sup_{t \in [0,h]} \|\bar{\xi}(t)\|^2 \\
\le & Ch^2 \Big(\|x\|^2 + h^2 \|v\|^2 + h^4 \Big\| \frac{3}{h^2}\Big((x' - x - vh\Big) - \frac{v' - v}{h} \Big\|^2 + h^6 \Big\| \frac{v' + v}{h^2} - \frac{2}{h^3}(x' - x) \Big\|^2 \Big).
\end{aligned}$$

[3]The correct statement of [DPZ14, Eq. (47)] is $\|\ddot{\bar{\xi}}\|_2^2 \le C\big(h^{-3}\|q - q'\|^2 + h^{-1}\|p - p'\|^2 + \|p\|^2 + \|p'\|^2\big)$.

Hence we obtain

$$c_h(x,v;x',v') \leq C\Bigg(h^2\Big\|\frac{3}{h^2}\Big(x'-x-vh\Big)-\frac{v'-v}{h}\Big\|^2+h^4\Big\|\frac{v'+v}{h^2}-\frac{2}{h^3}\Big(x'-x\Big)\Big\|^2$$
$$+h^2\Big(\|x\|^2+h^2\|v\|^2+h^4\Big\|\frac{3}{h^2}\Big(x'-x-vh\Big)-\frac{v'-v}{h}\Big\|^2+h^6\Big\|\frac{v'+v}{h^2}-\frac{2}{h^3}\Big(x'-x\Big)\Big\|^2\Big)\Bigg).$$

So considering $c_h(x,v;\mathcal{T}_h(x,v)-(\sigma z,\sigma w))$, we have

$$c_h(x,v;\mathcal{T}(x,v)-(\sigma z,\sigma w)) \leq C\Bigg(h^2\|\frac{3}{h^2}(-\sigma z)-\frac{\sigma w}{h}\|^2+h^4\|\frac{\sigma w}{h^2}-\frac{2}{h^3}\sigma z\|^2$$
$$+h^2\Big(\|x\|^2+h^2\|v\|^2+h^4\|\frac{3}{h^2}(-\sigma z)-\frac{\sigma w}{h}\|^2+h^6\|\frac{\sigma w}{h^2}-\frac{2}{h^3}\sigma z\|^2\Big)\Bigg),$$

which proves (4.2.11). Lastly the Lipschitz property of f gives (4.2.12), which completes the verification of Assumption 4.2.8. □

Proof of Proposition 4.3.4. By Theorem 4.2.13 one only needs to check that Assumptions 4.2.1, 4.2.3, 4.2.5, 4.2.8, and 4.2.10 hold. The Assumptions 4.2.1, 4.2.3, and 4.2.10 follow directly from the statement of the proposition and hence their verification is omitted.

We now check Assumption 4.2.5 on the cost function. The conditions (4.2.7), (4.2.9), (4.2.10), on c_h are easy to verify. For (4.2.8) see [DPZ14, Eqs. (39b),(39c)]. Lastly for (4.2.6) we again take inspiration from [DPZ14] and define for all $h>0$

$$B_h := \begin{pmatrix} -\frac{h^2}{6} & \frac{h}{2} \\ -\frac{h}{2} & 0 \end{pmatrix},$$

where again, in the matrix B_h, each entry is a $\tilde{d}\times\tilde{d}$-dimensional matrix of that entry multiplied by the identity matrix. One can see from [DPZ14, Eq. (60)] does ensure that (4.2.6) holds.

For Assumption 4.2.8 take $\mathcal{T}_h(x,v)=(x+hv,v)$, we have

$$c_h(x,v;\mathcal{T}_h(x,v)-(\sigma z,\sigma w)) = \|h\nabla g(x)-\sigma z\|^2+12\|\frac{1}{2}\sigma w-\frac{1}{h}\sigma z\|^2 \leq C\Big(h^2\|x\|^2+\|\frac{\sigma}{h}z\|^2+\|\sigma w\|^2\Big),$$

which proves (4.2.11). Lastly the Lipschitz property of f gives (4.2.12), which completes the verification of Assumption 4.2.8. □

4.B.3 A degenerate diffusion equation of Kolmogorov-type

The vector $\mathbf{b}$ and matrix $\mathcal{M}$ which define the cost function (4.3.21) are of the form

$$\mathbf{b}(h,\mathbf{x},\mathbf{y}) = \begin{pmatrix} y_1-x_1-\frac{h}{1}x_2-\ldots-\frac{h^{n-1}}{(n-1)!}x_n \\ \vdots \\ h^{i-1}\Big(y_i-\sum_{j=i}^n\frac{h^{j-i}}{(j-i)!}x_j\Big) \\ \vdots \\ h^{n-1}(y_n-x_n) \end{pmatrix}, \qquad \mathcal{M}=\mathcal{M}_1\mathcal{M}_2^{-1}, \tag{4.B.1}$$

with $\mathcal{M}_1, \mathcal{M}_2 \in \mathbb{R}^{\tilde{d}n\times\tilde{d}n}$ given by

$$(\mathcal{M}_1)_{ki} = \begin{cases} (-1)^{n-k}\frac{(n+i-1)!}{(k+i-n-1)!}, & \text{if} \quad k+i \geq n+1 \\ 0 & \text{if} \quad k+i < n+1, \end{cases}$$

$$\mathcal{M}_2 = \begin{bmatrix} 1 & \dots & 1 \\ \binom{n}{1} & \dots & \binom{2n-1}{1} \\ \vdots & \vdots & \vdots \\ k!\binom{n}{k} & \dots & k!\binom{2n-1}{k} \\ \vdots & \vdots & \vdots \\ (n-1)!\binom{n}{n-1} & \dots & (n-1)!\binom{2n-1}{n-1} \end{bmatrix},$$

where entry of these matrices is to be understood as a $\tilde{d}-$dimensional matrix that is equal to the entry multiplied but the $\tilde{d}-$dimensional identity matrix. The following matrices will also play an important role in the rest of the section

$$\mathcal{J}_1(h) := \mathrm{diag}(1, h, \cdots, h^{n-1}), \qquad \tilde{I} := \mathrm{diag}(0, \dots, 0, 1),$$

$$\mathcal{J}_2(h) := \begin{pmatrix} 1 & h & \frac{h^2}{2!} & \frac{h^3}{3!} & \cdots & \frac{h^{n-1}}{(n-1)!} \\ & h & h^2 & \frac{h^3}{2!} & \cdots & \frac{h^{n-1}}{(n-2)!} \\ & & h^2 & \frac{h^3}{1!} & \cdots & \frac{h^{n-1}}{(n-3)!} \\ & & & \ddots & \cdots & \vdots \\ & & & & & h^{n-1} \end{pmatrix}, \qquad Q := \begin{pmatrix} 0 & & & & \\ 1 & 0 & & & \\ & 1 & 0 & & \\ & & \ddots & \ddots & \\ & & & 1 & 0 \end{pmatrix}.$$

Omitting the h dependence in $\mathcal{J}_1, \mathcal{J}_2$ for the sake of clarity, we also define

$$\begin{aligned} T_1 &:= (2n-1)\mathcal{J}_1^T\mathcal{M}\mathcal{J}_1 - 2h(\mathcal{J}_1')^T\mathcal{M}\mathcal{J}_1 - h^{2-2n}\mathcal{J}_1^T\mathcal{M}\mathcal{J}_2\tilde{I}\mathcal{J}_2^T\mathcal{M}\mathcal{J}_1, \\ T_2 &:= (1-2n)\mathcal{J}_2^T\mathcal{M}\mathcal{J}_1 + h\big((\mathcal{J}_2')^T\mathcal{M}\mathcal{J}_1 + \mathcal{J}_2^T\,\mathcal{M}\,\mathcal{J}_1'\big) - hQ\mathcal{J}_2^T\mathcal{M}\mathcal{J}_1 + \mathcal{J}_2^T\mathcal{M}\mathcal{J}_0\mathcal{M}\mathcal{J}_1, \\ T_3 &:= (2n-1)\mathcal{J}_2^T\mathcal{M}\mathcal{J}_2 - 2h(\mathcal{J}_2')^T\mathcal{M}\mathcal{J}_2 + 2hQ\mathcal{J}_2^T\mathcal{M}\mathcal{J}_2 - h^{2-2n}\mathcal{J}_2^T\mathcal{M}\mathcal{J}_2\tilde{I}\mathcal{J}_2^T\mathcal{M}\mathcal{J}_2. \end{aligned}$$

Note that, again, $\mathcal{J}_1, \mathcal{J}_2, Q, \tilde{I} \in \mathbb{R}^{\tilde{d}n\times\tilde{d}n}$. Each entry of these matrices should be understood as a matrix of order $\tilde{d}$ that equals the entry multiplied with the $\tilde{d}$-dimensional identity matrix.

We now state a series of results from [DT18] which will assist us in proving Proposition 4.3.1.

Lemma 4.B.1 (Proposition 2 of [DT18])**.** The following assertions hold: (1) T_1 is antisymmetric, (2) $T_2 = 0$, (3) T_3 is antisymmetric, and (4) $\mathrm{Trace}(\tilde{I}\mathcal{J}_2^T\mathcal{M}\mathcal{J}_2) = n^2\tilde{d}h^{2(n-1)}$.

Lemma 4.B.2 (Lemma 4.3 of [DT18])**.** $\mathcal{J}_2^{-1}\mathcal{J}_1 = \mathcal{J}$ where

$$\mathcal{J}_{ij} = \begin{cases} 0, & \text{if } j < i \\ (-1)^{j-i}\frac{h^{j-i}}{(j-i)!}, & \text{if } j \geq i. \end{cases} \tag{4.B.2}$$

In particular $\mathcal{J}_{ii} = 1, \quad \mathcal{J}_{ii+1} = -h$ and $\mathcal{J}_{ij} = o(h^2)$ for $j \geq i+2$. Note that $\mathcal{J} \in \mathbb{R}^{\tilde{d}n\times\tilde{d}n}$ where $\mathcal{J}_{ij}$ should be understood as $\mathcal{J}_{ij}I_{\tilde{d}}$.

For any $h > 0$ define

$$\mathcal{K}_h = h^{2n-2}(\mathcal{J}_2^T\mathcal{M}\mathcal{J}_1)^{-1}. \tag{4.B.3}$$

Lemma 4.B.3 (Lemma 4.4 of [DT18])**.** For $\mathcal{K}_h$ defined in (4.B.3) we have

$$(\mathcal{K}_h)_{ij} = (-1)^{n-j}\frac{h^{2n-i-j}}{(2n-i-j+1)!}. \tag{4.B.4}$$

In particular, $(\mathcal{K}_h)_{nn} = 1$ and $(\mathcal{K}_h)_{ij} = o(h)$ for all $(i,j) \neq (n,n)$. Note also that $\mathcal{K}_h \in \mathbb{R}^{\tilde{d}n\times\tilde{d}n}$ where $(\mathcal{K}_h)_{ij}$ should be understood as $(\mathcal{K}_h)_{ij}I_{\tilde{d}}$.

With the use of the preceding lemmas we can prove the convergence of the proposed entropic regularised scheme for the degenerate diffusion of Kolmogorov type, Proposition 4.3.5.

Proof of Proposition 4.3.5. By Theorem 4.2.13 we just need to check Assumptions 4.2.1, 4.2.3, 4.2.5, 4.2.8, and 4.2.10 hold.

The scaling Assumption 4.2.10 and Assumption 4.2.1 on the internal and potential energy clearly hold. Similarly, its clear that Assumption 4.2.3 on b, D is also satisfied.

We now show the cost c_h defined in (4.3.21) satisfies Assumption 4.2.5, with b, D given by (4.3.15) and $D + B_h = \mathcal{K}_h$ defined in (4.B.3). Firstly for (4.2.8) we take the result directly from [DT18, Lemma 2.3]. Moreover, one can see that since $\mathcal{M}$ is constant and by definition of c_h that (4.2.9) holds with $C(h) = h^{2-2n}$. From [DT17, Lemma 2.2] we know that (4.2.10) holds.

Note we can rewrite $\mathbf{b}$ as

$$\mathbf{b}(h, \mathbf{x}, \mathbf{y}) = \begin{pmatrix} y_1 - x_1 - \frac{h}{1} x_2 - \dots - \frac{{}^{n-1}}{(n-1)!} x_n \\ \vdots \\ h^{i-1}\Big(y_i - \sum_{j=i}^n \frac{h^{j-i}}{(j-i)!} x_j\Big) \\ \vdots \\ h^{n-1}(y_n - x_n) \end{pmatrix}$$

$$= \begin{pmatrix} y_1 \\ hy_2 \\ h^2 y_3 \\ \vdots \\ h^{n-1} y_n \end{pmatrix} - \begin{pmatrix} 1 & h & \frac{h^2}{2!} & \frac{h^3}{3!} & \cdots & \frac{h^{n-1}}{(n-1)!} \\ & h & h^2 & \frac{h^3}{2!} & \cdots & \frac{h^{n-1}}{(n-2)!} \\ & & h^2 & \frac{h^3}{1!} & \cdots & \frac{h^{n-1}}{(n-3)!} \\ & & & \ddots & \cdots & \vdots \\ & & & & & h^{n-1} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = J_1 \mathbf{y} - J_2 \mathbf{x}.$$

Therefore, we have

$$\begin{aligned} c_h(\mathbf{x}, \mathbf{y}) &= h^{2-2n} [\mathbf{y}^T J_1^T - \mathbf{x}^T J_2^T]\, \mathcal{M}\, [J_1 \mathbf{y} - J_2 \mathbf{x}] \\ &= h^{2-2n} \Big[\mathbf{y}^T J_1^T\, \mathcal{M}\, J_1 \mathbf{y} - \mathbf{x}^T J_2^T\, \mathcal{M}\, J_1 \mathbf{y} - \mathbf{y}^T J_1^T\, \mathcal{M}\, J_2 \mathbf{x} + \mathbf{x}^T J_2^T \mathcal{M} J_2 \mathbf{x}\Big] \\ &= h^{2-2n} \Big[\mathbf{y}^T J_1^T\, \mathcal{M}\, J_1 \mathbf{y} - 2\mathbf{x}^T J_2^T\, \mathcal{M}\, J_1 \mathbf{y} + \mathbf{x}^T J_2^T \mathcal{M} J_2 \mathbf{x}\Big]. \end{aligned}$$

Therefore,

$$\nabla_{\mathbf{y}} c_h(\mathbf{x}, \mathbf{y}) = 2h^{2-2n} J_1^T \mathcal{M}(J_1 \mathbf{y} - J_2 \mathbf{x}),$$

so that (4.2.7) holds with $C(h) = h^{2-2n}$. Hence we are left to prove (4.2.6). Let $\eta \in \mathbb{R}^{\tilde{d}n}$. We choose $\tilde{\eta} \in \mathbb{R}^{\tilde{d}n}$ such that

$$\begin{pmatrix} \tilde{\eta}_1 \\ \vdots \\ \tilde{\eta}_n \end{pmatrix} = \mathcal{K}_h \begin{pmatrix} \eta_1 \\ \vdots \\ \eta_n \end{pmatrix} = \mathcal{K}_h \eta,$$

where $\mathcal{K}_h$ is given in Lemma 4.B.3, implying that $h^{2-2n} \mathcal{K}_h^T (J_1^T M J_2) = I$.

Using Lemmas 4.B.2 and 4.B.3, we compute

$$\begin{aligned} \Big\langle \nabla_{\mathbf{y}} c_h(\mathbf{x}, \mathbf{y}), \tilde{\eta} \Big\rangle = \Big\langle \nabla_{\mathbf{y}} c_h(\mathbf{x}, \mathbf{y}), \mathcal{K}_h \eta \Big\rangle &= 2\Big[(J_2^{-1} J_1 - I)\mathbf{y} \cdot \eta + (\mathbf{y} - \mathbf{x}) \cdot \eta\Big] \\ &= 2(\mathbf{y} - \mathbf{x}) \cdot \eta - 2h \sum_{i=2}^n y_i \cdot \eta_{i-1} + O(h^2)\|\mathbf{y}\|. \end{aligned}$$

For Assumption 4.2.8, define $\hat{\mathbf{x}}$ as $\hat{\mathbf{x}}_i := \sum_{j=i}^n \frac{t^{j-i}}{(j-i)!} \mathbf{x}_j$ for $i = 1, \dots, n$, and consider the change of variable $\mathcal{T}_h(\mathbf{x}) = \hat{\mathbf{x}}$. Assumption 4.2.8 holds with this change of variable and, indeed, one can easily check that

$$c_h(\mathbf{x}, \mathcal{T}_h(\mathbf{x}) + \sigma \mathbf{z}) \leq C h^{2-2n} \sigma^2 \|\mathbf{z}\|^2, \qquad \text{and} \qquad |f(\mathcal{T}_h(\mathbf{x}) + \sigma \mathbf{z}) - f(\mathbf{x})| \leq C \|\sigma z_n\|.$$

$\square$

Part II

Large Deviations for a Class of Reflected McKean-Vlasov SDE

Chapter 5

Freidlin–Wentzell Large Deviations for a Class of Reflected McKean-Vlasov SDE

This part of the thesis is self contained, the framework, notation, objectives, and mathematical tools, will change significantly from Part I. We no longer focus on the Kolmogorov forward equation, instead we study the underlying stochastic dynamics, and don't assume any gradient flow structure. The material contained here is taken from our publication [ADRR$^+$22].

5.1 Introduction

In this chapter we study $\mathbb{R}^d$-valued *Stochastic Differential Equations* (SDE) whose dynamics are confined to a subset $\mathcal{D} \subset \mathbb{R}^d$, namely, the solution X_t is repelled away from the boundary $\partial\mathcal{D}$ by a reflection mechanism defined in terms of the outward normal and a local time at the boundary. These *reflected SDEs*, enable one to model an impenetrable frontier at which the process is "constrained" and have advanced as a rich field within the applied probability theory. They are used to model physical transport processes [Cos91], molecular dynamics [Sai94], biological systems [DKB12, NBC16] and appear in mathematical finance [HHL16] and stochastic control [Kru00, Ram06]. Lastly, this reflection problem, the so-called *Skorokhod problem* [Sko61, Sko62], has also proven particularly useful in analysing a variety of queuing and communication networks. The literature on the latter is vast, see [WG03, RR03] or [CY01].

In this work, we focus on the general class of *reflected McKean-Vlasov equations*

$$\begin{aligned} X_t^i =& X_0 + \int_0^t b(s, X_s^i, \mu_s)ds + \int_0^t f * \mu_s(X_s^i)ds + \int_0^t \sigma(s, X_s^i, \mu_s)dW_s^i - k_t^i, \\ |k^i|_t =& \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^i)d|k^i|_s, \qquad k_t^i = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^i)\mathbf{n}(X_s^i)d|k^i|_s, \qquad \mu_t(dx) = \mathbb{P}\big[X_t^i \in dx\big], \end{aligned} \tag{5.1.1}$$

where $\mathbf{n}$ is a vector field on the boundary of the domain $\mathcal{D}$ in an outward normal direction, W is a Brownian motion and k is a bounded variation process with variation $|k|$ acting as a local time that constrains the process to the domain $\mathcal{D}$. Thus, the instant the path attains the boundary $\partial\mathcal{D}$ of the domain, k increases creating a contribution that ensures the path remains inside the domain. μ is the law of the solution process X and the coefficients b and f are locally Lipschitz over the domain $\mathcal{D}$. We denote by $f * \mu(\cdot)$ the convolution of a function f with the measure μ.

The law of the above diffusion solves the nonlinear Fokker-Planck equation with a Neumann boundary condition (see also [Wan21]), formally

$$\begin{aligned} &\partial_t\mu_t(x) = \nabla \cdot \Big(\tfrac{1}{2}\nabla^T \cdot (\sigma \cdot \sigma^T)(t, x, \mu_t)\mu_t(x) - b(s, x, \mu_t)\mu_t(x) - f * \mu_t(x)\mu_t(x)\Big) \\ &\Big\langle \mathbf{n}(x), \tfrac{1}{2}\nabla^T \cdot (\sigma \cdot \sigma^T)(t, x, \mu_t)\mu_t(x) - b(t, x, \mu_t)\mu_t(x) - f * \mu_t(x)\mu_t(x)\Big\rangle = 0 \quad \forall x \in \partial\mathcal{D}. \end{aligned} \tag{5.1.2}$$

It is widely known that McKean-Vlasov equations arise as the mean field limit of a system of interacting particles, the so-called *Propagation of Chaos* (PoC): for $N \in \mathbb{N}$ and $i \in \{1, ..., N\}$, the system of equations

$$
\begin{aligned}
X_t^{i,N} =& X_0 + \int_0^t b(s, X_s^{i,N}, \mu_s^N) ds + \int_0^t f * \mu_s^N (X_s^{i,N}) ds + \int_0^t \sigma(s, X_s^{i,N}, \mu_s^N) dW_s^{i,N} - k_t^{i,N}, \\
|k^{i,N}|_t =& \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^{i,N}) d|k^{i,N}|_s, \qquad k_t^{i,N} = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^{i,N}) \mathbf{n}(X_s^{i,N}) d|k^{i,N}|_s, \qquad \mu_t^N = \tfrac{1}{N}\sum_{j=1}^N \delta_{X_t^{j,N}},
\end{aligned}
\tag{5.1.3}
$$

has a dynamics that converges as $N \to \infty$ to that of Equation (5.1.1),

The problem of confining a stochastic process to a domain was first posed by Skorokhod in [Sko61]. The seminal works [Tan79], [LS84] and [Sai87] prove that such solutions exist and are unique in the multi-dimensional case for different classes of domain. [Tan79] works with processes on a convex domain while [Sai87] studies domains that satisfy a “Uniform Exterior Sphere” and “Uniform Interior Cone” condition but imposes more restrictive assumptions on the equation’s coefficients. [Szn84] was the first to prove wellposedness of reflected McKean-Vlasov equations in smooth bounded domains. The above works impose strong restrictions on the coefficients, usually requiring that they are Lipschitz and bounded. We prove the existence and uniqueness for a broader class of McKean-Vlasov reflected SDE in general convex domains, crucially not requiring global Lipschitz continuity, nor bounded coefficients, nor a bounded domain. We allow for superlinear growth components in both space and in the convolution component (the measure component). Very recently, [Wan21] contributes new wellposedness results under singular coefficients and establishes exponential ergodicity under a variety of conditions.

In this work we focus on reflections according to an outward normal of the solution’s path as $X_t \in \partial\mathcal{D}$, but other types of reflections exist. *Oblique reflected SDEs* are reflected SDEs where the vector field $\mathbf{n}$ is not normal but oblique to the boundary. Wellposedness is studied in [LS84, AO76] and in [Cos92, DI08] for non-smooth domains. *Elastic reflections* appears in [Spi07]. A recently introduced form of reflections motivated by financial applications, see [BEH18], is the *reflection in mean* where the reflection happens at the level of the distribution and is generally weaker than the classical pathwise constraint. A typical mean reflection constraint asks for the expected value (of a given function of the solution) to be non-negative, e.g. $\mathbb{E}[h(X_t)] \geq 0$. See [BCdRGL20] for a particle system approximation of mean reflected SDE and its numerics. The particle system approximations are similar to the classical McKean-Vlasov setting. Lastly, a Large Deviation Principle for mean reflected SDE is achieved in [Li18] while the exit-time problem, in the likes of our study in Section 5.5 below, is open.

Large Deviations and Exit-times

The second part of this work focuses in obtaining a *Large Deviations Principle* and the characterisation of the exit-time from a subdomain $\mathfrak{D} \subsetneq \mathcal{D}$ for the small noise limit for the reflected McKean-Vlasov equation

$$
\begin{aligned}
X_t^\varepsilon &= X_0 + \int_0^t b(s, X_s^\epsilon, \mu_s^\varepsilon) ds + \int_0^t f * \mu_s^\varepsilon (X_s^\varepsilon) ds + \sqrt{\varepsilon} \int_0^t \sigma(s, X_s^\varepsilon, \mu_s^\varepsilon) dW_s - k_t^\varepsilon, \\
|k^\varepsilon|_t &= \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^\varepsilon) d|k^\varepsilon|_s, \qquad k_t^\varepsilon = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^\varepsilon) \mathbf{n}(X_s^\varepsilon) d|k^\varepsilon|_s, \qquad \mu_t^\varepsilon(dx) = \mathbb{P}\big[X_t^\varepsilon \in dx\big].
\end{aligned}
\tag{5.1.4}
$$

The asymptotic theory of Large Deviations Principles (LDP) [DZ98] quantifies the rate of convergence for the probability of rare events. First developed by Schilder in [Sch66], an LDP is equivalent to convergence in probability with the addition that the rate of convergence is a specific speed controlled by the rate function. Consider a drift term b that has some basin of attraction and assume the noise in our system is small. Under such conditions, it is common for the system to exhibit a meta-stable behaviour. Loosely speaking, this terminology refers to when a particle is forced towards a basin of attraction and spends long periods of time there before moving to the next basin of attraction. The particle only leaves after receiving a large ‘kick’ from its noise which in the small noise limit, i.e., as the noise vanishes, is an increasingly rare event. This property of the dynamics poses a difficulty for numerical simulations since the numerical scheme takes an impractical amount of time to observe any deviations from the basin. LDPs help by quantifying the probability of this rare event.

A Freidlin–Wentzell LDP provides an estimate for the probability that the sample path of an Itô diffusion will stray far from the mean path when the size of the driving Brownian motion is small with respect to a pathspace norm. Freidlin-Wentzell LDPs for reflected SDEs have been explored in a number of works. For bounded and Lipschitz coefficients, [Dup87] provides the LDP in general convex domains. For smooth domains, [AO76] obtains the LDP under the assumption of bounded and Lipschitz coefficients. Additional references on LDPs for reflected processes can be found in [Pri82].

Close to our work is [LSZZ20] where large and moderate deviations for non-reflected McKean-Vlasov equations with jumps is addressed via the Dupuis-Ellis weak convergence framework [DE97]. Their comprehensive wellposedness results [LSZZ20, Proposition 5.3] are established under a uniformly Lipschitz measure assumption on the coefficients (their assumption A1 and A2) while here we allow for fully super-linear growth in both measure and space components.

LDPs are a suitable language for studying the rare event of exiting from a basin of attraction. For classical reflected SDEs the exit-time from a subdomain $\mathfrak{D} \subsetneq \mathcal{D}$ is a trivial problem as one exits the subdomain $\mathfrak{D}$ before hitting the boundary of $\mathcal{D}$, and hence, the exit-time result for $\mathfrak{D}$ is recovered from standard SDE counterpart. This is a priori *not* the case for reflected McKean-Vlasov equations where the reflection term affects the law and is thus different from the law of the non-reflected McKean-Vlasov.

In the small noise limit the exit-problem for non-reflected SDEs is well documented. A great introduction to the subject can be found in [DZ98, Section 5.7]; for an in-depth study with slowly-varying time-dependent coefficients see [HIPP14, Section 4]; the excellent work [HIP08] characterises the exit-time of a McKean-Vlasov equation after obtaining a large deviation principle; see [Tug16] for a simpler proof relying only on classical Freidlin-Wentzell estimates; and [Tug12], where the same results are obtained by transference from the particle system to the McKean-Vlasov system via propagation of chaos and Freidlin-Wentzell estimates.

Our motivation and contributions

Our *contributions* are threefold: (i) existence and uniqueness results for McKean-Vlasov SDEs constrained to a convex domain $\mathcal{D} \subseteq \mathbb{R}^d$ with coefficients that have superlinear growth in space and are non-Lipschitz in measure; (ii) a large deviations principle for this class of processes; and, (iii) the explicit characterisation of the first exit-time of the solution process from a subdomain $\mathfrak{D} \subsetneq \mathcal{D}$.

For (i), unlike previous works on reflected SDEs, we do not rely on the domain as a way of ensuring the coefficients are bounded or Lipschitz. We work with drift terms that satisfy a one-sided Lipschitz condition over the (possibly unbounded) domain and are locally Lipschitz. Further, we do not restrict ourselves to measure dependencies that are Lipschitz on the domain, but additionally work with a drift term that satisfies a self-stabilizing assumption that ensures any particle is attracted towards the mean of the distribution/particle system. Critically, in a convex domain this will always be away from the boundary.

From a technical point of view, the non-Lipschitz measure component, f in (5.1.1), destroys the standard contraction argument. Nonetheless, we are able to establish an intermediate fixed point argument which decouples f, leaving b to be dealt with. The main workaround result is Lemma 5.3.10 in combination with a specific moment estimate mechanism. The closest result to ours is that of [HIP08]. There, specific structural assumptions are required: drift of specific polynomial form, σ is constant, no-time dependencies, deterministic coefficients and, critically, b and f need to be combined into a mean-field interaction term of order 1. We lift all these constraints.

To the best of our knowledge, the scope of our well-posedness results for McKean-Vlasov equations, and separately for reflected SDEs, are not found in the literature. Thus, our contributions extend known results for McKean-Vlasov equations and reflected SDEs.

For (ii), our study of the LDPs is based on techniques which directly address the presence of the law in the coefficients and avoid the associated particle system. Methodologically, our approach relies on the classical mechanism of exponentially good approximations but employing judiciously chosen auxiliary processes and less standard tricks to obtain the main results. As in [dRST19], it turns out that the correct LDP rate function for McKean-Vlasov equations can be found through certain ODE equations (skeletons) where the McKean-Vlasov's noise and distributions are replaced by smooth functions and the degenerate distribution corresponding to the ODE's solution respectively.

For (iii), the LDP results are the intermediate step necessary to study the exit-time of X^ε from an open subdomain $\mathfrak{D} \subsetneq \mathcal{D}$. Motivated by numerical applications, as in [DGLLPN17, DGLLPN19], we provide the *explicit form of the rate function* for the exit-time distribution (the exit-cost Δ in Theorem 5.5.11).

Intuitively, the solution to (5.1.4) depends on its own law, hence one expects its exit-time from a subdomain to differ from the exit-time of its non-reflected analogue. Similarly, the exit-time of one of the particles in the system (5.1.3) will be altered by the presence of the reflection since this particle will interact with other particles which have already been reflected. However, we will show that, in the small noise limit the exit-time of our McKean-Vlasov reflected SDE is unaltered and we are able to establish a familiar Eyring-Kramer's type law.

The *motivation* of our work stems from numerical considerations around the simulation of McKean-Vlasov equations (reflected or not) where the measure component is non-Lipschitz, in finite and infinite time horizon, and non-constant diffusion coefficients. For instance, reflected McKean-Vlasov equations appear in [LW19] and [AHLW19] as models for bio-chemistry and our framework allows us to study the Granular media equation (see (5.1.2))

$$\partial_t \mu_t(x) = \tfrac{1}{2}\nabla^2 \mu_t(x) + \nabla \cdot \Big(\nabla B(x)\mu_t(x) + \nabla F * \mu_t(x)\mu_t(x) \Big),$$

where B is the constraining potential and F is the interactive potential. This models the velocity distribution in the hydrodynamic limit of a collection of inelastic particles. In the case where the potentials B and F are convex, it is well known that the solution rapidly converges (as $t \to \infty$) towards an invariant distribution [BGG12]. Our work opens a clear pathway to analyse the behaviour of (5.1.1) and (5.1.3) as $t \to \infty$.

An important and fully unanswered question left open by this work relates to effective numerical methods for this class of McKean-Vlasov equationss (even in the non-reflected case). On one hand the penalisation methodology of [Sło13] seem feasible, where the reflection on the bounded domain enforces boundedness of the solution process and the compact support of its law (a trick exploited in [BTWZ17]). On the other hand, explicit step Euler-type discretizations [dRES2101] for super-linear drifts have been shown to work but only for drifts that are Lipschitz in the measure components.

This work is organised as follows. Section 5.2 introduces notation, setting and objects of interest. In Section 5.3 we address the wellposedness of the reflected McKean-Vlasov equations, of the associated reflected interacting particle system and present a Propagation of Chaos result. Sections 5.4 and 5.5 cover the Freidlin-Wentzell Large deviations and exit-time results respectively.

5.2 Preliminaries

We denote by $\mathbb{N} = \{1, 2, \cdots\}$ the set of natural numbers; $\mathbb{Z}$ and $\mathbb{R}$ denote the set of integers and real numbers respectively, with the real positive half-line set as $\mathbb{R}_+ = [0, \infty)$. For $t \in \mathbb{R}$, we denote its floor as $\lfloor t \rfloor$ (the largest integer less than or equal to t). For any $x, y \in \mathbb{R}^d$, $\langle x, y\rangle$ stands for the usual Euclidean inner product and $\|x\| = \langle x, x\rangle^{1/2}$ the usual Euclidean distance. Let A be a $d \times d'$ matrix, we denote the transpose of A by A' and let $\|A\|$ be the Hilbert-Schmidt norm. Define the derivative of a function $f : \mathbb{R} \to \mathbb{R}^d$ as $\dot{f}$.

For sequences $(f_n)_{n\in\mathbb{N}}$ and $(g_n)_{n\in\mathbb{N}}$, we use the symbols $\lesssim, \gtrsim$ in the following way:

$$f_n \lesssim g_n \quad \iff \quad \limsup_{n\to\infty} \frac{f_n}{g_n} \leq C, \text{ for some } C > 0,$$

and

$$f_n \gtrsim g_n \quad \iff \quad \liminf_{n\to\infty} \frac{f_n}{g_n} \geq C, \text{ for some } C > 0.$$

For a set $\mathcal{D} \subset \mathbb{R}^d$, we denote its interior (largest open subset) by $\mathcal{D}^\circ$, its closure (smallest closed cover) by $\overline{\mathcal{D}}$ and the boundary by $\partial\mathcal{D} = \overline{\mathcal{D}} \backslash \mathcal{D}^\circ$. For $x \in \mathbb{R}^d$,$r \geq 0$, denote $B_r(x) \subset \mathbb{R}^d$ as the open ball of radius r centred at x.

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a differentiable function. Then we denote by ∇f the gradient operator and $\nabla^2 f$ to be the Hessian operator. Let $C([0, T]; \mathbb{R}^d)$ be the space of continuous function $f : [0, T] \to \mathbb{R}^d$ endowed with the supremum norm $\| \cdot \|_{\infty,[0,T]}$. For $x \in \mathbb{R}^d$ let $C_x([0, T]; \mathbb{R}^d)$ be the subspace of $C([0, T]; \mathbb{R}^d)$ of functions $f : [0, T] \to \mathbb{R}^d$ with $f(0) = x$.

Let $\tilde{\Omega} = C_0([0,T];\mathbb{R}^{d'})$ be the canonical d'-dimensional Wiener space and let W be the Wiener process with law $\tilde{\mathbb{P}}$. Let $(\tilde{\mathcal{F}}_t)_{t\in[0,T]}$ be the standard augmentation of the filtration generated by the Brownian motion. Then we have the probability space $(\tilde{\Omega}, \tilde{\mathcal{F}}, (\tilde{\mathcal{F}}_t)_{t\in[0,T]}, \tilde{\mathbb{P}})$. Additionally, let $([0,1], \mathcal{B}([0,1]), \overline{\mathbb{P}})$ be a probability space with the Lebesgue measure $\overline{\mathbb{P}}$. Our probability space is structured as follows:

1. The sample space will be $\Omega = [0,1] \times \tilde{\Omega}$,
2. The σ-algebra over this space will be $\mathcal{F} = \sigma(\mathcal{B}([0,1]) \times \tilde{\mathcal{F}})$ with filtration $\mathcal{F}_t = \sigma(\mathcal{B}([0,1]) \times \tilde{\mathcal{F}}_t)$,
3. The probability measure will be the product measure $\mathbb{P} = \overline{\mathbb{P}} \times \tilde{\mathbb{P}}$.

For $p \geq 1$, let $L^p(\Omega, \mathcal{F}, \mathbb{P}; \mathcal{D})$ be the space of random variables over the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with state space $\mathcal{D}$ and finite p moments. For $p \geq 1$, let $\mathcal{S}^p([0,T];\mathbb{R}^d)$ be the space of $(\tilde{\mathcal{F}}_t)_{t\in[0,T]}$-adapted processes $X : \Omega \times [0,T] \to \mathcal{D}$ satisfying $\mathbb{E}[\|X\|_{\infty,[0,T]}^p]^{1/p} < \infty$ where $\|X\|_{\infty,[0,T]} := \sup_{s\in[0,T]} \|X_s\|$.

Let $\mathcal{H}_1^0$ be the Cameron Martin Hilbert space for Brownian motion: the space of all absolutely continuous paths on the interval $[0,T]$ which start at 0 and have a derivative almost everywhere which is $L^2([0,T];\mathbb{R}^{d'})$ integrable

$$\mathcal{H}_1^0 := \big\{h : [0,T] \to \mathbb{R}^{d'},\ h(0) = 0,\ h(\cdot) = \int_0^{\cdot} \dot{h}(s)ds,\ \dot{h} \in L^2([0,T];\mathbb{R}^{d'})\big\}.$$

Let $\mathcal{D}$ (possibly unbounded) be a subset of $\mathbb{R}^d$ and $\mathcal{B}_{\mathcal{D}}$ be the Borel σ-algebra over $\mathcal{D}$. Let $\mathcal{P}_r(\mathcal{D})$ be the set of all Borel probability measures which have finite r^{th} moment.

Definition 5.2.1. Let $r \geq 1$. Let $(\mathcal{D}, d)$ be a metric space with Borel σ-algebra $\mathcal{B}_{\mathcal{D}}$. Let $\mu, \nu \in \mathcal{P}_r(\mathcal{D})$. We define the Wasserstein r-distance $\mathbb{W}_{\mathcal{D}}^{(r)} : \mathcal{P}_r(\mathcal{D}) \times \mathcal{P}_r(\mathcal{D}) \to \mathbb{R}_+$ to be

$$\mathbb{W}_{\mathcal{D}}^{(r)}(\mu,\nu) = \Big(\inf_{\pi\in\Pi_r(\mu,\nu)} \int_{\mathcal{D}\times\mathcal{D}} d(x,y)^r \pi(dx,dy)\Big)^{\frac{1}{r}},$$

where $\Pi_r(\mu,\nu) \subset \mathcal{P}_r(\mathcal{D}\times\mathcal{D})$ is the space of joint distributions over $\mathcal{D}\times\mathcal{D}$ with marginals μ and ν.

Domain, outward normal vectors and properties

The processes that we consider in this chapter are confined to a domain $\mathcal{D}$.

Definition 5.2.2. Let $\mathcal{D}$ be a subset of $\mathbb{R}^d$ that has non-zero Lebesgue measure interior. For $x \in \partial\mathcal{D}$, define

$$\mathcal{N}_{x,r} := \{\mathbf{n} \in \mathbb{R}^d : \|\mathbf{n}\| = 1, B_r(x + r\mathbf{n}) \cap \mathcal{D}^\circ = \emptyset\} \quad \text{and} \quad \mathcal{N}_x := \cup_{r>0}\mathcal{N}_{x,r}.$$

We call the set $\mathcal{N}_x$ the outward normal vectors.

For general domains, the set $\mathcal{N}_x$ can be empty, for example if the boundary contains a concave corner. Furthermore if the boundary is not smooth at x then it may be the case that $|\mathcal{N}_{x,r}| = \infty$.

Definition 5.2.3. Let $\mathcal{D} \subset \mathbb{R}^d$ with non-zero Lebesgue measure interior. We say that $\mathcal{D}$ has a *Uniform Exterior Sphere* if $\exists r_0 > 0$ such that $\forall x \in \partial\mathcal{D}$, $\mathcal{N}_{x,r_0} \neq \emptyset$.

The existence of a uniform exterior sphere ensures there is at least one outward normal vector at every point on the boundary. When this is not the case, there is no canonical choice for the reflective vector field. The following property of convex domains will be used extensively.

Lemma 5.2.4. Let $\mathcal{D} \subset \mathbb{R}^d$ be a convex domain with interior that has non-zero Lebesgue measure. Then $\mathcal{D}$ has a Uniform Exterior Sphere, and for any $x \in \partial\mathcal{D}$ and $\mathbf{n}(x) \in \mathcal{N}_x$ it holds that

$$\langle \mathbf{n}(x), y - x\rangle \leq 0,\ \forall y \in \mathcal{D}. \tag{5.2.1}$$

Proof. First we prove that $\mathcal{D}$ has a Uniform Exterior Sphere. Let $r > 0$ be fixed and let $x \in \partial\mathcal{D}$. If $\mathcal{D}$ is a convex subspace of $\mathbb{R}^d$, then there exists a semi-plane $(\mathcal{S})$ which contains $\mathcal{D}$. Thus we have a hyperplane $\mathcal{H}_x$ that contains x and $\mathcal{D}^\circ \cap \mathcal{H}_x = \emptyset$. Then, $\exists \mathbf{n}$ such that $\forall y \in \mathcal{H}_x$ we have $\langle y, \mathbf{n}\rangle = 0$. Without loss of generality, $\mathbf{n}$ can be chosen to be an exiting vector from $\mathcal{D}$. Consider the open ball $B_r(x + r\mathbf{n})$. This is an open set contained in the complement of the closed semi-plane $(\mathcal{S}^c)$. Thus $B_r(x + r\mathbf{n}) \cap \mathcal{D}^\circ = \emptyset$. Hence $\mathcal{N}_{x,r} \neq \emptyset$. Now we show (5.2.1), For $x \in \partial\mathcal{D}$, we have just shown that a vector $\mathbf{n}(x) \in \mathcal{N}_x$ exists. Further, $\exists r > 0$ such that $\mathbf{n} \in \mathcal{N}_{x,r}$ and denote $z = x + r\mathbf{n}(x)$. Then

$$\inf_{y\in\mathcal{D}} \|z - y\| = \|z - x\|.$$

If this is not the case the ball of radius r centred at y would intersect with the $\mathcal{D}^\circ$ and hence

$$\|(x - z) + (y - x)\| \geq \|z - x\| \quad \Rightarrow \quad \langle x - z, y - x\rangle \geq 0,$$

rearranging this yields that (5.2.1). ☐

Motivated by this lemma, we will make the following assumption throughout this chapter.

Assumption 5.2.5. Let $\mathcal{D} \subset \mathbb{R}^d$ be a closed, convex set with non-zero Lebesgue measure interior.

For example, if $d = 2$ a possible choice is $\mathcal{D} = [0,\infty)^2$ or $\mathcal{D} = [0, a] \times (-\infty, \infty)$ for some $a > 0$, stressing the fact that we allow for unbounded domains with non-smooth boundaries.

At this point it is worth mentioning that if the domain is non-convex, it may not satisfy such helpful conditions. For example both [Sai87] and [LS84] assume the uniform exterior sphere condition and cannot access Lemma 5.2.4, whereas [Tan79] relies on Lemma 5.2.4.

Reflective boundaries and the Skorokhod problem

We are now in the position to formulate the Skorokhod problem which was first stated and studied in [Sko61, Sko62].

A path $\gamma : [0, T] \to \mathbb{R}^d$ is said to be càdlàg if it is right continuous and has left limits.

Definition 5.2.6. Let $\gamma : [0, T] \to \mathbb{R}^d$ be a càdlàg path and let $\mathcal{D}$ be a subset of $\mathbb{R}^d$. Suppose additionally that $\gamma_0 \in \mathcal{D}$. For each $x \in \partial\mathcal{D}$, suppose that $\mathcal{N}_x \neq \emptyset$. Let $\mathbf{n} : \partial\mathcal{D} \to \mathbb{R}^d$ such that $\mathbf{n}(x) \in \mathcal{N}_x$. The triple $(\gamma, \mathcal{D}, \mathbf{n})$ denotes the *Skorokhod problem.*

We say that the pair (η, k) is a solution to the Skorokhod problem $(\gamma, \mathcal{D}, \mathbf{n})$ if $\eta : [0, T] \to \overline{\mathcal{D}}$ is a càdlàg path, $k : [0, T] \to \mathbb{R}^d$ is a bounded variation path and

$$\eta_t = \gamma_t - k_t, \quad k_t = \int_0^t \mathbf{n}(\eta_s)\mathbb{1}_{\partial\mathcal{D}}(\eta_s)d|k|_s, \quad |k|_t = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(\eta_s)d|k|_s, \tag{5.2.2}$$

where $\mathbf{n}(x) \in \mathcal{N}_x$ when $x \in \partial\mathcal{D}$ and $\mathbf{n}(x) = 0$ otherwise.

This problem was first studied in the deterministic setting in [CMEKM80] and in the stochastic setting in [Tan79]. For general domains, one may be unable to show uniqueness, or even existence of a solution to the Skorokhod problem. We emphasise that this will not be an issue that we explore. Note the following result of [Tan79, Theorem 3.1].

Theorem 5.2.7. Let $\mathcal{D}$ satisfy Assumption 5.2.5. Let $(\Omega, \mathcal{F}, (\mathcal{F}_t)_{t\in[0,T]}, \mathbb{P})$ be a filtered probability space. Let $\gamma = (\gamma_t)_{t\in[0,T]}$ be an $\mathcal{F}_t$-adapted $\mathbb{R}^d$-valued semimartingale with $\gamma_0 \in \mathcal{D}$.

Then there exists a unique solution to the Skorokhod problem $(\gamma, \mathcal{D}, \mathbf{n})$ $\mathbb{P}$-a.s.

5.3 Existence, uniqueness and propagation of chaos

In this section, we prove that under appropriate assumptions there exists a unique solution to the Stochastic Differential Equations (5.1.1) In the subsequent step, we address the *Propagation of Chaos* result regarding convergence of the solution of the particle system (5.1.3) to the solution of the McKean-Vlasov (5.1.1). The phrase "*Propagation of Chaos*" refers to the process in which a system of interacting particles decouples as the number of particles tends to infinity. In this limit, any one particle can then be described by the same governing equation.

In Section 5.3.1 we prove *existence and uniqueness for a broad class of classical reflected SDEs* where the coefficients are assumed random, time-dependent and satisfying a superlinear growth condition. Crucially, we do not restrict ourselves to a bounded domain. In Section 5.3.2 we prove *existence and uniqueness for reflected McKean-Vlasov SDEs* satisfying a $\mathbb{W}^{(2)}$-Lipschitz condition in the measure component. This is *generalised in Theorem 5.3.5 to coefficients that are locally Lipschitz in measure*, although in this final step we necessarily restrict to deterministic coefficients; the proof of the result is provided in Section 5.3.3.

Lastly, in Section 5.3.4, we prove that the limit of a single equation within the system of interacting equations (5.1.3) converges to the dynamics of Equation (5.1.1), i.e. *Propagation of Chaos (PoC)*.

5.3.1 Existence and uniqueness for reflected SDEs

Let $t \geq 0$. We commence by studying classical reflected SDEs of the form

$$\begin{aligned} X_t =&\theta + \int_0^t b(s, X_s) ds + \int_0^t \sigma(s, X_s) dW_s - k_t, \\ |k|_t =& \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s) d|k|_s, \qquad k_t = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s)\mathbf{n}(X_s) d|k|_s. \end{aligned} \tag{5.3.1}$$

This first result is a generalisation of Tanaka's classical results in [Tan79] extended to the case where the drift and diffusion terms are random and time dependent, and the drift term satisfies a one-sided Lipschitz condition.

Theorem 5.3.1. Let $\mathcal{D}$ satisfy Assumption 5.2.5. Let $p \geq 2$. Let W be a d' dimensional Brownian motion. Let $\theta : \Omega \to \mathcal{D}$, $b : [0, T] \times \Omega \times \mathcal{D} \to \mathbb{R}^d$ and $\sigma : [0, T] \times \Omega \times \mathcal{D} \to \mathbb{R}^{d \times d'}$ be progressively measurable maps. Suppose that

- $\theta \in L^p(\mathcal{F}_0, \mathbb{P}; \mathcal{D})$.
- $\exists x_0 \in \mathcal{D}$ such that b and σ satisfy the integrability conditions
$$\mathbb{E}\Big[\Big(\int_0^T \|b(s, x_0)\| ds\Big)^p\Big] \vee \mathbb{E}\Big[\Big(\int_0^T \|\sigma(s, x_0)\|^2 ds\Big)^{p/2}\Big] < \infty.$$
- $\exists L > 0$ such that for almost all $(s, \omega) \in [0, T] \times \Omega$ and $\forall x, y \in \mathcal{D}$,
$$\big\langle b(s, x) - b(s, y), x - y\big\rangle \leq L\|x - y\|^2 \quad \text{and} \quad \|\sigma(s, x) - \sigma(s, y)\| \leq L\|x - y\|,$$
- $\forall n \in \mathbb{N}$, $\exists L_n >$ such that $\forall x, y \in \mathcal{D}_n = \mathcal{D} \cap \overline{B_n(x_0)}$,
$$\|b(s, x) - b(s, y)\| \leq L_n\|x - y\| \quad \text{for almost all } (s, \omega) \in [0, T] \times \Omega.$$

Then there exists a unique solution to the reflected Stochastic Differential Equation (5.3.1) in $\mathcal{S}^p([0, T])$ and

$$\mathbb{E}\Big[\|X - x_0\|_{\infty,[0,T]}^p\Big] \lesssim \mathbb{E}\Big[\|\theta - x_0\|^p\Big] + \mathbb{E}\Big[\Big(\int_0^T \|b(s, x_0)\| ds\Big)^p\Big] + \mathbb{E}\Big[\Big(\int_0^T \|\sigma(s, x_0)\|^2 ds\Big)^{p/2}\Big].$$

The proof is given in Appendix 5.B.

5.3.2 Existence and uniqueness for McKean-Vlasov equations

Next, for $t \geq 0$, we study reflected McKean-Vlasov equations, i.e. stochastic processes of the form

$$\begin{aligned} X_t =&\theta + \int_0^t b(s, X_s, \mu_s) ds + \int_0^t \sigma(s, X_s, \mu_s) dW_s - k_t, \quad \mathbb{P}\big[X_t \in dx\big] = \mu_t(dx), \\ |k|_t =& \int_0^t \mathbb{1}_{\partial D}(X_s) d|k|_s, \qquad k_t = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s)\mathbf{n}(X_s) d|k|_s. \end{aligned} \tag{5.3.2}$$

Theorem 5.3.2. Let $\mathcal{D}$ satisfy Assumption 5.2.5. Let $p \geq 2$. Let W be a d' dimensional Brownian motion. Let $\theta : \Omega \to \mathcal{D}$, $b : [0,T] \times \Omega \times \mathcal{D} \times \mathcal{P}_2(\mathcal{D}) \to \mathbb{R}^d$ and $\sigma : [0,T] \times \Omega \times \mathcal{D} \times \mathcal{P}_2(\mathcal{D}) \to \mathbb{R}^{d \times d'}$ be progressively measurable maps. Assume that

- $\theta \in L^p(\mathcal{F}_0, \mathbb{P}; \mathcal{D})$ and $\theta \sim \mu_\theta$.
- $\exists x_0 \in \mathcal{D}$ such that b and σ satisfy the integrability conditions

$$\mathbb{E}\Big[\Big(\int_0^T \|b(s,x_0,\delta_{x_0})\| ds\Big)^p\Big] \vee \mathbb{E}\Big[\Big(\int_0^T \|\sigma(s,x_0,\delta_{x_0})\|^2 ds\Big)^{p/2}\Big] < \infty.$$

- $\exists L > 0$ such that for almost all $(s,\omega) \in [0,T] \times \Omega$, $\forall \mu, \nu \in \mathcal{P}_2(\mathcal{D})$ and $\forall x, y \in \mathbb{R}^d$,

$$\Big\langle b(s,x,\mu) - b(s,y,\mu), x-y \Big\rangle \leq L\|x-y\|^2, \quad \|\sigma(s,x,\mu) - \sigma(s,y,\mu)\| \leq L\|x-y\|,$$
$$\|b(s,x,\mu) - b(s,x,\nu)\| \leq L\mathbb{W}^{(2)}_{\mathcal{D}}(\mu,\nu), \quad \|\sigma(s,x,\mu) - \sigma(s,x,\nu)\| \leq L\mathbb{W}^{(2)}_{\mathcal{D}}(\mu,\nu).$$

- $\forall n \in \mathbb{N}$, $\exists L_n >$ such that $\forall x, y \in \mathcal{D} \cap \overline{B_n(x_0)}$,

$$\|b(s,x,\mu) - b(s,y,\mu)\| \leq L_n\|x-y\| \quad \text{for almost all } (s,\omega) \in [0,T] \times \Omega.$$

Then there exists a unique solution to the reflected McKean-Vlasov equation (5.3.2) in $\mathcal{S}^p([0,T])$ and

$$\mathbb{E}\Big[\|X - x_0\|^p_{\infty,[0,T]}\Big] \lesssim \mathbb{E}\Big[\|\theta - x_0\|^p\Big] + \mathbb{E}\Big[\Big(\int_0^T \|b(s,x_0,\delta_{x_0})\| ds\Big)^p\Big] + \mathbb{E}\Big[\Big(\int_0^T \|\sigma(s,x_0,\delta_{x_0})\|^2 ds\Big)^{p/2}\Big].$$

Proof. Throughout this proof, we distinguish between measures $\nu \in \mathcal{P}_2\big(C([0,T];\mathcal{D})\big)$ and their pushforward measure with respect to path evaluation $\nu_t \in \mathcal{P}_2(\mathcal{D})$.

Then for $\nu^1, \nu^2 \in \mathcal{P}_2\big(C([0,T];\mathcal{D})\big)$, we have

$$\sup_{t \in [0,T]} \mathbb{W}^{(2)}_{\mathcal{D}}\Big(\nu^1_t, \nu^2_t\Big) \leq \mathbb{W}^{(2)}_{C([0,T];\mathcal{D})}\Big(\nu^1, \nu^2\Big). \tag{5.3.3}$$

For $\nu \in \mathcal{P}_2(C([0,T];\mathcal{D}))$, we define the reflected Stochastic Differential Equation

$$\begin{aligned} X^{(\nu)}_t =& \theta + \int_0^t b(s, X^{(\nu)}_s, \nu_s) ds + \int_0^t \sigma(s, X^{(\nu)}_s, \nu_s) dW_s - k^{(\nu)}_t, \\ |k^{(\nu)}|_t =& \int_0^t \mathbb{1}_{\partial D}(X^{(\nu)}_s) d|k^{(\nu)}|_s, \quad k^{(\nu)}_t = \int_0^t \mathbb{1}_{\partial \mathcal{D}}(X^{(\nu)}_s) \mathbf{n}(X^{(\nu)}_s) d|k^{(\nu)}|_s. \end{aligned} \tag{5.3.4}$$

Let $x_0 \in \mathcal{D}$. For $\mu_0 \in \mathcal{P}_2(\mathcal{D})$, let $\mu_0' \in \mathcal{P}_2\big(C([0,T];\mathcal{D})\big)$ be the law of the constant path with initial distribution μ_0. Using the Lipschitz condition for the measure dependency of b and σ, we have

$$\begin{aligned} \mathbb{E}\Big[\Big(\int_0^T \|b(s,x_0,\nu_s)\| ds\Big)^p\Big] \leq& \mathbb{E}\Big[\Big(\int_0^T \|b(s,x_0,\mu_0)\| ds + L\int_0^T \mathbb{W}^{(2)}_{\mathcal{D}}(\nu_s,\mu_0) ds\Big)^p\Big] \\ \leq& 2^{p-1}\mathbb{E}\Big[\Big(\int_0^T \|b(s,x_0,\mu_0)\| ds\Big)^p\Big] + 2^{p-1}L^pT^p\mathbb{W}^{(2)}_{C([0,T];\mathcal{D})}(\nu,\mu_0')^p, \\ \mathbb{E}\Big[\Big(\int_0^T \|\sigma(s,x_0,\nu_s)\|^2 ds\Big)^{p/2}\Big] \leq& \mathbb{E}\Big[\Big(2\int_0^T \|\sigma(s,x_0,\mu_0)\|^2 ds + 2L^2\int_0^T \mathbb{W}^{(2)}_{\mathcal{D}}(\nu_s,\mu_0) ds\Big)^{p/2}\Big] \\ \leq& 2^{p-1}\mathbb{E}\Big[\Big(\int_0^T \|\sigma(s,x_0,\mu_0)\|^2 ds\Big)^{p/2}\Big] + 2^{p-1}L^pT^{p/2}\mathbb{W}^{(2)}_{C([0,T];\mathcal{D})}(\nu,\mu_0')^p. \end{aligned}$$

Therefore, by Theorem 5.3.1, we have existence and uniqueness of Equation (5.3.4). Consider the operator $\Xi : \mathcal{P}_2\big(C([0,T];\mathbb{R}^d)\big) \to \mathcal{P}_2\big(C([0,T];\mathbb{R}^d)\big)$ defined by

$$\Xi[\nu] := \mu^{(\nu)},$$

where $\mu^{(\nu)}$ is the law of the solution to Equation (5.3.4). Now, for any two measures $\nu^1, \nu^2 \in \mathcal{P}_2\big(C([0,T];\mathcal{D})\big)$,

$$\begin{aligned}\Big\|X_t^{(\nu^1)} - X_t^{(\nu^2)}\Big\|^2 \leq& 2\int_0^t \Big\langle X_s^{(\nu^1)} - X_s^{(\nu^2)}, b(s, X_s^{(\nu^1)}, \nu_s^1) - b(s, X_s^{(\nu^2)}, \nu_s^2)\Big\rangle ds\\ &+ 2\int_0^t \Big\langle X_s^{(\nu^1)} - X_s^{(\nu^1)}, \Big(\sigma(s, X_s^{(\nu^1)}, \nu_s^1) - \sigma(s, X_s^{(\nu^2)}, \nu_s^2)\Big) dW_s\Big\rangle\\ &+ \int_0^t \Big\|\sigma(s, X_s^{(\nu^1)}, \nu_s^1) - \sigma(s, X_s^{(\nu^2)}, \nu_s^2)\Big\|^2 ds - 2\int_0^t \Big\langle X_s^{(\nu^1)} - X_s^{(\nu^2)}, dk_s^{(\nu^1)} - dk_s^{(\nu^2)}\Big\rangle.\end{aligned}$$

The reflective term in the above expression is negative due to the convexity of the domain and Lemma 5.2.4. Therefore, taking a supremum over time, expectations, and using Burkholder-Davis-Gundy inequality, we get

$$\begin{aligned}&\mathbb{E}\Big[\|X^{(\nu^1)} - X^{(\nu^2)}\|_{\infty,[0,T]}^2\Big]\\ &\leq 2L\int_0^T \mathbb{E}\Big[\|X^{(\nu^1)} - X^{(\nu^2)}\|_{\infty,[0,t]}^2\Big]dt + 2L\mathbb{E}\Big[\|X^{(\nu^1)} - X^{(\nu^2)}\|_{\infty,[0,T]} \cdot \int_0^T \sup_{s\in[0,t]} \mathbb{W}_{\mathcal{D}}^{(2)}(\nu_s^1, \nu_s^2)dt\Big]\\ &\quad + 4C_1L\mathbb{E}\Big[\|X^{(\nu^1)} - X^{(\nu^2)}\|_{\infty,[0,T]}\Big(\int_0^T \sup_{s\in[0,t]} \mathbb{W}_{\mathcal{D}}^{(2)}(\nu_s^1, \nu_s^2)^2 dt\Big)^{1/2}\Big]\\ &\quad + 4C_1L\mathbb{E}\Big[\|X^{(\nu^1)} - X^{(\nu^2)}\|_{\infty,[0,T]}\Big(\int_0^T \|X^{(\nu^1)} - X^{(\nu^2)}\|_{\infty,[0,t]}^2 dt\Big)^{1/2}\Big]\\ &\quad + 2L^2\int_0^T \mathbb{E}\Big[\|X^{(\nu^1)} - X^{(\nu^2)}\|_{\infty,[0,t]}^2 dt + 2L^2\int_0^T \sup_{s\in[0,t]} \mathbb{W}_{\mathcal{D}}^{(2)}(\nu_s^1, \nu_s^2)^2 dt.\end{aligned}$$

Careful application of Young's Inequality, Grönwall's inequality and Equation (5.3.3) yields that there exists a constant $K > 0$ such that

$$\mathbb{W}_{C([0,T];\mathcal{D})}^{(2)}\Big(\Xi[\nu^1], \Xi[\nu^2]\Big)^2 \leq \mathbb{E}\Big[\|X^{(\nu^1)} - X^{(\nu^1)}\|_{\infty,[0,T]}^2\Big] \leq K\int_0^T \mathbb{W}_{C([0,t];\mathcal{D})}^{(2)}\Big(\nu^1, \nu^2\Big)^2 dt.$$

Iteratively applying the operator Ξ n times gives

$$\begin{aligned}\mathbb{W}_{C([0,T];\mathcal{D})}^{(2)}\Big(\Xi^n[\nu^1], \Xi^n[\nu^2]\Big)^2 \leq& K^n\int_0^T\int_0^{t_1}...\int_0^{t_{n-1}} \mathbb{W}_{C([0,t_n];\mathcal{D})}^{(2)}\Big(\nu^1, \nu^2\Big)^2 dt_n...dt_2dt_1\\ \leq& \frac{K^n}{n!}\mathbb{W}_{C([0,T];\mathcal{D})}^{(2)}\Big(\nu^1, \nu^2\Big)^2.\end{aligned}$$

Choosing $n \in \mathbb{N}$ such that $\frac{K^n}{n!} < 1$, we obtain that the operator Ξ^n is a contraction operator, so a unique fixed point on the metric space $\mathcal{P}_2\big(C([0,T];\mathcal{D})\big)$ paired with the Wasserstein metric must exist.

This unique fixed point is the law of the McKean-Vlasov equation (5.3.2). □

Remark 5.3.3. It is worth remarking that the framework of coefficients that satisfy a Lipschitz condition in their measure dependency with respect to the Wasserstein distance is broad, but in this manuscript we are predominantly interested in coefficients where the measure dependency is not Lipschitz.

Main result: existence and uniqueness for McKean-Vlasov equations under reflection

We next study McKean-Vlasov equations with the addition of a self-stabilizing drift term that does not satisfy a Lipschitz condition with respect to the Wasserstein distance. For example, in Equation (5.1.1), we have $f * \mu_t(x) := \int_{\mathcal{D}} f(x-y)\mu_t(dy)$, the convolution of the vector field f with the measure μ_t. Consider

$$\begin{aligned}X_t =& \theta + \int_0^t b(s, X_s, \mu_s)ds + \int_0^t \sigma(s, X_s, \mu_s)dW_s + \int_0^t f * \mu_s(X_s)ds - k_t,\\ |k|_t =& \int_0^t \mathbb{1}_{\partial D}(X_s)d|k|_s, \qquad k_t = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s)\mathbf{n}(X_s)d|k|_s, \qquad \mathbb{P}\Big[X_t \in dx\Big] = \mu_t(dx).\end{aligned} \tag{5.3.5}$$

We show existence of a solution to the above reflected McKean-Vlasov equation under the following assumption.

Assumption 5.3.4. Let $r > 1$ and $p > 2r$. Let $\theta : \Omega \to \mathcal{D}$, $b : [0,T] \times \mathcal{D} \times \mathcal{P}_2(\mathcal{D}) \to \mathbb{R}^d$, $f : \mathbb{R}^d \to \mathbb{R}^d$ and $\sigma : [0,T] \times \mathcal{D} \times \mathcal{P}_2(\mathcal{D}) \to \mathbb{R}^{d\times d'}$. Assume that

- $\theta \in L^p(\mathcal{F}_0, \mathbb{P}; \mathcal{D})$ and $\theta \sim \mu_\theta$,
- $\exists x_0 \in \mathcal{D}$ such that b and σ satisfy the integrability conditions

$$\int_0^T \|b(s, x_0, \delta_{x_0})\| ds \vee \int_0^T \|\sigma(s, x_0, \delta_{x_0})\|^2 ds < \infty.$$

- $\exists L > 0$ such that for almost all $s \in [0,T]$, $\forall \mu, \nu \in \mathcal{P}_2(\mathcal{D})$ and $\forall x, y \in \mathcal{D}$,

$$\Big\langle b(s,x,\mu) - b(s,y,\mu), x-y \Big\rangle \le L\|x-y\|^2, \quad \|\sigma(s,x,\mu) - \sigma(s,y,\mu)\| \le L\|x-y\|,$$
$$\|b(s,x,\mu) - b(s,x,\nu)\| \le L\mathbb{W}^{(2)}_{\mathcal{D}}(\mu,\nu), \quad \|\sigma(s,x,\mu) - \sigma(s,x,\nu)\| \le L\mathbb{W}^{(2)}_{\mathcal{D}}(\mu,\nu),$$

- $f(0) = 0$, $f(x) = -f(-x)$ and $\exists L > 0$ such that $\forall x, y \in \mathbb{R}^d$, $\big\langle f(x) - f(y), x-y \big\rangle \le L\|x-y\|^2$,
- $\forall n \in \mathbb{N}$, $\exists L_n >$ such that $\forall x, y \in \mathcal{D} \cap \overline{B_n(x_0)}$,

$$\|b(s,x,\mu) - b(s,y,\mu)\| \le L_n\|x-y\| \quad \text{for almost all } (s,\omega) \in [0,T] \times \Omega,$$

- $\exists L > 0$ such that $\forall x, y \in \mathbb{R}^d$

$$\|f(x) - f(y)\| \le C\|x-y\|\big(1 + \|x\|^{r-1} + \|y\|^{r-1}\big), \quad \|f(x)\| \le C\big(1 + \|x\|^r\big).$$

Theorem 5.3.5. Let $\mathcal{D} \subseteq \mathbb{R}^d$ (not necessarily bounded) satisfy Assumption 5.2.5. Let $r > 1$ and $p > 2r$. Let W be a d' dimensional Brownian motion. Let θ, b, σ and f satisfy Assumption 5.3.4.

Then there exists a unique solution to the reflected McKean-Vlasov equation (5.3.5) in $\mathcal{S}^p([0,T])$ (explicit $\mathcal{S}^p$-norm bounds are given below in (5.3.17)).

The proof of this theorem is the content of the next section.

Remark 5.3.6. A nuanced detail of the following proof is the calculation of moments and potentially singular and non-integrable drifts. In [IdRS19], the authors studied processes where the drift term could have polynomial growth that was greater than the moments of the final solution. The conclusion was that time integrals of these drift terms "smooth out" the non-integrability.

In this chapter, we only require a one-sided Lipschitz condition for the spatial variable. However, we were unable to remove the polynomial growth condition for the self-stabilizing term f. This is because one needs integrability of the convolution of the law of the solution with the vector field f before the self-stabilisation acts to push deviating paths back towards the mean of the distribution.

5.3.3 Proof of Theorem 5.3.5

This proof is inspired by [BRTV98]. Unlike the proof of Theorem 5.3.2 which constructs a contraction operator on the space of measures, we construct a fixed point on a space of functions. Each function will give rise to a McKean-Vlasov process by substituting it into the equation as a drift term. Then, the law of this McKean-Vlasov equation is convolved with the vector field f to obtain a new function. This trick allows us to bypass the non-Lipschitz property of the functional $g(x,\mu) := f * \mu(x)$ while still exploiting the one-sided Lipschitz condition in the spatial variable.

Our contributions in this section include developing this method to allow for diffusion terms that are not constant. This is novel, even before the addition of a domain of constraint. The non-constant diffusion complicates the computation of moment estimates which are key to this method. Of particular interest is Proposition 5.3.13, which diverges from previous literature.

Definition 5.3.7. Let $r>1$. Let $x_0\in\mathcal{D}$ and $L>0$ be as in Assumption 5.3.4. For $g:[0,T]\times\mathcal{D}\to\mathbb{R}^d$, let

$$\|g\|_{[0,T],r}:=\sup_{t\in[0,T]}\left(\sup_{x\in\mathcal{D}}\frac{\|g(t,x)\|}{1+\|x-x_0\|^r}\right).$$

Let $\Lambda_{[0,T],r}$ be the space of all functions $g:[0,T]\times\mathcal{D}\to\mathbb{R}^d$ such that $\|g\|_{[0,T],r}<\infty$ and

$$\langle g(t,x)-g(t,y),x-y\rangle\le L\|x-y\|^2\qquad\forall xy,\in\mathcal{D},\ t\in[0,T].$$

The space $\Lambda_{[0,T],r}$ is a Banach space. For $g\in\Lambda_{[0,T],r}$, consider the reflected McKean-Vlasov equation

$$\begin{aligned}X_t^{(g)}=&\theta+\int_0^t b(s,X_s^{(g)},\mu_s^{(g)})ds+\int_0^t\sigma(s,X_s^{(g)},\mu_s^{(g)})dW_s+\int_0^t g(s,X_s^{(g)})ds-k_t^{(g)},\\|k^{(g)}|_t=&\int_0^t\mathbb{1}_{\partial D}(X_s^{(g)})d|k^{(g)}|_s,\quad k_t^{(g)}=\int_0^t\mathbb{1}_{\partial\mathcal{D}}(X_s^{(g)})\mathbf{n}(X_s^{(g)})d|k^{(g)}|_s,\quad\mathbb{P}\Big[X_t^{(g)}\in dx\Big]=\mu_t^{(g)}(dx).\end{aligned}\tag{5.3.6}$$

By Theorem 5.3.2, we know that there exists a unique solution to this McKean-Vlasov equation for every choice of $g\in\Lambda_{[0,T],r}$ and every $r\ge1$. Further, we have the moment estimate that for $\varepsilon>0$ and $T_0\in[0,T-\varepsilon]$,

$$\begin{aligned}&\sup_{t\in[T_0,T_0+\varepsilon]}\mathbb{E}\Big[\|X_t^{(g)}-x_0\|^p\Big]\\&\le\Bigg(4\mathbb{E}\Big[\|X_{T_0}^{(g)}-x_0\|^p\Big]+\big(4(p-1)\big)^{p-1}\bigg(\Big(\int_{T_0}^{T_0+\varepsilon}\|b(r,x_0,\delta_{x_0})\|dr\Big)^p+\Big(\int_{T_0}^{T_0+\varepsilon}\|g(r,x_0)\|dr\Big)^p\bigg)\\&\quad+2(p-1)^{p/2}\cdot(p-2)^{(p-2)/2}\cdot4^{p/2}\Big(\int_{T_0}^{T_0+\varepsilon}\|\sigma(r,x_0,\delta_{x_0})\|^2dr\Big)^{\frac{p}{2}}\Bigg)\cdot\exp\Big(\big(4pL+2p(p-1)L^2\big)\varepsilon\Big).\end{aligned}\tag{5.3.7}$$

Our challenge will be to find a g such that $g(t,x)=f*\mu_t^{(g)}(x)$.

Definition 5.3.8. Let b, σ and f satisfy Assumption 5.3.4. Let $g\in\Lambda_{[0,T],r}$. Let $X^{(g)}$ be the unique solution to the McKean-Vlasov equation (5.3.6) with law $\mu^{(g)}$. Let $\Gamma:\Lambda_{[0,T],r}\to C([0,T]\times\mathcal{D};\mathbb{R}^d)$ be defined by

$$\Gamma[g](t,x):=f*\mu_t^{(g)}(x)=\mathbb{E}\big[f(x-X_t^{(g)})\big].$$

Our goal is to demonstrate that the operator Γ has a fixed point g'. Then the McKean-Vlasov equation $X^{(g')}$ that solves (5.3.6) will be the solution to the McKean-Vlasov equation (5.3.5).

Lemma 5.3.9. Let Γ be the operator defined in Definition 5.3.8. Then $\forall T_0\in[0,T]$ and $\forall\varepsilon>0$ such that $T_0+\varepsilon<T$, Γ maps $\Lambda_{[T_0,T_0+\varepsilon],r}$ to $\Lambda_{[T_0,T_0+\varepsilon],r}$.

Proof. Fix $T_0\in[0,T]$ and $\varepsilon>0$ appropriately. Let $g\in\Lambda_{[T_0,T_0+\varepsilon],r}$. Then $\forall x,y\in\mathbb{R}^d$ and $\forall t\in[T_0,T_0+\varepsilon]$,

$$\Big\langle x-y,\Gamma[g](t,x)-\Gamma[g](t,y)\Big\rangle=\int_{\mathcal{D}}\Big\langle x-y,f(x-u)-f(y-u)\Big\rangle d\mu_t^{(g)}(u)\le L\|x-y\|^2.$$

Secondly,

$$\begin{aligned}\mathbb{E}\Big[f(X_t^{(g)}-x)\Big]\le&2C+\big(C+2^r\big)\Big(\|x-x_0\|^r+\mathbb{E}\Big[\|X_t^{(g)}\|^r\Big]\Big)\\\le&\Big(2C+2^{r+1}\Big)\Big(1+\|x-x_0\|^r\Big)\Big(1+\mathbb{E}\Big[\|X_t^{(g)}-x_0\|^r\Big]\Big).\end{aligned}$$

By Assumption 5.3.4, we know the process $X^{(g)}$ has finite moments of order $p>2r$. Thus

$$\Big\|\Gamma[g]\Big\|_{[T_0,T_0+\varepsilon],r}\le\Big(2C+2^{r+1}\Big)\cdot\Big(1+\sup_{t\in[T_0,T_0+\varepsilon]}\mathbb{E}\Big[\|X_t^{(g)}-x_0\|^r\Big]\Big).\tag{5.3.8}$$

Combining these with Equation (5.3.7) and using that

$$\Big(\int_{T_0}^{T_0+\varepsilon}\|g(s,x_0)\|ds\Big)^p\le\varepsilon^p\|g\|^p_{[T_0,T_0+\varepsilon],r},$$

we obtain that

$$\begin{aligned}\Big\|\Gamma[g]\Big\|_{[T_0,T_0+\varepsilon],r}\le&\Big(2C+2^{r+1}\Big)\Big(1+\sup_{t\in[0,T_0]}\mathbb{E}\Big[\|X_t^{(g)}-x_0\|^r\Big]\Big)\\&+\Bigg(\Big(4(p-1)\Big)^{p-1}\Bigg(\Big(\int_{T_0}^{T_0+\varepsilon}\|b(s,x_0,\delta_{x_0})\|ds\Big)^p+\Big(\int_{T_0}^{T_0+\varepsilon}\|g(s,x_0)\|ds\Big)^p\Bigg)\\&\quad+2(p-1)^{p/2}\cdot(p-2)^{(p-2)/2}\cdot4^{p/2}\Big(\int_{T_0}^{T_0+\varepsilon}\|\sigma(s,x_0,\delta_{x_0})\|^2ds\Big)^{\frac{p}{2}}\Bigg)\\&\quad\cdot\exp\Big(\big(4pL+2p(p-1)L^2\big)\varepsilon\Big).\end{aligned}\tag{5.3.9}$$

Taking $T_0=0$ and $\varepsilon=T$, we get $\Big\|\Gamma[g]\Big\|_{[0,T],r}<\infty$ for any $g\in\Lambda_{[0,T],r}$.

□

Lemma 5.3.10. Let $T_0\in[0,T]$ and let $\varepsilon>0$ such that $T_0+\varepsilon<T$. Let Γ be the operator given in Definition 5.3.8. Then there exists a constant K such that $\forall g_1,g_2\in\Lambda_{[T_0,T_0+\varepsilon],r}$ with $g_1(t)=g_2(t)$ $\forall t\in[0,T_0]$ we have

$$\Big\|\Gamma[g_1]-\Gamma[g_2]\Big\|_{[T_0,T_0+\varepsilon],r}\le\|g_1-g_2\|_{[T_0,T_0+\varepsilon],r}K\sqrt{\varepsilon}e^{K\varepsilon}.$$

Proof. Let $g_1,g_2:[0,T]\times\mathcal{D}\to\mathbb{R}^d$ such that $g_1(t)=g_2(t)$ for $t\in[0,T_0]$. Let $X^{(g_1)}$ and $X^{(g_2)}$ be solutions to Equation (5.3.6). Firstly, for $t\in[T_0,T_0+\varepsilon]$ we have, applying Itô's formula,

$$\begin{aligned}&\|X_t^{(g_1)}-X_t^{(g_2)}\|^2\\&=2\int_{T_0}^t\Big\langle X_s^{(g_1)}-X_s^{(g_2)},b(s,X_s^{(g_1)},\mu_s^{(g_1)})-b(s,X_s^{(g_2)},\mu_s^{(g_2)})\Big\rangle ds\\&\quad+2\int_{T_0}^t\Big\langle X_s^{(g_1)}-X_s^{(g_2)},g_1(X_s^{(g_1)})-g_1(X_s^{(g_2)})\Big\rangle ds+2\int_{T_0}^t\Big\langle X_s^{(g_1)}-X_s^{(g_2)},g_1(X_s^{(g_2)})-g_2(X_s^{(g_2)})\Big\rangle ds\\&\quad+2\int_{T_0}^t\Big\langle X_s^{(g_1)}-X_s^{(g_2)},\Big(\sigma(s,X_s^{(g_1)},\mu_s^{(g_1)})-\sigma(s,X_s^{(g_2)},\mu_s^{(g_2)})\Big)dW_s\Big\rangle\\&\quad+\int_{T_0}^t\Big\|\sigma(s,X_s^{(g_1)},\mu_s^{(g_1)})-\sigma(s,X_s^{(g_2)},\mu_s^{(g_2)})\Big\|^2ds-2\int_{T_0}^t\Big\langle X_s^{(g_1)}-X_s^{(g_2)},dk_s^{(g_1)}-dk_s^{(g_2)}\Big\rangle.\end{aligned}$$

Taking expectations, a supremum over time and applying Lemma 5.2.4, we get

$$\begin{aligned}\sup_{t\in[T_0,T_0+\varepsilon]}\mathbb{E}\Big[\|X_t^{(g_1)}-X_t^{(g_2)}\|^2\Big]\le&(6L+4L^2)\int_{T_0}^{T_0+\varepsilon}\sup_{s\in[T_0,T_0+t]}\mathbb{E}\Big[\|X_s^{(g_1)}-X_s^{(g_2)}\|^2\Big]dt\\&+2\int_{T_0}^{T_0+\varepsilon}\mathbb{E}\Big[\|X_t^{(g_1)}-X_t^{(g_2)}\|\cdot\|g_1-g_2\|_{[T_0,T_0+t],r}\Big(1+\|X_t^{(g_2)}-x_0\|^r\Big)\Big]dt.\end{aligned}$$

An application of Grönwall's Inequality yields

$$\begin{aligned}&\sup_{t\in[T_0,T_0+\varepsilon]}\mathbb{E}\Big[\|X_t^{(g_1)}-X_t^{(g_2)}\|^2\Big]\\&\le8\|g_1-g_2\|^2_{[T_0,T_0+\varepsilon],r}\cdot\varepsilon\cdot e^{(8L^2+12L)\varepsilon}\cdot\Bigg(1+\sup_{t\in[T_0,T_0+\varepsilon]}\mathbb{E}\Big[\|X_t^{(g_2)}-x_0\|^{2r}\Big]\Bigg).\end{aligned}\tag{5.3.10}$$

Let $x \in \mathcal{D}$. Using the polynomial growth assumption of f, we have that

$$\begin{aligned}
&\mathbb{E}\Big[f(x - X_t^{(g_1)}) - f(x - X_t^{(g_2)})\Big]\\
&\leq (C + 2^r)\mathbb{E}\Big[\|X_t^{(g_1)} - X_t^{(g_2)}\| \cdot \big(1 + \|x - x_0\|^r\big) \cdot \big(1 + \|X_t^{(g_1)} - x_0\|^r + \|X_t^{(g_2)} - x_0\|^r\big)\Big]\\
&\leq (C + 2^r) \cdot \Big(1 + \|x - x_0\|^r\Big)\mathbb{E}\Big[\|X_t^{(g_1)} - X_t^{(g_2)}\|^2\Big]^{\frac{1}{2}} \cdot \mathbb{E}\Big[\Big(1 + \|X_t^{(g_1)} - x_0\|^r + \|X_t^{(g_2)} - x_0\|^r\Big)^2\Big]^{\frac{1}{2}}. \quad (5.3.11)
\end{aligned}$$

By Assumption 5.3.4 and (5.3.7) we have that

$$\sup_{t \in [0,T]} \mathbb{E}\Big[\|X_t^{(g_1)} - x_0\|^{2r}\Big], \quad \sup_{t \in [0,T]} \mathbb{E}\Big[\|X_t^{(g_2)} - x_0\|^{2r}\Big] < \infty.$$

Further, these bounds are uniform and depend only on b and σ.

Substituting Equation (5.3.10) into Equation (5.3.11), we get

$$\begin{aligned}
\Big\|\Gamma[g_1] - \Gamma[g_2]\Big\|_{[T_0,T_0+\varepsilon],r} &= \sup_{t \in [T_0,T_0+\varepsilon]} \sup_{x \in \mathcal{D}} \frac{\mathbb{E}\Big[f(x - X_t^{(g_1)}) - f(x - X_t^{(g_2)})\Big]}{1 + |x - x_0|^r}\\
&\leq (C + 2^r)3\sqrt{8}\|g_1 - g_2\|_{[T_0,T_0+\varepsilon],r}\sqrt{\varepsilon}e^{(4L^2+6L)\varepsilon}\left(1 + \sup_{t \in [T_0,T_0+\varepsilon]} \mathbb{E}\Big[\|X_t^{(g_1)}\|^{2r} + \|X_t^{(g_2)}\|^{2r}\Big]\right). \quad (5.3.12)
\end{aligned}$$

□

Next, our goal is to establish a subset on which this operator is a contraction operator.

Definition 5.3.11. Let $K > 0$. For $T > 0$ and $r > 1$, we define

$$\Lambda_{[0,T],r,K} := \Big\{g \in \Lambda_{[0,T],r} : \|g\|_{[0,T],r} \leq K\Big\}.$$

Our goal is to choose T and K so that Γ is a contraction operator when restricted to $\Lambda_{[0,T],r,K}$.

Proposition 5.3.12. Let $\Gamma : \Lambda_{[0,T],r} \to \Lambda_{[0,T],r}$ be as defined in Definition 5.3.8. Then $\exists K_1, \varepsilon > 0$ such that,

$$\Gamma\Big[\Lambda_{[0,\varepsilon],r,K_1}\Big] \subset \Lambda_{[0,\varepsilon],r,K_1}, \qquad \text{and} \qquad \forall g_1, g_2 \in \Lambda_{[0,\varepsilon],r,K_1} \quad \Big\|\Gamma[g_1] - \Gamma[g_2]\Big\|_{[0,\varepsilon],r} \leq \frac{1}{2}\Big\|g_1 - g_2\Big\|_{[0,\varepsilon],r}.$$

As such, there exists a unique solution to Equation (5.3.5) on the interval $[0, \varepsilon]$.

Proof. Let $\varepsilon > 0$. Let $g \in \Lambda_{[0,\varepsilon],r,K_1}$. Taking Equation (5.3.9) with $T_0 = 0$ provides

$$\begin{aligned}
&\Big\|\Gamma[g]\Big\|_{[0,\varepsilon],r}\\
&\leq \Big(2C + 2^{r+1}\Big)\Big(1 + \mathbb{E}\Big[|\theta - x_0|^r\Big]\Big) + \Bigg(\Big(4(p-1)\Big)^{p-1}\bigg(\Big(\int_0^\varepsilon |b(s, x_0, \delta_{x_0})|ds\Big)^p + \Big(\varepsilon K_1\Big)^p\bigg)\\
&\quad + 2(p-1)^{p/2} \cdot (p-2)^{(p-2)/2} \cdot 4^{p/2}\Big(\int_0^\varepsilon |\sigma(s, x_0, \delta_{x_0})|^2 ds\Big)^{\frac{p}{2}}\Bigg) \cdot \exp\Big(\big(4pL + 2p(p-1)L^2\big)\varepsilon\Big).
\end{aligned}$$

Choose $K_1 = 2(2C + 2^{r+1})\Big(1 + \mathbb{E}\Big[\|\theta - x_0\|^p\Big]\Big)$. We have the limit

$$\lim_{\varepsilon \to 0} \Big(\int_0^\varepsilon \|b(s, x_0, \delta_{x_0})\|ds\Big)^p + \Big(\int_0^\varepsilon \|\sigma(s, x_0, \delta_{x_0})\|^2 ds\Big)^{\frac{p}{2}} = 0.$$

Then we can choose $\varepsilon' > 0$ such that $\Big\|\Gamma[g]\Big\|_{[0,\varepsilon'],r} < K_1$.

Secondly, using Equation (5.3.12) we choose $\varepsilon'' > 0$ such that

$$\Big\|\Gamma[g_1] - \Gamma[g_2]\Big\|_{[0,\varepsilon''],r} < \frac{\|g_1 - g_2\|_{[0,\varepsilon''],r}}{2}.$$

We emphasise that the choice of $\varepsilon = \min\{\varepsilon', \varepsilon''\}$ is dependent on the choice of K_1.

Define $d : \Lambda_{[0,\varepsilon],r} \times \Lambda_{[0,\varepsilon],r} \to \mathbb{R}_+$ to be the metric $d(g_1, g_2) = \|g_1 - g_2\|_{[0,\varepsilon],r}$. The metric space $(\Lambda_{[0,\varepsilon],r,K_1}, d)$ is non-empty, complete and $\Gamma : \Lambda_{[0,\varepsilon],r,K_1} \to \Lambda_{[0,\varepsilon],r,K_1}$ is a contraction operator. Therefore, $\exists g' \in \Lambda_{[0,\varepsilon],r,K_1}$ such that $\Gamma[g'] = g'$. Thus $\forall t \in [0,\varepsilon]$,

$$g'\Big(t, X_t^{(g')}\Big) = f * \mu_t^{(g')}(X_t^{(g')}).$$

Substituting this into (5.3.6), we obtain (5.3.5). Thus a solution to (5.3.5) exists in $\mathcal{S}^p([0,\varepsilon])$. □

Our challenge now is to find a solution over the whole interval $[0, T]$.

Proposition 5.3.13. Let $\mathcal{D}$ satisfy Assumption 5.2.5. Let $r > 1$ and $p > 2r$. Let W be a d' dimensional Brownian motion. Let b, σ and f satisfy Assumption 5.3.4. Suppose that a solution X to the McKean-Vlasov equation (5.3.5) exists in $\mathcal{S}^p([0, T_0])$ for some $0 < T_0 < T$. Then there exists a constant $K_2 = K_2(p, T)$ such that

$$\left(\sup_{t\in[0,T_0]} \mathbb{E}\Big[\|X_t - x_0\|^p\Big]\right) \vee \left(\mathbb{E}\Big[\|X - x_0\|^p_{\infty,[0,T_0]}\Big]\right) < K_2.$$

The challenge of this proof is that the symmetry trick for establishing 2nd moments (see Equation (5.3.13)) does not hold for higher moments. However, if we try to bypass this using the methods of [HIP08], the non-constant diffusion terms yields integrals that blow up. Arguing by induction on m, we fix this by considering

$$\sup_{t\in[0,T]} \mathbb{E}\Big[\|X_t - x_0\|^{2m}\Big] + \mathbb{E}\Big[\|X_t - \tilde{X}_t\|^{2m}\Big],$$

and demonstrating via a Grönwall argument that this is finite, even though a similar argument would not work for either of these terms on their own.

Proof. Suppose that $t \in [0, T_0]$. Let (X_t, k_t), $(\tilde{X}_t, \tilde{k}_t)$ and $(\overline{X_t}, \overline{k_t})$ be independent, identically distributed solutions of Equation (5.3.5).

Consider the two processes

$$\begin{aligned}
\|X_t - x_0\|^2 = \|\theta - x_0\|^2 &+ 2\int_0^t \Big\langle X_s - x_0, b(s, X_s, \mu_s)\Big\rangle ds + 2\int_0^t \Big\langle X_s - x_0, \sigma(s, X_s, \mu_s) dW_s\Big\rangle \\
&+ \int_0^t \Big\|\sigma(s, X_s, \mu_s)\Big\|^2 ds + 2\int_0^t \Big\langle X_s - x_0, \overline{\mathbb{E}}\Big[f(X_s - \overline{X_s})\Big]\Big\rangle ds - 2\int_0^t \Big\langle X_s - x_0, dk_s\Big\rangle, \\
\|X_t - \tilde{X}_t\|^2 = \|\theta - \tilde{\theta}\|^2 &+ 2\int_0^t \Big\langle X_s - \tilde{X}_s, b(s, X_s, \mu_s) - b(s, \tilde{X}_s, \mu_s)\Big\rangle ds \\
&+ 2\int_0^t \Big\langle X_s - \tilde{X}_s, \sigma(s, X_s, \mu_s) dW_s - \sigma(s, \tilde{X}_s, \mu_s) d\tilde{W}_s\Big\rangle \\
&+ \int_0^t \Big\|\sigma(s, X_s, \mu_s)\Big\|^2 + \Big\|\sigma(s, \tilde{X}_s, \mu_s)\Big\|^2 ds \\
&+ 2\int_0^t \Big\langle X_s - \tilde{X}_s, \overline{\mathbb{E}}\Big[f(X_s - \overline{X_s}) - f(\tilde{X}_s - \overline{X_s})\Big]\Big\rangle ds - 2\int_0^t \Big\langle X_s - \tilde{X}_s, dk_s - d\tilde{k}_s\Big\rangle.
\end{aligned}$$

We remark that since f is symmetric we have the identity

$$\mathbb{E}\Big[\Big\langle X_s - x_0, \overline{\mathbb{E}}\Big[f(X_s - \overline{X_s})\Big]\Big\rangle\Big] \le L \cdot \mathbb{E}\Big[\overline{\mathbb{E}}\Big[\|X_s - \overline{X_s}\|^2\Big]\Big]. \tag{5.3.13}$$

Taking expectations of both processes (and no longer distinguishing between the integral operators $\mathbb{E}$ and $\tilde{\mathbb{E}}$) and adding them together, we get

$$\begin{aligned}\mathbb{E}\Big[\|X_t - x_0\|^2 + \|X_t - \tilde{X}_t\|^2\Big] \leq& \mathbb{E}\Big[\|\theta - x_0\|^2\Big] + \mathbb{E}\Big[\|\theta - \tilde{\theta}\|^2\Big] \\ &+ (4L + 12L^2)\int_0^t \mathbb{E}\Big[\|X_s - x_0\|^2\Big] ds + 2\int_0^t \mathbb{E}\Big[\|X_s - x_0\|\Big] \cdot \|b(s, x_0, \delta_{x_0})\| ds \\ &+ 6\int_0^t \|\sigma(s, x_0, \delta_{x_0})\|^2 ds + 6L\int_0^t \mathbb{E}\Big[\|X_s - \tilde{X}_s\|^2\Big] ds.\end{aligned}$$

Taking a supremum over $t \in [0, T_0]$, then applying Young's inequality followed by Grönwall's inequality, we obtain

$$\begin{aligned}\sup_{t\in[0,T_0]} \mathbb{E}\Big[\|X_t - x_0\|^2 + \|X_t - \tilde{X}_t\|^2\Big] \leq& 2\Bigg(\mathbb{E}\Big[\|\theta - x_0\|^2\Big] + \mathbb{E}\Big[\|\theta - \tilde{\theta}\|^2\Big] \\ &+ \Big(\int_0^T \Big\|b(s, x_0, \delta_{x_0})\Big\| ds\Big)^2 + \int_0^T \Big\|\sigma(s, x_0, \delta_{x_0})\Big\|^2 ds\Bigg) e^{(4L+12L^2)T}.\end{aligned}$$

We proceed via induction. Let

$$Y_t = X_t - \mathbb{E}[X_t]$$

be the centred process. Then

$$\mathbb{E}\Big[\|X_t - x_0\|^{2m}\Big] \leq 2^{2m-1}\Big(\mathbb{E}\Big[\|X_t - x_0\|^2\Big]^m + \mathbb{E}\Big[\|Y_t\|^{2m}\Big]\Big). \tag{5.3.14}$$

Let ξ and $\tilde{\xi}$ be independent copies of a scalar random variable with mean 0. Then by the Binomial Theorem, we have that for $m \in \mathbb{N}$,

$$\mathbb{E}\Big[(\xi - \tilde{\xi})^{2m}\Big] = \sum_{k=0}^{2m} (-1)^k \binom{2m}{k} \mathbb{E}\Big[\xi^k\Big]\mathbb{E}\Big[\xi^{2m-k}\Big],$$

and therefore from [HIP08, Proposition 2.12]

$$2\mathbb{E}\Big[\|Y_t\|^{2m}\Big] \leq c(m,d)\Big(\mathbb{E}\Big[\|X_t - \tilde{X}_t\|^{2m}\Big] + \Big(1 + \mathbb{E}\Big[\|Y_t\|^{2m-2}\Big]\Big)^2\Big), \tag{5.3.15}$$

for a constant $c(m,d)$ depending only on m and d. In what follows we write $c(m,d,L)$ for a constant possibly changing on each line, but dependent only on m, d and Lipshitz constant L. We combine Equations (5.3.14) and Equation (5.3.15) to get

$$\begin{aligned}&\mathbb{E}\Big[\|X_t - x_0\|^{2m}\Big] + \mathbb{E}\Big[\|X_t - \tilde{X}_t\|^{2m}\Big] \\ &\quad \leq c(m,d,L)\Big(\mathbb{E}\Big[\|X_t - x_0\|^2\Big]^m + \Big(1 + \mathbb{E}\Big[\|Y_t\|^{2m-2}\Big]\Big)^2\Big) + c(m,d,L)\mathbb{E}\Big[\|X_t - \tilde{X}_t\|^{2m}\Big].\end{aligned} \tag{5.3.16}$$

We use Itô's formula to get that

$$\begin{aligned}\|X_t - \tilde{X}_t\|^{2m} =& \|\theta - \tilde{\theta}\|^{2m} + 2m\int_0^t \|X_s - \tilde{X}_s\|^{2m-2}\Big\langle X_s - \tilde{X}_s, b(s, X_s, \mu_s) - b(s, \tilde{X}_s, \mu_s)\Big\rangle ds \\ &+ 2m\int_0^t \|X_s - \tilde{X}_s\|^{2m-2}\Big\langle X_s - \tilde{X}_s, \overline{\mathbb{E}}\Big[f(X_s - \overline{X}_s) - f(\tilde{X}_s - \overline{X}_s)\Big]\Big\rangle ds \\ &+ 2m\int_0^t \|X_s - \tilde{X}_s\|^{2m-2}\Big\langle X_s - \tilde{X}_s, \sigma(s, X_s, \mu_s)dW_s - \sigma(s, \tilde{X}_s, \mu_s)d\tilde{W}_s\Big\rangle \\ &+ m(2m-1)\int_0^t \|X_s - \tilde{X}_s\|^{2m-2}\Big(\|\sigma(s, X_s, \mu_s)\|^2 + \|\sigma(s, \tilde{X}_s, \mu_s)\|^2\Big) ds - 2m\int_0^t \Big\langle X_s - \tilde{X}_s, dk_s - d\tilde{k}_s\Big\rangle,\end{aligned}$$

Now for any $K > 0$,

$$
\begin{aligned}
&K \sup_{t\in[0,T]} \mathbb{E}\Bigg[\int_0^t \|X_s - \tilde{X}_s\|^{2m-2}\Big(\|\sigma(s, X_s, \mu_s)\|^2 + \|\sigma(s, \tilde{X}_s, \mu_s)\|^2\Big) ds\Bigg] \\
\leq& 12L^2 K \int_0^T \mathbb{E}\Big[\|X_s - \tilde{X}_s\|^{2m}\Big] ds + \tfrac{12L^2 K}{m} \int_0^T \mathbb{E}\Big[\|X_s - x_0\|^{2m}\Big] ds \\
&+ \sup_{t\in[0,T]} \frac{\mathbb{E}\Big[\|X_t - \tilde{X}_t\|^{2m}\Big]}{2} + \big[2(m-1)\big]^{m-1} \cdot \Big[\tfrac{6K}{m}\Big]^m \cdot \Big(\int_0^T \Big|\sigma(s, x_0, \delta_{x_0})\Big|^2 ds\Big)^m.
\end{aligned}
$$

Applying this with Equation (5.3.16) yields

$$
\begin{aligned}
&\sup_{t\in[0,T]} \mathbb{E}\Big[\|X_t - x_0\|^{2m}\Big] + \mathbb{E}\Big[\|X_t - \tilde{X}_t\|^{2m}\Big] \\
&\leq c(m, d, L)\Bigg(\mathbb{E}\Big[\|X_t - x_0\|^2\Big]^m + \Big(1 + \mathbb{E}\Big[\|Y_t\|^{2m-2}\Big]\Big)^2 + \mathbb{E}\Big[\|\theta - \tilde{\theta}\|^{2m}\Big] + \Big(\int_0^T \|\sigma(s, x_0, \delta_{x_0})\|^2 ds\Big)^m \\
&+ \int_0^T \sup_{s\in[0,t]} \mathbb{E}\Big[\|X_s - \tilde{X}_s\|^{2m}\Big] + \mathbb{E}\Big[\|X_s - x_0\|^{2m}\Big] dt\Bigg) + \frac{1}{2} \sup_{t\in[0,T]} \mathbb{E}\Big[\|X_t - \tilde{X}_t\|^{2m}\Big].
\end{aligned}
$$

Combining all terms together, we get that there exist a constant $c = c(m, d, L, T)$, dependent only on m, d, L, T and not T_0 such that

$$
\sup_{t\in[0,T_0]} \mathbb{E}\Big[\|X_t - x_0\|^{2m} + \|X_t - \tilde{X}_t\|^{2m}\Big] \leq c\Bigg(1 + \int_0^{T_0} \sup_{s\in[0,t]} \mathbb{E}\Big[\|X_s - x_0\|^{2m} + \|X_s - \tilde{X}_s\|^{2m}\Big] dt\Bigg).
$$

Thus via Grönwall

$$
\sup_{t\in[0,T_0]} \mathbb{E}\Big[\|X_t - x_0\|^{2m} + \|X_t - \tilde{X}_t\|^{2m}\Big] \leq c e^{cT_0} < c e^{cT}.
$$

Hence, by induction we have finite moment estimates for all $m \in \mathbb{N}$ such that $2m \leq p$. In particular, this is true for $2m \geq 2r$. For sharp moment estimates, we use the methods from the proof of Theorem 5.3.1 to get

$$
\begin{aligned}
\mathbb{E}\Big[\|X - x_0\|_{\infty,[0,T_0]}^p\Big] \lesssim& \mathbb{E}\Big[\|\theta - x_0\|^p\Big] + \Big(\int_0^{T_0} \|b(s, x_0, \delta_{x_0})\| ds\Big)^p \\
&+ \Big(\int_0^{T_0} \|\sigma(s, x_0, \delta_{x_0})\|^2 ds\Big)^{p/2} + \Big(\int_0^{T_0} \Big\|\tilde{\mathbb{E}}\Big[f(\tilde{X}_s - x_0)\Big]\Big\| ds\Big)^p \\
\lesssim& \mathbb{E}\Big[\|\theta - x_0\|^p\Big] + \Big(\int_0^T \|b(s, x_0, \delta_{x_0})\| ds\Big)^p \\
&+ \Big(\int_0^T \|\sigma(s, x_0, \delta_{x_0})\|^2 ds\Big)^{p/2} + \Big(TC \sup_{t\in[0,T_0]} \mathbb{E}\Big[\|X_t - x_0\|^r + 1\Big]\Big)^p.
\end{aligned} \tag{5.3.17}
$$

□

Finally, we are in position to prove Theorem 5.3.5.

Proof of Theorem 5.3.5. By Proposition 5.3.12, we have that a unique solution to Equation (5.3.5) exists on the interval $[0, \varepsilon]$. Let $\delta > 0$ and $g \in \Lambda_{[\varepsilon,\varepsilon+\delta],r}$. Then again by (5.3.9)

$$
\begin{aligned}
\Big\|\Gamma[g]\Big\|_{[\varepsilon,\varepsilon+\delta],r} \leq & \Big(2C+2^{r+1}\Big)\Big(1+\sup_{t\in[0,\varepsilon]}\mathbb{E}\Big[\|X_t-x_0\|^r\Big]\Big) \\
& + \Bigg(\Big(4(p-1)\Big)^{p-1}\bigg(\Big(\int_\varepsilon^{\varepsilon+\delta}\|b(s,x_0,\delta_{x_0})\|ds\Big)^p + \Big(\delta\|g\|_{[\varepsilon,\varepsilon+\delta],r}\Big)^p\bigg) \\
& \quad + 2(p-1)^{p/2}\cdot(p-2)^{(p-2)/2}\cdot 4^{p/2}\Big(\int_\varepsilon^{\varepsilon+\delta}\|\sigma(s,x_0,\delta_{x_0})\|^2 ds\Big)^{\frac{p}{2}}\Bigg) \\
& \quad \cdot \exp\Big(\big(4pL+2p(p-1)L^2\big)\delta\Big).
\end{aligned}
$$

By Proposition 5.3.13, we know that

$$
2\Big(2C+2^{r+1}\Big)\Big(1+\sup_{t\in[0,\varepsilon]}\mathbb{E}\Big[\|X_t-x_0\|^r\Big]\Big) < K_5,
$$

for some K_5 independent of ε. Then for $\|g\|_{[\varepsilon,\varepsilon+\delta],r} < K_5$, we get

$$
\begin{aligned}
\Big\|\Gamma[g]\Big\|_{[\varepsilon,\varepsilon+\delta],r} \leq & \tfrac{K_5}{2} + \Bigg(\Big(4(p-1)\Big)^{p-1}\bigg(\Big(\int_\varepsilon^{\varepsilon+\delta}\|b(s,x_0,\delta_{x_0})\|ds\Big)^p + \big(\delta K_5\big)^p\bigg) \\
& \quad + 2(p-1)^{p/2}\cdot(p-2)^{(p-2)/2}\cdot 4^{p/2}\Big(\int_\varepsilon^{\varepsilon+\delta}\|\sigma(s,x_0,\delta_{x_0})\|^2 ds\Big)^{\frac{p}{2}}\Bigg) \\
& \quad \cdot \exp\Big(\big(4pL+2p(p-1)L^2\big)\delta\Big).
\end{aligned}
$$

By the uniform continuity of the mappings

$$
\delta \mapsto \int_\varepsilon^{\varepsilon+\delta}\|b(s,x_0,\delta_{x_0})\|ds \quad \text{and} \quad \delta \mapsto \int_\varepsilon^{\varepsilon+\delta}\|\sigma(s,x_0,\delta_{x_0})\|^2 ds,
$$

we choose $\delta' > 0$ (independently of ε) so that $\|\,\Gamma[g]\,\|_{[\varepsilon,\varepsilon+\delta'],r} < K_5$. Next, we use Equation (5.3.12) to get

$$
\begin{aligned}
&\Big\|\Gamma[g_1]-\Gamma[g_2]\Big\|_{[\varepsilon,\varepsilon+\delta],r} \\
&\quad \leq (C+2^r)3\sqrt{8}\|g_1-g_2\|_{[\varepsilon,\varepsilon+\delta],r}\sqrt{\delta}e^{(4L^2+6L)\delta}\Bigg(1+\sup_{t\in[\varepsilon,\varepsilon+\delta]}\mathbb{E}\Big[\|X_t^{(g_1)}-x_0\|^{2r}+\|X_t^{(g_2)}-x_0\|^{2r}\Big]\Bigg).
\end{aligned}
$$

Next, using Equation (5.3.7), we get

$$
\begin{aligned}
\Big\|\Gamma[g_1]-\Gamma[g_2]\Big\|_{[\varepsilon,\varepsilon+\delta],r} \leq & (C+2^r)3\sqrt{8}\|g_1-g_2\|_{[\varepsilon,\varepsilon+\delta],r}\sqrt{\delta}e^{(4L^2+6L)\delta}\Bigg(1+8\sup_{t\in[0,\varepsilon]}\mathbb{E}\Big[|X_t-x_0|^{2r}\Big] \\
& + 2\big(4(2r-1)\big)^{2r-1}\bigg(\Big(\int_\varepsilon^{\varepsilon+\delta}|b(s,x_0,\delta_{x_0})|ds\Big)^{2r} + \big(\delta K_5\big)^{2r}\bigg) \\
& + 4(2r-1)^r\cdot(2r-2)^{r-1}\cdot 4^r\Big(\int_\varepsilon^{\varepsilon+\delta}|\sigma(s,x_0,\delta_{x_0})|^2 ds\Big)^r\Bigg)e^{\big(8rL+4r(2r-1)L^2\big)\delta}.
\end{aligned}
$$

Finally, by Proposition 5.3.13, we choose $\delta'' > 0$ (independently of ε) such that

$$
\Big\|\Gamma[g_1]-\Gamma[g_2]\Big\|_{[\varepsilon,\varepsilon+\delta''],r} \leq \frac{1}{2}\|g_1-g_2\|_{[\varepsilon,\varepsilon+\delta''],r}.
$$

Let $\delta = \min\{\delta',\delta''\}$.

Define $d : \Lambda_{[\varepsilon,\varepsilon+\delta],r} \times \Lambda_{[\varepsilon,\varepsilon+\delta],r} \to \mathbb{R}_+$ be the metric $d(g_1, g_2) = \|g_1 - g_2\|_{[\varepsilon,\varepsilon+\delta],r}$. The metric space $(\Lambda_{[\varepsilon,\varepsilon+\delta],r,K_3}, d)$ is non-empty, complete and $\Gamma : \Lambda_{[\varepsilon,\varepsilon+\delta],r,K_3} \to \Lambda_{[\varepsilon,\varepsilon+\delta],r,K_3}$ is a contraction operator. Therefore, $\exists g' \in \Lambda_{[\varepsilon,\varepsilon+\delta],r,K_3}$ such that $\Gamma[g'] = g'$.

Thus $\forall t \in [\varepsilon, \varepsilon + \delta]$,

$$g'\big(t, X_t^{(g')}\big) = f * \mu_t^{(g')}\big(X_t^{(g')}\big).$$

Repeating this argument and concatenating, we obtain a function $g \in \Lambda_{[0,T],r}$ such that $\forall t \in [0, T]$

$$g\big(t, X_t^{(g)}\big) = f * \mu_t^{(g)}\big(X_t^{(g)}\big).$$

Substituting this into Equation (5.3.6), we obtain Equation (5.3.5) over the interval $[0, T]$. □

5.3.4 Propagation of chaos

We are interested in the ways in which the dynamics of a single equation within a system of reflected interacting equations of the form (5.1.3) converges to the dynamics of the reflected McKean-Vlasov equation.

Let $N \in \mathbb{N}$ and let $i \in \{1, ..., N\}$. We now study the law of a solution to the interacting particle system

$$\begin{aligned} X_t^{i,N} =& \theta^i + \int_0^t b(s, X_s^{i,N}, \mu_s^N)ds + \int_0^t \sigma(s, X_s^{i,N}, \mu_s^N)dW_s^{i,N} + \int_0^t f * \mu_s^N(X_s^{i,N})ds - k_t^{i,N}, \\ |k^{i,N}|_t =& \int_0^t \mathbb{1}_{\partial D}(X_s^{i,N})d|k^{i,N}|_s, \qquad k_t^{i,N} = \int_0^t \mathbb{1}_{\partial \mathcal{D}}(X_s^{i,N})\mathbf{n}(X_s^{i,N})d|k^{i,N}|_s, \qquad \mu_t^N = \tfrac{1}{N}\sum_{j=1}^N \delta_{X_t^{j,N}}. \end{aligned} \tag{5.3.18}$$

We demonstrate Propagation of Chaos (PoC), that is for a finite time interval $[0, T]$ the trajectories of the particle system on average converge to that of the McKean-Vlasov equation.

Theorem 5.3.14 (Propagation of Chaos (PoC))**.** Let $\mathcal{D} \subset \mathbb{R}^d$ satisfy Assumption 5.2.5. Let θ^i be independent identically distributed copies of θ, and let θ, b, σ and f satisfy Assumption 5.3.4. Let $W^{i,N}$ be a sequence of independent Brownian motions taking values on $\mathbb{R}^{d'}$. Additionally, suppose that $p > \max\{2r, 4\}$. Let X_t^i be a sequence of strong solutions to Equation (5.3.5) driven by the Brownian motion $W^{i,N}$, and with initial conditions θ^i. Let $X_t^{i,N}$ be the solution to particle system (5.3.18).

Then there exists a constant $c = c(T) > 0$, depending only on T, such that

$$\sup_{t\in[0,T]} \mathbb{E}\Big[\|X_t^{i,N} - X_t^i\|^2\Big] \le c(T) \begin{cases} N^{-1/2}, & d < 4, \\ N^{-1/2}\log N, & d = 4, \\ N^{\frac{-2}{d+4}}, & d > 4. \end{cases} \tag{5.3.19}$$

Proof. Firstly, we assume that the noise driving the McKean-Vlasov equation (5.3.5) and the noise driving the particle system (5.3.18) have correlation 1. Using Itô's formula, summing over i and taking expectations,

$$\begin{aligned} \sum_{i=1}^N \mathbb{E}\Big[\|X_t^{i,N} - X_t^i\|^2\Big] \le& 2L\int_0^t \sum_{i=1}^N \mathbb{E}\Big[\|X_s^{i,N} - X_s^i\|^2\Big]ds + 2L\int_0^t \sum_{i=1}^N \mathbb{E}\Big[\|X_s^{i,N} - X_s^i\| \cdot \mathbb{W}_{\mathcal{D}}^{(2)}(\mu_s^N, \mu_s)\Big]ds \\ &+ 4L^2\int_0^t \sum_{i=1}^N \mathbb{E}\Big[\|X_s^{i,N} - X_s^i\|^2 + \mathbb{W}_{\mathcal{D}}^{(2)}\Big(\mu_s^N, \mu_s\Big)^2\Big]ds \\ &+ 2\int_0^t \sum_{i=1}^N \mathbb{E}\Big[\Big\langle X_s^{i,N} - X_s^i, \tfrac{1}{N}\sum_{j=1}^N f(X_s^{i,N} - X_s^{j,N}) - f(X_s^i - X_s^j)\Big\rangle\Big]ds \qquad (5.3.20) \\ &+ 2\int_0^t \sum_{i=1}^N \mathbb{E}\Big[\Big\langle X_s^{i,N} - X_s^i, \tfrac{1}{N}\sum_{j=1}^N f(X_s^i - X_s^j) - f * \mu_s(X_s^i)\Big\rangle\Big]ds. \qquad (5.3.21) \end{aligned}$$

Re-arranging the double sum and using that f is odd, we can rewrite the integrand of (5.3.20) as

$$\sum_{i,j=1}^{N}\mathbb{E}\Big[\Big\langle X_s^{i,N}-X_s^i, f(X_s^{i,N}-X_s^{j,N})-f(X_s^i-X_s^j)\Big\rangle\Big]$$
$$=\frac{1}{2}\sum_{i,j=1}^{N}\mathbb{E}\Big[\Big\langle (X_s^{i,N}-X_s^{j,N})-(X_s^i-X_s^j), f(X_s^{i,N}-X_s^{j,N})-f(X_s^i-X_s^j)\Big\rangle\Big], \quad (5.3.22)$$

and thus using the one-sided Lipschitz property of f we can bound (5.3.22) by $L\sum_{i=1}^{N}\mathbb{E}\big[\|X_s^{i,N}-X_s^i\|^2\big]$.

Consider the sum over j in the integrand of (5.3.21). One observes that after using the Cauchy-Schwarz inequality we have the product of the two terms

$$\mathbb{E}\Big[\Big\langle X_s^{i,N}-X_s^i, \sum_{j=1}^{N}\big(f(X_s^i-X_s^j)-f*\mu_s(X_s^i)\big)\Big\rangle\Big]$$
$$\leq \mathbb{E}\Big[\|X_s^{i,N}-X_s^i\|\Big]^{1/2}\mathbb{E}\Big[\Big\|\sum_{j=1}^{N}\big(f(X_s^i-X_s^j)-f*\mu_s(X_s^i)\big)\Big\|^2\Big]^{1/2}. \quad (5.3.23)$$

We next show that the second of these terms is bounded by $C\sqrt{N}$ for some fixed constant $C>0$. We have

$$\begin{aligned}\mathbb{E}\Big[\Big\|\sum_{j=1}^{N}\big(f(X_s^i-X_s^j)-f*\mu_s(X_s^i)\big)\Big\|^2\Big] &= \sum_{j,k=1}^{N}\mathbb{E}\Big[\big\langle f(X_s^i-X_s^j)-f*\mu_s(X_s^i), f(X_s^i-X_s^k)-f*\mu_s(X_s^i)\big\rangle\Big]\\ &= \sum_{j=1}^{N}\mathbb{E}\Big[\big\|f(X_s^i-X_s^j)-f*\mu_s(X_s^i)\big\|^2\Big] \quad (5.3.24)\\ &\leq CN \quad (5.3.25)\end{aligned}$$

where (5.3.24) is due to the fact that the cross terms (i.e., $i\neq j$) are all zero since in this case X^j is independent of X^k, and (5.3.25) follows from the polynomial growth of f and the control on the moments $\mathbb{E}[\|X_s^i\|^{2r}]$. Using (5.3.23) in conjunction with (5.3.25), it is clear that the integrand in (5.3.21) is some constant multiple of $\sqrt{N}+\frac{1}{\sqrt{N}}\sum_{i=1}^{N}\mathbb{E}[\|X_s^{i,N}-X_s^i\|^2]$ (from the inequality $|x|\leq 1+|x|^2$). Next, dealing with the $\mathbb{W}_{\mathcal{D}}^{(2)}(\mu_\cdot^N,\mu_\cdot)$ terms, set $\nu_\cdot^N=\frac{1}{N}\sum_{j=1}^{N}\delta_{X_\cdot^j}$. By the triangle inequality, we get

$$\mathbb{E}\Big[\mathbb{W}_{\mathcal{D}}^{(2)}(\mu_s^N,\mu_s)\Big]\leq \mathbb{E}\Big[\Big(\tfrac{1}{N}\sum_{i=1}^{N}\|X_s^{i,N}-X_s^i\|^2\Big)^{1/2}+\mathbb{W}_{\mathcal{D}}^{(2)}(\nu_s^N,\mu_s)\Big]. \quad (5.3.26)$$

Assembling all the previous bounds with the estimate obtained after applying Itô's formula, we get

$$\sum_{i=1}^{N}\mathbb{E}\Big[\|X_t^{i,N}-X_t^i\|^2\Big]\lesssim\int_0^t\sum_{i=1}^{N}\mathbb{E}\Big[\|X_s^{i,N}-X_s^i\|^2\Big]ds+t\sqrt{N}+N\int_0^t\mathbb{W}_{\mathcal{D}}^{(2)}(\mu_s^N,\mu_s)\Big]ds.$$

Noting that the particles are exchangeable, and taking the supremum over $t\in[0,T]$ we find that

$$\sup_{t\in[0,T]}\mathbb{E}\Big[\|X_t^{i,N}-X_t^i\|^2\Big]\lesssim\int_0^T\sup_{t\in[0,s]}\mathbb{E}\Big[\|X_s^{i,N}-X_s^i\|^2\Big]ds+T\Big(\frac{1}{\sqrt{N}}+\sup_{t\in[0,T]}\mathbb{E}\Big[\mathbb{W}_{\mathcal{D}}^{(2)}\Big(\nu_t^N,\mu_t\Big)^2\Big]\Big).$$

Applying Grönwall inequality yields

$$\sup_{t\in[0,T]}\mathbb{E}\Big[\|X_t^{i,N}-X_t^i\|^2\Big]\lesssim T\Big(\frac{1}{\sqrt{N}}+\sup_{t\in[0,T]}\mathbb{E}\Big[\mathbb{W}_{\mathcal{D}}^{(2)}\Big(\nu_t^N,\mu_t\Big)^2\Big]\Big).$$

Finally, by assumption on p all processes have moments larger the 4th one, thus one can use the well known rate of convergence for an empirical distribution to the true law, see [CD18, Theorem 5.8], and obtain

$$\mathbb{E}\Big[\mathbb{W}^{(2)}_{\mathcal{D}}\Big(\nu^N_t,\mu_t\Big)^2\Big] \lesssim \begin{cases} N^{-1/2}, & d<4,\\ N^{-1/2}\log N, & d=4,\\ N^{\frac{-2}{d+4}}, & d>4,\end{cases}$$

to conclude. Note that the latter convergence rate dominates the $T/\sqrt{N}$ element in the main error estimate. $\square$

5.3.5 An example

A key advantage of the framework that we consider for Theorem 5.3.2 and Theorem 5.3.5 is that the drift term b is locally Lipschitz over $\mathcal{D}$. We demonstrate that the measure dependencies allowed for with the self-stabilizing term $f*\mu$ do not satisfy a Lipschitz condition with respect to the Wasserstein distance.

Example 5.3.15. Let $\mathcal{D}=\mathbb{R}_+$. Let $F(x)=-x^4/4$ so that $f(x)=\nabla F(x)=-x^3$. Consider the dynamics

$$X_t = W_t - \int_0^t \int_{\mathcal{D}} (X_s-y)^3 \mu_t(dy)ds - k_t, \quad \mu_t(dx)=\mathbb{P}\big[X_t\in dx\big], \quad X_0=1.$$

Without entering details and assuming $\mu,\nu\in\mathcal{P}_4(\mathcal{D})$, the Lions derivative of $\mu\mapsto\Psi_x(\mu):=-\int_{\mathcal{D}}(x-y)^3\mu(dy)$ is unbounded, meaning that the Lipschitz constant of $\mu\mapsto\Psi_x(\mu)$ depends on x in an unbounded way since $\mathcal{D}$ is unbounded.

For the reader familiarised with the theory, see [CD18, Section 5], the Lions derivative of the functional $\Psi_x(\cdot)$ follows from Example 1 in Section 5.2.2 (p385) and is given by $\partial_\mu\psi_x(\mu)(Z)=f'(x-Z)$ for $Z\sim\mu$. Their Remark 5.27 (p384) and Remark 5.28 (p390) connect to the Lipschitz constant.

5.4 Large Deviation Principles

Throughout this section let $\varepsilon>0$, all results hold under the following assumptions:

Assumption 5.4.1. Suppose that $\mathcal{D}\subset\mathbb{R}^d$ satisfies Assumption 5.2.5. Suppose that b,σ, and f satisfy Assumptions 5.3.4. Additionally, suppose that $\exists L>0, \exists\beta\in(0,1]$ such that $\forall s,t\in[0,T]$, $\forall\mu\in\mathcal{P}_2(\mathcal{D})$ and $\forall x\in\mathcal{D}$,

$$\|\sigma(t,x,\mu)-\sigma(s,x,\mu)\|\leq L\|t-s\|^\beta.$$

The regularity on σ imposed above will allow us to make an Euler scheme approximation to the dynamics. We begin by reminding the reader of the definition of a Freidlin-Wentzell Large Deviation Principle.

Definition 5.4.2. Let E be a metric space. A function $I:E\to[0,\infty]$ is said to be a *rate function* if it is lower semi-continuous and the level sets of I are closed. A *good rate function* is a rate function whose level sets are compact.

The rate function is used to encode the asymptotic rate for a convergence in probability statement that is called a Large Deviations Principle.

Definition 5.4.3. Let $x\in\mathcal{D}$. A family of probability measures $\{\mu^\varepsilon\}_{\varepsilon>0}$ on $C_x([0,T];\mathcal{D})$ is said to satisfy a Large Deviations Principle with rate function I if

$$-\inf_{h\in G^\circ} I(h) \leq \liminf_{\varepsilon\to0}\varepsilon\log\mu^\varepsilon[G^\circ] \leq \limsup_{\varepsilon\to0}\varepsilon\log\mu^\varepsilon[\overline{G}] \leq -\inf_{h\in\overline{G}} I(h), \tag{5.4.1}$$

for all Borel subsets G of the space $C_x([0,T];\mathcal{D})$.

We prove a Freidlin-Wentzell Large Deviation Principle for the class of reflected McKean-Vlasov equations studied in Section 5.3. The inclusion of non-Lipschitz measure dependence and reflections extends the classical Freidlin-Wentzell results for SDEs found in [DZ98, DS89, dH00].

Our approach uses sequences of exponentially good approximations, inspired by the methods of [HIP08] and [dRST19]. As with previous works proving Freidlin-Wentzell LDP results for McKean-Vlasov SDEs, the non-Lipschitz measure dependency is accounted for by establishing an LDP for a diffusion that is an exponentially tight approximation.

The section is structured as follows, first a deterministic path is identified which the solution to (5.4.2) approaches as $\varepsilon \to 0$. Definition (5.4.7) then introduces an approximation of (5.4.2) where the law is replaced by this deterministic path. An LDP is established for this approximation by first obtaining an LDP for its Euler scheme in Lemma 5.4.10, and then transferring it via the method of exponential approximations in Lemmas 5.4.11 and 5.4.12. Finally the LDP for the object of interest (5.4.2) is acquired by establishing exponential equivalence between it and the approximation of Definition 5.4.6.

5.4.1 Convergence of the law

Recall that the key point of an LDP is to characterise the rate at which the probability of rare events decreases as we change a parameter in our experiment. In the case of path space LDP for a stochastic processes this relies on identifying a path which the diffusion increasingly concentrates around as the noise decays. The dynamics of the process can then be seen as small perturbations from this fixed path, often referred to as the skeleton path. Consider the reflected McKean-Vlasov SDE

$$\begin{aligned} X^\varepsilon_t =& x_0 + \int_0^t b(s, X^\varepsilon_s, \mu^\varepsilon_s) ds + \int_0^t f * \mu^\varepsilon_s(X^\varepsilon_s) ds + \sqrt{\varepsilon}\int_0^t \sigma(s, X^\varepsilon_s, \mu^\varepsilon_s) dW_s - k^\varepsilon_t, \\ |k^\varepsilon|_t =& \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X^\varepsilon_s) d|k^\varepsilon|_s, \quad k^\varepsilon_t = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X^\varepsilon_s)\mathbf{n}(X^\varepsilon_s) d|k^\varepsilon|_s. \end{aligned} \tag{5.4.2}$$

Heuristically, as $\varepsilon \to 0$ the noise term in (5.4.2) vanishes, the law of X^ε tends to a Dirac measure of its own deterministic trajectory and hence the interaction term vanishes. Therefore in the small noise limit the dynamics is governed by b and the diffusion behaves like the solution to the following deterministic Skorokhod problem.

Definition 5.4.4. Define ψ^{x_0} to be the solution to the reflected ODE

$$\begin{aligned} \psi^{x_0}(t) =& x_0 + \int_0^t b(s, \psi^{x_0}(s), \delta_{\psi^{x_0}(s)}) ds - k^\psi_t, \\ |k^\psi|_t =& \int_0^t \mathbb{1}_{\partial\mathcal{D}}(\psi(s)) d|k^\psi|_s, \quad k^\psi_t = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(\psi(s))\mathbf{n}(\psi(s)) d|k^\psi|_s, \end{aligned} \tag{5.4.3}$$

on the interval $[0,T]$. We define the Skeleton operator $H : \mathcal{H}^0_1 \to C_{x_0}([0,T];\mathcal{D})$ by $h \mapsto H[h]$ where

$$\begin{aligned} H[h]_t =& x_0 + \int_0^t b(s, H[h]_s, \delta_{\psi^{x_0}(s)}) ds + \int_0^t f(H[h]_s - \psi^{x_0}(s)) ds + \int_0^t \sigma(s, H[h]_s, \delta_{\psi^{x_0}(s)}) dh_s - k^h_t, \\ |k^h|_t =& \int_0^t \mathbb{1}_{\partial\mathcal{D}}(H[h]_s) d|k^h|_s, \quad k^h_t = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(H[h]_s)\mathbf{n}(H[h]_s) d|k^h|_s. \end{aligned} \tag{5.4.4}$$

The existence of a unique solution to the Skorokhod problem for a continuous path into a convex domain [Tan79, Theorem 2.1] ensures the existence and uniqueness of a solution to Equation (5.4.4), this can we proved in a similar and fashion to [Tan79, Theorem 4.1]. Hence the operator $H[h]$ is well defined.

The following lemma proves that, for small ϵ, the solution X^ϵ to (5.4.2) will remain close to the trajectory ψ^{x_0} of the skeleton ODE (5.4.3). Moreover the law μ^ε can be shown to tend to the Dirac measure of ψ^{x_0}.

Lemma 5.4.5. Let X^ε be the solution to (5.4.2) and μ^ε its law. Let ψ^{x_0} be the solution of (5.4.3). Then we have for any $T > 0$,

$$\sup_{t\in[0,T]} \mathbb{E}\Big[\|X^\varepsilon_t - \psi^{x_0}(t)\|^2\Big] \le \varepsilon T e^{cT}, \tag{5.4.5}$$

for a constant c independent of ε and x_0. Moreover for any $x \in \mathbb{R}^d$ we have that

$$\lim_{\varepsilon \to 0} \|f * \mu_t^\varepsilon(x) - f(x - \psi^{x_0}(t))\|_{\infty,[0,T]} = 0. \tag{5.4.6}$$

Proof. Let $t \in [0,T]$. We have

$$\begin{aligned}\|X_t^\varepsilon - \psi^{x_0}(t)\|^2 =&2\int_0^t \Big\langle X_s^\varepsilon - \psi^{x_0}(s), b(s, X_s^\varepsilon, \mu_s^\varepsilon) - b(s, \psi^{x_0}(s), \delta_{\psi^{x_0}(s)})\Big\rangle ds\\ &+ \sqrt{\varepsilon}\int_0^t \Big\langle X_s^\varepsilon - \psi^{x_0}(s), \sigma(s, X_s^\varepsilon, \mu_s) dW_s\Big\rangle + \varepsilon\int_0^t \|\sigma(s, X_s^\varepsilon, \mu_s^\varepsilon)\|^2 ds\\ &+ \int_0^t \Big\langle X_s^\varepsilon - \psi^{x_0}(s), f(X_s^\varepsilon) * \mu_s^\varepsilon\Big\rangle ds - \int_0^t \Big\langle X_s^\varepsilon - \psi^{x_0}(s), dk_s^\varepsilon - dk_s^\psi\Big\rangle.\end{aligned}$$

Thus

$$\begin{aligned}\sup_{t\in[0,T]} \mathbb{E}\Big[\|X_t^\varepsilon - \psi^{x_0}(t)\|^2\Big] \le& 6L\int_0^T \sup_{s\in[0,t]} \mathbb{E}\Big[\|X_s^\varepsilon - \psi^{x_0}(s)\|^2\Big] ds\\ &+ C\cdot \sup_{t\in[0,T]} \mathbb{E}\Big[\Big(1 + \|X_t^\varepsilon - \psi(t)\|^r\Big)^2\Big]^{1/2} \cdot \int_0^T \sup_{s\in[0,t]} \mathbb{E}\Big[\|X_s^\varepsilon - \psi^{x_0}(s)\|^2\Big] dt\\ &+ \varepsilon\Big(6TL^2 \sup_{t\in[0,T]} \mathbb{E}\Big[\|X_t^\varepsilon - x_0\|^2\Big] + 3\int_0^T \|\sigma(t, x_0, \delta_{x_0})\|^2 dt\Big).\end{aligned}$$

Therefore we can conclude (5.4.5) from the finite moment estimates proved in Proposition 5.3.13 and Grönwall's inequality. Next, (5.4.6) follows from (5.4.5)

$$\begin{aligned}&\sup_{t\in[0,T]} \|f * \mu_t^\varepsilon(x) - f(x - \psi^{x_0}(t)\|\\ &\qquad\le C \sup_{t\in[0,T]} \mathbb{E}\Big[\|X_t^\varepsilon - \psi^{x_0}(t)\|^2\Big]^{1/2} \cdot \mathbb{E}\Big[\Big(1 + \|X_t^\varepsilon\|^{r-1} + \|\psi^{x_0}(t)\|^{r-1}\Big)^2\Big]^{1/2} \xrightarrow[\varepsilon\to 0]{} 0.\end{aligned}$$

□

5.4.2 A classical Freidlin-Wentzell result

Since the law μ^ε tends to the Dirac mass of the path ψ^{x_0}, we will first study SDEs where the law in the coefficients of the McKean-Vlasov equation has been replaced by $\delta_{\psi^{x_0}}$.

Definition 5.4.6. Let Y^ε be the solution of

$$\begin{aligned}Y_t^\varepsilon =&x_0 + \int_0^t b(s, Y_s^\varepsilon, \delta_{\psi^{x_0}(s)}) ds + \int_0^t f\Big(Y_s^\varepsilon - \psi^{x_0}(s)\Big) ds + \sqrt{\varepsilon}\int_0^t \sigma(s, Y_s^\varepsilon, \delta_{\psi^{x_0}(s)}) dW_s - k_t^Y,\\ |k^Y|_t =& \int_0^t \mathbb{1}_{\partial\mathcal{D}}(Y_s^\varepsilon) d|k^Y|_s, \qquad k_t^Y = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(Y_s^\varepsilon)\mathbf{n}(Y_s^\varepsilon) d|k^Y|_s.\end{aligned} \tag{5.4.7}$$

The dynamics of (5.4.7) satisfy those of Theorem 5.3.1, so the existence and uniqueness of a solution is established. Further, we introduce the follow approximation of (5.4.7).

Definition 5.4.7. Let $n \in \mathbb{N}$. Let $Y^{n,\varepsilon}$ be the solution of

$$\begin{aligned}Y_t^{n,\varepsilon} =&x_0 + \int_0^t b(s, Y_s^{n,\varepsilon}, \delta_{\psi^{x_0}(s)}) + f\Big(Y_s^{n,\varepsilon} - \psi^{x_0}(s)\Big) ds\\ &\sqrt{\varepsilon}\sum_{i=0}^{\lfloor \frac{tn}{T}\rfloor - 1} \sigma\Big(\tfrac{iT}{n}, Y_{\frac{iT}{n}}^{n,\varepsilon}, \delta_{\psi^{x_0}\left(\frac{iT}{n}\right)}\Big) \cdot \Big(W_{\frac{(i+1)T}{n}} - W_{\frac{iT}{n}}\Big)\\ &+ \sqrt{\varepsilon}\sigma\Big(\tfrac{T\lfloor \frac{tn}{T}\rfloor}{n}, Y_{\frac{T\lfloor \frac{tn}{T}\rfloor}{n}}^{n,\varepsilon}, \delta_{\psi^{x_0}\left(\frac{T\lfloor \frac{tn}{T}\rfloor}{n}\right)}\Big)\Big(W_{\frac{T\lceil \frac{tn}{T}\rceil}{n}} - W_{\frac{T\lfloor \frac{tn}{T}\rfloor}{n}}\Big) n\Big(t - \tfrac{T\lfloor \frac{tn}{T}\rfloor}{n}\Big) - k_t^{Y^{n,\varepsilon}}\\ |k^{Y^{n,\varepsilon}}|_t =& \int_0^t \mathbb{1}_{\partial\mathcal{D}}(Y_s^{n,\varepsilon}) d|k^{Y^{n,\varepsilon}}|_s, \qquad k_t^{Y^{n,\varepsilon}} = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(Y_s^{n,\varepsilon})\mathbf{n}(Y_s^{n,\varepsilon}) d|k^{Y^{n,\varepsilon}}|_s.\end{aligned} \tag{5.4.8}$$

On a subset of measure 1, Equation (5.4.8) determines the dynamics of a random ODE for which the Skorokhod problem has already been solved, so existence and uniqueness are already assured.

Definition 5.4.8. Let $I' : C_0([0,T];\mathbb{R}^d) \to \mathbb{R}$ be the rate function of Schilder's Theorem [DZ98, Theorem 5.2.3],

$$I'(g) = \begin{cases} \frac{1}{2}\int_0^T \|\dot{g}(t)\|^2 dt & \text{if } g \in \mathcal{H}_1^0, \\ \infty & \text{otherwise,} \end{cases}$$

where $\mathcal{H}_1^0$ is the Cameron Martin space for Brownian motion defined in Section 5.2.

Define the functional $H^n : C_0([0,T];\mathbb{R}^d) \to C_{x_0}([0,T];\mathbb{R}^d)$, which maps the Brownian path to the reflected path of (5.4.8), that is

$$\begin{aligned} H^n[h](t) =& x_0 + \int_0^t b\big(s, H^n[h](s), \delta_{\psi^{x_0}(s)}\big) + f\Big(H^n[h](s) - \psi^{x_0}(s)\Big) ds - k_t^{h,n} \\ &+ \sum_{i=0}^{\lfloor \frac{tn}{T} \rfloor -1} \sigma\Big(\frac{iT}{n}, H^n[h]\Big(\frac{iT}{n}\Big), \delta_{\psi^{x_0}(\frac{iT}{n})}\Big)\Big(h\Big(\frac{(i+1)T}{n}\Big) - h\Big(\frac{iT}{n}\Big)\Big) \\ &+ \sigma\Big(\frac{T\lfloor \frac{tn}{T}\rfloor}{n}, H^n[h]\Big(\frac{T\lfloor \frac{tn}{T}\rfloor}{n}\Big), \delta_{\psi^{x_0}(\frac{T\lfloor \frac{tn}{T}\rfloor}{n})}\Big)\Big(h\Big(\tfrac{T\lceil \frac{tn}{T}\rceil}{n}\Big) - h\Big(\tfrac{T\lfloor \frac{tn}{T}\rfloor}{n}\Big)\Big)\frac{n}{T}\Big(t - \frac{T\lfloor \frac{tn}{T}\rfloor}{n}\Big), \end{aligned} \tag{5.4.9}$$

$$|k^{h,n}|_t = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(H^n[h](s)) d|k^{h,n}|_s, \quad k_t^{h,n} = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(H^n[h](s))\mathbf{n}(H^n[h](s)) d|k^{h,n}|_s.$$

When restricted to $\mathcal{H}_1^0$, the operator H^n represents a Skeleton operator for the random ODE (5.4.8). Equation (5.4.7) is a classical reflected SDE and [Dup87, Theorem 3.1] proves a Freidlin-Wentzell type LDP for such reflected SDEs when the coefficients are bounded and Lipschitz. The following lemma extends this result to unbounded domains and allows for unbounded locally Lipschitz coefficients, this is done via the contraction principle [DZ98, Theorem 4.2.1]. For convenience of notation let

$$\hat{t} := \frac{T\lceil \frac{tn}{T}\rceil}{n}, \ \check{t} := \frac{T\lfloor \frac{tn}{T}\rfloor}{n}, \text{ and } \hat{s} := \frac{T\lceil \frac{sn}{T}\rceil}{n}, \ \check{s} := \frac{T\lfloor \frac{sn}{T}\rfloor}{n}.$$

Lemma 5.4.9. For each $n \in \mathbb{N}$, the mapping $H^n : C_0([0,T];\mathbb{R}^d) \to C_{x_0}([0,T];\mathbb{R}^d)$ defined by (5.4.9) is continuous.

Proof. Let $\{h_m : m \in \mathbb{N}\} \subset C_0([0,T];\mathbb{R}^d)$ and suppose $\lim_{m\to\infty} \|h_m - h\|_{\infty,[0,T]} = 0$. We denote $\phi = H^n[h]$ and $\phi_m = H^n[h_m]$. Then

$$\begin{aligned} \|\phi(t) - \phi_m(t)\|^2 =& 2\int_0^t \Big\langle \phi(s) - \phi_m(s), b(s,\phi(s),\delta_{\psi(s)}) - b(s,\phi_m(s),\delta_{\psi(s)})\Big\rangle ds \\ &+ 2\int_0^t \Big\langle \phi(s) - \phi_k(s), f(\phi(s) - \psi(s)) - f(\phi_m(s) - \psi(s))\Big\rangle ds \\ &- 2\int_0^t \Big\langle \phi(s) - \phi_m(s), dk_s^{h,n} - dk_s^{h_m,n}\Big\rangle \\ &+ 2n\int_0^t \Big\langle \phi(s) - \phi_m(s), \sigma(\check{s},\phi(\check{s}),\delta_{\psi(\check{s})})\Big(h(\hat{s}) - h(\check{s})\Big) \\ &\qquad - \sigma(\check{s},\phi_m(\check{s}),\delta_{\psi(\check{s})})\Big(h_m(\hat{s}) - h_m(\check{s})\Big)\Big\rangle ds. \end{aligned}$$

Hence

$$\begin{aligned} \Big\|\phi(t) - \phi_m(t)\Big\|^2 \leq& 4L\int_0^t \Big\|\phi(s) - \phi_m(s)\Big\|^2 ds \\ &+ 2n\int_0^t \Big\langle \phi(s) - \phi_m(s), \Big(\sigma(\check{s},\phi(\check{s}),\delta_{\psi(\check{s})}) - \sigma(\check{s},\phi_m(\check{s}),\delta_{\psi(\check{s})})\Big)\cdot\Big(h_m(\hat{s}) - h_m(\check{s})\Big) ds \\ &+ 2n\int_0^t \Big\langle \phi(s) - \phi_m(s), \sigma(\check{s},\phi(\check{s}),\delta_{\psi(\check{s})})\cdot\Big((h - h_m)(\hat{s}) - (h - h_m)(\check{s})\Big\rangle ds. \end{aligned}$$

Using the Lipschitz properties of σ combined with n being fixed, we get

$$\begin{aligned}\|\phi-\phi_m\|^2_{\infty,[0,T]} \leq & \Big(8L+8n\|h\|_{\infty,[0,T]}\Big)\int_0^t \Big\|\phi(s)-\phi_m(s)\Big\|^2 ds \\ & + 16n^2\|h-h_m\|^2_{\infty,[0,T]}\Big(\int_0^T \sigma(\check{s},\phi(\check{s}),\delta_{\psi(\check{s})})ds\Big)^2.\end{aligned}$$

As the integral $\int_0^T \sigma(\check{s},\phi(\check{s}),\delta_{\psi(\check{s})})ds$ will be finite for any choice of n and h, we apply Grönwall inequality to conclude

$$\|\phi-\phi_m\|^2_{\infty,[0,T]} \lesssim \|h-h_m\|^2_{\infty,[0,T]}.$$

□

Lemma 5.4.10. Let $Y^{n,\varepsilon}$ be the solution to (5.4.8). Then $Y^{n,\varepsilon}$ satisfies an LDP on the space $C_{x_0}([0,T];\mathbb{R}^d)$, with a good rate function given by

$$I^{n,T}_{x_0}(\phi) := \inf_{\{h\in\mathcal{H}^0_1\,:\,H^n(h)=\phi\}} I'(h). \tag{5.4.10}$$

Proof. The result is a straightforward application of the contraction principle [DZ98, Theorem 4.2.1] using the continuous map H^n as established in Lemma 5.4.9). □

Next we use that $Y^{n,\varepsilon}$ is an approximation of Y^ε in the appropriate sense to obtain an LDP for Y^ε via [DZ98, Theorem 4.2.23].

Lemma 5.4.11. Let Y^ε be the solution to (5.4.7), and $Y^{n,\varepsilon}$ be the solution to (5.4.8). Then for every $\delta>0$

$$\limsup_{n\to\infty}\limsup_{\epsilon\to 0}\epsilon\log\mathbb{P}\Big[\sup_{t\in[0,T]}\|Y^{n,\varepsilon}_t-Y^\varepsilon_t\|>\delta\Big]=-\infty. \tag{5.4.11}$$

That is $Y^{n,\varepsilon}$ is an exponentially good approximation of Y^ε, in the sense of [DZ98, Definition 4.2.14].

Proof. The proof makes use of the LDP for $Y^{n,\varepsilon}$ established in Lemma 5.4.10. We follow a similar strategy as [dRST19, Lemma 4.6], requiring an adapted version of [DZ98, Lemma 5.6.18] stated here in Lemma 5.A.1.

Define the process $Z^\varepsilon := Y^\varepsilon - Y^{n,\varepsilon}$, so that

$$Z^\varepsilon_t = \int_0^t b_s ds + \int_0^t \sigma_s ds + k^{Y^n}_t - k^Y_t,$$

where

$$\begin{aligned} b_t :=& b\Big(t,Y^\varepsilon_t,\delta_{\psi(t)}\Big) - b\Big(t,Y^{n,\varepsilon}_t,\delta_{\psi(t)}\Big) + f\Big(Y^\varepsilon_t-\psi(t)\Big) - f\Big(Y^{n,\varepsilon}_t-\psi(t)\Big),\\ \sigma_t :=& \sigma\Big(t,Y^\varepsilon_t,\delta_{\psi(t)}\Big) - \sigma\Big(\check{t},Y^{n,\varepsilon}_{\check{t}},\delta_{\psi(\check{t})}\Big).\end{aligned}$$

Next we define the stopping time

$$\tau_{R+1} := \min\Big\{T, \inf\{t\geq 0 : \|Y^\varepsilon_t\|\geq R+1\}, \inf\{t\geq 0: \|Y^{n,\varepsilon}_t\|\geq R+1\}\Big\}.$$

Note that for $t\in[0,\tau_{R+1}]$ by the local Lipschitz property of b and f, we have

$$\|b_t\| \leq L_R\|Z^\varepsilon_t\|,$$

for a constant L_R only depending on R. Also note that

$$\begin{aligned}\|\sigma_t\| \leq & \Big\|\sigma\Big(t,Y^\varepsilon_t,\delta_{\psi(t)}\Big)-\sigma\Big(\check{t},Y^\varepsilon_t,\delta_{\psi(t)}\Big)\Big\| + \Big\|\sigma\Big(\check{t},Y^{n,\varepsilon}_{\check{t}},\delta_{\psi(t)}\Big)-\sigma\Big(\check{t},Y^\varepsilon_t,\delta_{\psi(t)}\Big)\Big\| \\ & + \Big\|\sigma\Big(\check{t},Y^{n,\varepsilon}_{\check{t}},\delta_{\psi(\check{t})}\Big)-\sigma\Big(\check{t},Y^{n,\varepsilon}_{\check{t}},\delta_{\psi(t)}\Big)\Big\| \\ \leq & L\Big(\|t-\check{t}\|^\beta + \|Z^\varepsilon_t\| + \|\psi(t)-\psi(\check{t})\|\Big) \\ \leq & M(\rho(n)+\|Z_t\|),\end{aligned}$$

for some M large enough, and $\rho(n) \underset{n\to\infty}{\to} 0$. Thus the conditions of Lemma 5.A.1 are satisfied. Now fix any $\delta > 0$ and notice that

$$\Big\{ \sup_{t\in[0,T]} \|Y_t^\varepsilon - Y_t^{n,\varepsilon}\| \geq \delta \Big\} \subseteq \Big\{ \sup_{t\in[0,\tau_{R+1}]} \|Y_t^\varepsilon - Y_t^{n,\varepsilon}\| \geq \delta, \tau_{R+1} = T \Big\} \cup \Big\{ \sup_{t\in[0,T]} \|Y_t^\varepsilon - Y_t^{n,\varepsilon}\| \geq \delta, \tau_{R+1} < T \Big\}$$
$$\subseteq \Big\{ \sup_{t\in[0,\tau_{R+1}]} \|Y_t^\varepsilon - Y_t^{n,\varepsilon}\| \geq \delta \Big\} \cup \Big\{ \tau_{R+1} < T \Big\}.$$

By Lemma 5.A.1 we know that

$$\lim_{n\to\infty} \limsup_{\varepsilon\to 0} \varepsilon \log \Big(\mathbb{P}\Big[\sup_{t\in[0,\tau_{R+1}]} \|Y_t^\varepsilon - Y_t^{n,\varepsilon}\| \geq \delta \Big] \Big) = -\infty.$$

Furthermore define $\tau_R^{Y_n} = \inf\{t \geq 0 : \|Y_t^{n,\varepsilon}\| \geq R\}$, and notice

$$\Big\{ \tau_{R+1} < T \Big\} \subseteq \Big\{ \tau_{R+1} < T, \tau_R^{Y^n} \leq T \Big\} \cup \Big\{ \tau_{R+1} < T, \tau_R^{Y^n} > T \Big\}$$
$$\subseteq \Big\{ \tau_R^{Y^n} \leq T \Big\} \cup \Big\{ \|Y_{\tau_{R+1}}^\varepsilon - Y_{\tau_{R+1}}^{n,\varepsilon}\| \geq 1 \Big\}.$$

Again, by Lemma 5.A.1 and setting $\delta = 1$ we have that

$$\lim_{n\to\infty} \limsup_{\varepsilon\to 0} \varepsilon \log \Big(\mathbb{P}\Big[\sup_{t\in[0,\tau_{R+1}]} \|Y_t^\varepsilon - Y_t^{n,\varepsilon}\| \geq 1 \Big] \Big) = -\infty.$$

Recalling the identity, for positive $\alpha_\varepsilon, \beta_\varepsilon$

$$\limsup_{\varepsilon\to 0} \varepsilon \log \Big(\alpha_\varepsilon + \beta_\varepsilon \Big) = \limsup_{\varepsilon\to 0} \varepsilon \log \Big(\max \Big\{ \alpha_\varepsilon, \beta_\varepsilon \Big\} \Big),$$

and appealing to the LDP satisfied by $Y^{n,\varepsilon}$, we are left with

$$\lim_{n\to\infty} \limsup_{\varepsilon\to 0} \varepsilon \log \Big(\mathbb{P}\Big[\sup_{t\in[0,T]} \|Y_t^\varepsilon - Y_t^{n,\varepsilon}\| \geq \delta \Big] \Big) \leq \lim_{n\to\infty} \limsup_{\varepsilon\to 0} \varepsilon \log \Big(\mathbb{P}\Big[\sup_{t\in[0,T]} \|Y_t^{n,\varepsilon}\| \geq R \Big] \Big)$$
$$\leq \lim_{n\to\infty} - \inf_{\phi\in C_{x_0}([0,T];\mathbb{R}^d) : \sup_{t\in[0,T]} \|\phi(t)\| \geq R} I_{x_0}^{n,T}(\phi).$$

Hence to conclude (5.4.11) we show that

$$\lim_{R\to\infty} \lim_{n\to\infty} \inf_{\phi\in C_{x_0}([0,T];\mathbb{R}^d) : \sup_{t\in[0,T]} \|\phi(t)\| \geq R} I_{x_0}^{n,T}(\phi) = \infty. \tag{5.4.12}$$

Indeed, let $\phi \in C_{x_0}([0,T];\mathbb{R}^d)$ be such that $\sup_{s\in[0,T]} \|\phi(s)\| \geq R$. Let $h \in \mathcal{H}_1^0$ be a function such that $H^n[h] = \phi$, recall that if $h \notin \mathcal{H}_1^0$ we immediately have that $I'(h) = \infty$. Via a concatenation argument it is simple to show that we can assume the path ϕ is increasing on $[0,T]$. Assuming ϕ is increasing we have $\forall s_1 \leq s_2$ the bound

$$\|\phi(s_1) - x_0\| \leq 3\|\phi(s_2) - x_0\| + 2\|x_0\|. \tag{5.4.13}$$

Note that

$$\|\phi(t) - x_0\|^2 = 2\int_0^t \Big\langle \phi(s) - x_0, b(s, \phi(s), \delta_{\psi(s)}) + f(\phi(s) - \delta_{\psi(s)}) \Big\rangle ds$$
$$+ \int_0^t \Big\langle \phi(s) - x_0, \sigma(\check{s}, \phi(\check{s}), \delta_{\psi(\check{s})}) \frac{n}{T} \Big(h(\hat{s}) - h(\check{s}) \Big) \Big\rangle ds$$
$$- 2\int_0^t \Big\langle \phi(s) - x_0, \mathbf{n}(\phi(s)) \Big\rangle |k^{h,n}|_s.$$

By Cauchy–Schwarz and the one-sided Lipschitz properties of b and f we can bound the drift term by

$$\begin{aligned}&\Big\langle \phi(s)-x_0, b(s,\phi(s),\delta_{\psi(s)})+f(h(s)-\delta_{\psi(s)})\Big\rangle\\&\quad\leq 2(L+2)\|\phi(s)-x_0\|^2+2\|f(x_0-\delta_{\psi(s)})\|^2+2\|b(s,x_0,\delta_{\psi(s)})\|^2.\end{aligned}$$

Using this bound, the integrability conditions of f and b, and Lemma 5.2.4 we have for a constant $c_1 = c_1(L,x_0)$ independent of t

$$\begin{aligned}\|\phi(t)-x_0\|^2 &= c_1\Big(1+\int_0^t\|\phi(s)-x_0\|^2ds\Big)\\&\quad+\int_0^t\Big\langle\phi(s)-x_0,\sigma(\check{s},\phi(\check{s}),\delta_{\check{s}})\frac{n}{T}\Big(h(\hat{s})-h(\check{s})\Big)\Big\rangle ds.\end{aligned}\tag{5.4.14}$$

We can further bound the above term by noting that for any vector $a\in\mathbb{R}^d$,

$$\begin{aligned}\Big\langle\phi(s)-x_0,\sigma(\check{s},\phi(\check{s}),\delta_{\check{s}})a\Big\rangle \leq & L\|\phi(s)-x_0\|\|\phi(\check{s})-x_0\|\|a\|\\&+\|\phi(s)-x_0\|\|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\|\|a\|.\end{aligned}$$

Since $\check{s}\leq s$ employing (5.4.13), and $c<c^2+1$ for $c\in\mathbb{R}$,we have for a constant $c_2=c_2(L,x_0)$ independent of t, n

$$\begin{aligned}\Big\langle\phi(s)-x_0,\sigma(\check{s},\phi(\check{s}),\delta_{\psi(\check{s})})a\Big\rangle \leq & c_2\Bigg(\|\phi(s)-x_0\|^2\Big(\|a\|+\|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\|\|a\|\Big)\\&+\|a\|+\|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\|\|a\|\Bigg).\end{aligned}$$

Setting

$$a=\frac{n}{T}\Big(h(\hat{s})-h(\check{s})\Big)=\frac{n}{T}\int_{\check{s}}^{\hat{s}}\dot{h}(u)du,$$

and substituting this bound into (5.4.14), we get that for a constant $c=c(L,x_0)$ independent of t or n

$$\begin{aligned}\|\phi(t)-x_0\|^2 \leq & c\Bigg(\int_0^t\Big\|\frac{n}{T}\int_{\check{s}}^{\hat{s}}\dot{h}(u)du\Big\|+\Big\|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\Big\|\Big\|\frac{n}{T}\int_{\check{s}}^{\hat{s}}\dot{h}(u)du\Big\|ds\\&+\int_0^t\|\phi(s)-x_0\|^2\Big(1+\Big\|\frac{n}{T}\int_{\check{s}}^{\hat{s}}\dot{h}(u)du\Big\|+\Big\|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\Big\|\Big\|\frac{n}{T}\int_{\check{s}}^{\hat{s}}\dot{h}(u)du\Big\|\Big)ds\Bigg).\end{aligned}\tag{5.4.15}$$

Also note that we have

$$\frac{n}{T}\int_0^t\int_{\check{s}}^{\hat{s}}\|\dot{h}(u)\|duds\leq\int_0^T\|\dot{h}(s)\|ds,$$

and similarly

$$\begin{aligned}\frac{n}{T}\int_0^t\|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\|\int_{\check{s}}^{\hat{s}}\|\dot{h}(u)\|duds =& \frac{n}{T}\int_0^t\int_{\check{s}}^{\hat{s}}\|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\|\|\dot{h}(u)\|duds\\ \leq & \int_0^T\|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\|\|\dot{h}(s)\|ds.\end{aligned}$$

By applying to Grönwall's Inequality in (5.4.15), and using the previous two observations, we have

$$\|\phi(t)-x_0\|^2 \le c\Bigg(\int_0^T \|\dot{h}(s)\| + \|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\|\|\dot{h}(s)\|ds \\ \cdot \exp\left(c\int_0^T 1+\|\dot{h}(s)\|+\|\sigma(\check{s},x_0,\delta_{\psi(\check{s})})\|\|\dot{h}(s)\|ds\right)\Bigg).$$

Now adding and subtracting the terms $\|\sigma(s,x_0,\delta_{\psi(\check{s})})\|, \|\sigma(\check{s},x_0,\delta_{\psi(s)})\|$, using the Triangle Inequality, Cauchy-Schwarz's inequality, the continuity of ψ, and recalling the Assumption 5.4.1 we obtain (5.4.12). $\square$

Lemma 5.4.12. Let Y^ε be the solution to (5.4.7). Then Y^ε satisfies an LDP on the space $C_{x_0}([0,T];\mathbb{R}^d)$ with the good rate function

$$I_{x_0}^T(\phi) = \inf_{\{h\in\mathcal{H}_1^0\,:\,H[h]=\phi\}} I'(h), \tag{5.4.16}$$

where the skeleton operator H was defined in (5.4.4).

Proof. The proof will follow by appealing to [DZ98, Theorem 4.2.23]. That is we need to show that for every $\alpha>0$

$$\lim_{n\to\infty}\sup_{\{h\in\mathcal{H}_1^0\,:\,\|h\|_{\mathcal{H}_1^0}<\alpha\}} \|H^n[h]-H[h]\| = 0. \tag{5.4.17}$$

Fix $\alpha<\infty$, $h\in\mathcal{H}_1^0$ with $\|h\|_{\mathcal{H}_1^0}<\alpha$. Denote $\phi^n = H^n(h)$, $\phi = H(h)$. Now by the one-sided Lipschitz property of the drift and Lemma 5.2.4,

$$\|\phi^n(t)-\phi(t)\|^2 \le 2\int_0^t \Big\langle \phi^n(s)-\phi(s), \sigma(\check{s},\phi^n(\check{s}),\delta_{\psi(\check{s})}h_n(s) \\ -\sigma\Big(s,\phi(s),\delta_{\psi(s)}\Big)\dot{h}(s)\Big\rangle ds + \int_0^t 4L\|\phi^n(s)-\phi(s)\|^2 ds, \tag{5.4.18}$$

where we have denoted $h_n(s) \coloneqq \frac{n}{T}\Big(h(\hat{s})-h(\check{s})\Big)$. Next notice that

$$\begin{aligned}\Big\|\sigma(\check{s},\phi^n(\check{s}),\delta_{\psi(\check{s})})-\sigma(s,\phi(s),\delta_{\psi(s)})\Big\| \le& \Big\|\sigma(\check{s},\phi^n(\check{s}),\delta_{\psi(\check{s})})-\sigma(s,\phi^n(\check{s}),\delta_{\psi(\check{s})})\Big\| \\ &+\Big\|\sigma(s,\phi^n(\check{s}),\delta_{\psi(\check{s})})-\sigma(s,\phi^n(\check{s}),\delta_{\psi(s)})\Big\| \\ &+\Big\|\sigma(s,\phi^n(\check{s}),\delta_{\psi(s)})-\sigma(s,\phi(s),\delta_{\psi(s)})\Big\| \\ \le& \rho^n(s)+L\|\phi^n(s)-\phi(s)\|,\end{aligned}$$

where $\sup_{s\in[0,T]}\rho^n(s) \underset{n\to\infty}{\to} 0$, by continuity of ψ and the Assumption 5.4.1. Hence

$$\Big\|\sigma(\check{s},\phi^n(\check{s}),\delta_{\psi(\check{s})})h_n(s)-\sigma\Big(s,\phi(s),\delta_{\psi(s)}\Big)\dot{h}(s)\Big\| \\ \le(\rho^n(s)+L\|\phi^n(s)-\phi(s)\|)\|h_n(s)\|+\|\sigma(s,\phi(s),\delta_{\psi(s)})\|\|\dot{h}(s)-h_n(s)\|.$$

Substituting this bound into (5.4.18) and applying Grönwall we get that for a constant c independent of n or t,

$$\begin{aligned}\|\phi^n(t)-\phi(t)\|^2 \le& c\exp\left(c\int_0^t 1+(\rho^n(s)+1)\|h_n(s)\|+\|\sigma(s,\phi(s),\delta_{\psi(s)})\|\cdot\|\dot{h}(s)-h_n(s)\|ds\right) \\ &\cdot\int_0^t(\rho^n(s)+1)\|h_n(s)\|+\|\sigma(s,\phi(s),\delta_{\psi(s)})\|\cdot\|\dot{h}(s)-h_n(s)\|ds \\ \le& c\exp\left(c\int_0^t 1+(\rho^n(s)+1)\cdot(\|\dot{h}(s)\|+\|h_n(s)-\dot{h}(s)\|)+\|\sigma(s,\phi(s),\delta_{\psi(s)})\|\cdot\|\dot{h}(s)-h_n(s)\|ds\right) \\ &\cdot\int_0^t(\rho^n(s)+1)\|\dot{h}(s)\|+(\rho^n(s)+1)\|h_n(s)-\dot{h}(s)\|+\|\sigma(s,\phi(s),\delta_{\psi(s)})\|\cdot\|\dot{h}(s)-h_n(s)\|ds.\end{aligned}$$

Applying Cauchy–Schwarz on the $\|\sigma(s,\phi(s),\delta_{\psi(s)})\|\cdot\|\dot{h}(s)-h_n(s)\|$ terms and sending $n\to\infty$ gives (5.4.17). The LDP for Y^ϵ with rate function (5.4.16) now follows by appealing to [DZ98, Theorem 4.2.23] and the fact that $Y^{n,\varepsilon}$ are exponentially good approximations of Y^ε Lemma 5.4.11. □

5.4.3 Freidlin-Wentzell results for reflected McKean-Vlasov equations

Next we pass the LDP from the process Y^ε to X^ε using exponential equivalence.

Theorem 5.4.13. Let $x_0^\varepsilon\in\mathbb{R}^d$, converge to $x_0\in\mathbb{R}^d$ as $\varepsilon\to 0$. Let Y^ε be the solution to (5.4.7), ψ^{x_0} the solution of (5.4.3), and X^ε be the solution to Equation (5.4.2) started at $X_0^\varepsilon=x_0^\varepsilon$. Then the reflected McKean-Vlasov equation X^ε satisfies an LDP on $C_{x_0}([0,T];\mathbb{R}^d)$ with rate function (5.4.16).

Proof. Firstly, one can quickly verify that $\|\psi^{x_0^\varepsilon}(t)-\psi^{x_0}(t)\|\underset{\varepsilon\to 0}{\to}0$. Let $Z_t^\varepsilon:=X_t^\varepsilon-Y_t^\varepsilon$. Then Z^ε satisfies

$$Z_t^\varepsilon=z_0+\int_0^t b_s ds+\int_0^t\sigma_s ds+k_t^{Y,\varepsilon}-k_t^\varepsilon,$$

where $z_0:=x_0^\epsilon-x_0$, $\sigma_t:=\sigma\big(t,X_t^\varepsilon,\mu_t^\varepsilon\big)-\sigma\big(t,Y_t^\varepsilon,\delta_{\psi^{x_0}(t)}\big)$ and

$$b_t:=b\Big(t,X_t^\varepsilon,\mu_t^\varepsilon\Big)-b\Big(t,Y_t^\varepsilon,\delta_{\psi^{x_0}(t)}\Big)+\int_{\mathbb{R}^d}f(X_t^\varepsilon-x)d\mu_t^\varepsilon-f(Y_t^\varepsilon-\psi^{x_0}(t)).$$

Let $R>0$ be large enough so that $x_0^\varepsilon,y\in B_{R+1}(0)$, and $\psi^{x_0}(t)$ does not leave $B_{R+1}(0)$ up to time T. We are able to do since ψ is non-explosive. Let $\tau_{R+1}:=\min\Big\{T,\inf\{t\geq 0:\|X_t^\varepsilon\|\geq R+1\},\inf\{t\geq 0:\|Y_t^\varepsilon\|\geq R+1\}\Big\}$. Notice that for all $t\in[0,\tau_{R+1}]$ we have

$$\begin{aligned}\Big\|b\Big(t,X_t^\varepsilon,\mu_t^\varepsilon\Big)&-b\Big(t,Y_t^\varepsilon,\delta_{\psi^{x_0}(t)}\Big)\Big\|\\&\leq\Big\|b\Big(t,X_t^\varepsilon,\mu_t^\varepsilon\Big)-b\Big(t,X_t^\varepsilon,\delta_{\psi^{x_0^\varepsilon}(t)}\Big)\Big\|+\Big\|b\Big(t,X_t^\varepsilon,\delta_{\psi^{x_0^\varepsilon}(t)}\Big)-b\Big(t,X_t^\varepsilon,\delta_{\psi^{x_0}(t)}\Big)\Big\|\\&\quad+\Big\|b\Big(t,X_t^\varepsilon,\delta_{\psi^{x_0}(t)}\Big)-b\Big(t,Y_t^\varepsilon,\delta_{\psi^{x_0}(t)}\Big)\Big\|\\&\leq L\mathbb{E}\Big[\|X_t^\varepsilon-\psi^{x_0^\varepsilon}(t)\|^2\Big]^{\frac{1}{2}}+L\|\psi^{x_0^\varepsilon}(t)-\psi^{x_0}(t)\|+L_R\|X_t^\varepsilon-Y_t^\varepsilon\|.\end{aligned}$$

Hence

$$\Big\|b\Big(t,X_t^\varepsilon,\mu_t^\varepsilon\Big)-b\Big(t,Y_t^\varepsilon,\delta_{\psi^{x_0}(t)}\Big)\Big\|\leq B_R^1\big(\rho^1(\varepsilon)+\|Z_t^\varepsilon\|^2\big)^{\frac{1}{2}},$$

for a constant B_R^1 large enough, and $\rho^1(\varepsilon):=\mathbb{E}\|X_t^\varepsilon-\psi^{x_0^\varepsilon}(t)\|^2+\|\psi^{x_0^\varepsilon}(t)-\psi^{x_0}(t)\|\underset{\varepsilon\to 0}{\to}0$ by (5.4.5). Furthermore for $t\in[0,\tau_{R+1}]$ we also have

$$\begin{aligned}\Big\|\int_{\mathbb{R}^d}&f(X_t^\varepsilon-x)d\mu_t^\varepsilon-f(Y_t^\varepsilon-\psi^{x_0}(t))\Big\|\\&\leq\Big\|\int_{\mathbb{R}^d}f(X_t^\varepsilon-x)-f(X_t^\varepsilon-\psi^{x_0^\varepsilon}(t))\Big\|+\Big\|f(X_t^\varepsilon-\psi^{x_0^\varepsilon}(t))-f(X_t^\varepsilon-\psi^{x_0}(t))\Big\|\\&\quad+\Big\|f(X_t^\varepsilon-\psi^{x_0}(t))-f(Y_t^\varepsilon-\psi^{x_0}(t))\Big\|\\&\leq\Big\|\int_{\mathbb{R}^d}f(X_t^\varepsilon-x)d\mu_t^\varepsilon-f(X-\psi^{x_0^\varepsilon}(t))\Big\|+L_R\Big\|\psi^{x_0^\varepsilon}(t)-\psi^{x_0}(t)\Big\|+L_R\|Z_t\|.\end{aligned}$$

Hence

$$\|b_t\|\leq B_R^2\Big(\rho^2(\varepsilon)+\|Z_t\|^2\Big)^{\frac{1}{2}},$$

for a constant B_R^2 and $\rho^2(\varepsilon) := \| \int_{\mathbb{R}^d} f(X_t^\varepsilon - x)d\mu_t^\varepsilon - f(X - \psi^{x_0^\varepsilon}(t))\| + \|\psi^{x_0^\varepsilon}(t) - \psi^{x_0}(t)\| \underset{\varepsilon\to 0}{\to} 0$, thanks to (5.4.6). Now for the diffusion term,

$$\begin{aligned}\|\sigma_t\| \le & \Big\|\sigma\Big(t, X_t^\varepsilon, \mu_t^\varepsilon\Big) - \sigma\Big(t, X_t^\varepsilon, \delta_{\psi^{x_0^\varepsilon}(t)}\Big)\Big\| + \Big\|\sigma\Big(t, X_t^\varepsilon, \delta_{\psi^{x_0^\varepsilon}(t)}\Big) - \sigma\Big(t, X_t^\varepsilon, \delta_{\psi^{x_0}(t)}\Big)\Big\| \\ & + \Big\|\sigma\Big(t, X_t^\varepsilon, \delta_{\psi^{x_0}(t)}\Big) - \sigma\Big(t, Y_t^\varepsilon, \delta_{\psi^{x_0}(t)}\Big)\Big\| \\ \le & L\Big(\mathbb{E}\Big[\|X_t^\varepsilon - \psi^{x_0^\varepsilon}(t)\|^2\Big]^{\frac{1}{2}} + \|\psi^{x_0^\varepsilon}(t) - \psi^{x_0}(t)\| + \|X_t^\varepsilon - Y_t^\varepsilon\|\Big).\end{aligned}$$

Hence

$$\|\sigma_t\| \le M\big(\rho(\varepsilon) + \|Z_t^\varepsilon\|^2\big)^{\frac{1}{2}}, \tag{5.4.19}$$

for a constant M and $\rho(\varepsilon) \underset{\varepsilon\to 0}{\to} 0$.

Now fix $\delta > 0$ and notice that

$$\begin{aligned}\Big\{\sup_{t\in[0,T]} \|X_t^\varepsilon - Y_t^\varepsilon\| \ge \delta\Big\} \subseteq & \Big\{\sup_{t\in[0,\tau_{R+1}]} \|X_t^\varepsilon - Y_t^\varepsilon\| \ge \delta, \tau_{R+1} = T\Big\} \cup \Big\{\sup_{t\in[0,T]} \|X_t^\varepsilon - Y_t^\varepsilon\| \ge \delta, \tau_{R+1} < T\Big\} \\ \subseteq & \Big\{\sup_{t\in[0,\tau_{R+1}]} \|X_t^\varepsilon - Y_t^\varepsilon\| \ge \delta\Big\} \cup \Big\{\tau_{R+1} < T\Big\}.\end{aligned}$$

By Lemma 5.A.1 we know that

$$\limsup_{\varepsilon\to 0} \varepsilon \log\Big(\mathbb{P}\Big[\sup_{t\in[0,\tau_{R+1}]} \|X_t^\varepsilon - Y_t^\varepsilon\| \ge \delta\Big]\Big) = -\infty.$$

Furthermore, define $\tau_R^Y := \inf\{t \ge 0 : \|Y_t^\varepsilon\| \ge R\}$, and notice that

$$\begin{aligned}\Big\{\tau_{R+1} < T\Big\} \subseteq & \Big\{\tau_{R+1} < T, \tau_R^Y \le T\Big\} \cup \Big\{\tau_{R+1} < T, \tau_R^Y > T\Big\} \\ \subseteq & \Big\{\tau_{R+1} < T\Big\} \cup \Big\{\|X_{\tau_R^Y}^\varepsilon - Y_{\tau_{R+1}}^\varepsilon\| \ge 1\Big\}.\end{aligned}$$

Again, setting $\delta = 1$ and using Lemma 5.A.1, we have that

$$\limsup_{\varepsilon\to 0} \varepsilon \log\Big(\mathbb{P}\Big[\sup_{t\in[0,\tau_{R+1}]} \|X_t^\varepsilon - Y_t^\varepsilon\| \ge 1\Big]\Big) = -\infty,$$

hence are left with

$$\limsup_{\varepsilon\to 0} \varepsilon \log\Big(\mathbb{P}\Big[\sup_{t\in[0,T]} \|X_t^\varepsilon - Y_t^\varepsilon\| \ge \delta\Big]\Big) \le \limsup_{\varepsilon\to 0} \varepsilon \log\Big(\mathbb{P}\Big[\sup_{t\in[0,T]} \|Y_t^\varepsilon\| \ge R\Big]\Big).$$

Applying the LDP proved for Y^ε in Lemma 5.4.12 we conclude,

$$\begin{aligned}&\limsup_{\varepsilon\to 0} \varepsilon \log\Big(\mathbb{P}\Big[\sup_{t\in[0,T]} \|X_t^\varepsilon - Y_t^\varepsilon\| \ge \delta\Big]\Big) \\ &\qquad \le - \inf_{\{\phi\in C_{x_0}([0,T];\mathbb{R}^d, \,:\, \sup_{t\in[0,T]} \|\phi(t)\| \ge R\}} I_{x_0}^T(\phi) \underset{R\to\infty}{\longrightarrow} -\infty,\end{aligned}$$

by the same arguments as the end of the proof of Lemma 5.4.11. ☐

An immediate consequence (choosing $x_0^\varepsilon = x_0$) we have an LDP for our reflected McKean-Vlasov equation's solution X^ε of (5.4.2) with $X_0^\varepsilon = x_0$. The point of allowing ε-dependent initial conditions for X^ε enables us to claim the LDP uniformly on compacts, similarly to [HIP08, Corollary 3.5], or [HIPP14, Propositions 4.6 and 4.8]. We provide a statement and a brief proof, the full justification is identical to those found in [HIP08, HIPP14].

Corollary 5.4.14. Let $\mathbb{P}_{x_0}[X^\varepsilon \in \cdot]$ be the law on $C_{x_0}([0,T];\mathbb{R}^d)$ of the solution X^ε to (5.4.2) with $X_0^\varepsilon = x_0$. Let $M \subset \mathbb{R}^d$ be a compact subset. Then, for any Borel set $A \subset C([0,T];\mathbb{R}^d)$, we have

$$\liminf_{\varepsilon\to 0} \varepsilon \log \sup_{x_0\in M} \mathbb{P}_{x_0}[X^\varepsilon \in A] \le - \inf_{x_0\in M} \inf_{\phi\in\overline{A}} I^T_{x_0}(\phi), \tag{5.4.20}$$

and

$$\liminf_{\varepsilon\to 0} \varepsilon \log \inf_{x_0\in M} \mathbb{P}_{x_0}[X^\varepsilon \in A] \ge - \sup_{x_0\in M} \inf_{\phi\in A^\circ} I^T_{x_0}(\phi). \tag{5.4.21}$$

Proof. Allowing ε-dependent initial conditions, implies that (otherwise we would contradict the LDP)

$$\limsup_{\substack{\varepsilon\to 0\\ x_\varepsilon\to x_0}} \varepsilon \log \mathbb{P}_{x_\varepsilon}[X^\varepsilon \in A] \le - \inf_{\phi\in\overline{A}} I^T_{x_0}(\phi),$$

then arguing as in [DZ98, Corollary 5.6.15] yields (5.4.20). The lower bound (5.4.21) is done similarly. $\square$

Furthermore, proceeding like in [HIP08] we could obtain uniform on compacts LDP for the process X^ε started at some later time $s > 0$, and initial condition x_s^ε. Such uniform LDP can be useful when obtaining exit-time results in the manner of [HIP08]. However we will not need them, and instead obtain exit-time results by the method of [Tug16].

5.5 Exit-time

In this section we obtain a characterisation of the exit-time of X^ε from an open subdomain $\mathfrak{D} \subset \mathcal{D}$ under several additional assumptions: strict convexity of potentials, the diffusion matrix is the identity matrix and time-homogeneity of the coefficients. These are motivated by applications (like [DGLLPN17, DGLLPN19]) where the exit-cost of the diffusion from a domain needs to be computed explicitly, here we refer to Δ in Theorem 5.5.11. The results obtained in this section are, from a methodological point of view, inspired by [Tug16].

Let us start by introducing the process of interest $(X_t^\varepsilon)_{t\ge 0}$ over $\mathbb{R}^d$ with dynamics

$$\begin{aligned} X_t^\varepsilon &= x_0 + \int_0^t b(X_s^\varepsilon)ds + \int_0^t f * \mu_s^\varepsilon(X_s^\varepsilon)ds + \sqrt{\varepsilon}W_t - k_t^\varepsilon, \quad \mathbb{P}\big[X_t^\varepsilon \in dx\big] = \mu_t^\varepsilon(dx), \\ |k^\varepsilon|_t &= \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^\varepsilon) d|k^\varepsilon|_s, \qquad k_t^\varepsilon = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^\varepsilon)\mathbf{n}(X_s^\varepsilon) d|k^\varepsilon|_s. \end{aligned} \tag{5.5.1}$$

Assumption 5.5.1. Let $\mathcal{D}$ satisfy Assumption 5.2.5. Let $r > 1$ and let $b : \mathcal{D} \to \mathbb{R}^d$, $f : \mathbb{R}^d \to \mathbb{R}^d$ satisfy

- There exist functions $B : \mathcal{D} \to \mathbb{R}$ and $F : \mathbb{R}^d \to \mathbb{R}$ such that

$$b(x) = \nabla B(x), \quad f(x) = \nabla F(x),$$

- B is uniformly strictly concave, $\exists L > 0$ such that $\forall x, y \in \mathcal{D}$,

$$\big\langle x - y, b(x) - b(y)\big\rangle \le -L\|x - y\|^2,$$

- $\exists G : \mathbb{R} \to \mathbb{R}$ a convex even polynomial such that $F(x) = G(\|x\|)$ of order r where

$$G(\|x\|) < C(1 + \|x\|^r),$$

  and $\forall x, y \in \mathbb{R}^d$ we have $\big\langle x - y, f(x) - f(y)\big\rangle \le 0$,

- $\exists \tilde{x} \in \mathcal{D}^\circ$ such that $\inf_{x\in\mathcal{D}} \|b(x)\| = \|b(\tilde{x})\| = 0$.

We study the metastability of the system around $\tilde{x}$ within the domain $\mathfrak{D}$. Intuitively, the dynamics of the process are similar to those of the non-reflected case, so that in the small noise limit the process spends most of its time around the stable point $\tilde{x}$ and with a high probability excursions from the stable point promptly return to it. Therefore, the only way to leave the domain $\mathfrak{D}$ is to receive a large shock from the driving noise, which is expected to take a long time to happen.

Definition 5.5.2. Let $\mathcal{G}$ be a subset of $\mathcal{D}$ and let $U : \mathcal{D} \to \mathbb{R}^d$. For all $x \in \mathcal{D}$, let φ be the dynamical system

$$\mathbb{R}^+ \ni t \mapsto \varphi_t(x) = x + \int_0^t U(\varphi_s(x))ds.$$

We say that the domain $\mathcal{G}$ is *stable by U* if $\forall x \in \mathcal{G}$,

$$\Big\{\varphi_t(x) : \ t \in \mathbb{R}^+\Big\} \subset \mathcal{G}.$$

This is also referred to as "positively invariant" in other works. We now introduce supplementary assumptions on the domain $\mathfrak{D}$ in order to obtain the exit-time. The first one is slightly different from the one in [HIP08] as we do not assume that $\mathfrak{D}$ is stable by b but instead we work with the following.

Assumption 5.5.3. Let $\mathfrak{D} \subset \mathcal{D}$ be an open, connected set containing $\tilde{x}$ such that $\overline{\mathfrak{D}} \subset \mathcal{D}$ and $\partial\mathcal{D} \cap \mathfrak{D} = \emptyset$.
Let $x_0 \in \mathfrak{D}$. Let $\psi_t = x_0 + \int_0^t b(\psi_s)ds$. The orbit

$$\Big\{\psi_t : t \in \mathbb{R}^+\Big\} \subset \mathfrak{D}.$$

Further domain $\mathfrak{D}$ is stable by $b(\cdot) + f(\cdot - \tilde{x})$.

Roughly speaking, when the time is small, the reflected self-stabilizing diffusion behaves like the dynamical system $\{\psi_t\}_{t\in[0,T]}$. As a consequence, and in order to have a non-trivial exit-time, we assume that the orbit of the dynamical system without noise stays in the domain $\mathfrak{D}$.

After a long time, the reflected self-stabilizing diffusion stays close to a linear reflected diffusion with potential $B(\cdot) + F * \delta_{\tilde{x}}$. It is then natural to assume that the domain is stable by $b(\cdot) + f(\cdot - \tilde{x})$.

Definition 5.5.4. Let $x \in \mathcal{D}$. Let $r > 1$ and let $\kappa > 0$. Let $\mathbb{B}_x^{\kappa,r} \subset \mathcal{P}_r(\mathcal{D})$ denote the set of all the probability measures such that

$$\int_{\mathcal{D}} \|y - x\|^r \mu(dy) \leq \kappa^r.$$

We study the distribution of the following stopping time.

Definition 5.5.5. Let $\mathfrak{D} \subset \mathbb{R}^d$, $x_0, \tilde{x} \in \mathbb{R}^d$ satisfy Assumption 5.5.3. Let $\varepsilon > 0$ and let X^ε be the solution to (5.5.1).

Define the exit-time $\tau_{\mathfrak{D}}(\varepsilon)$ of X^ε from the domain $\mathfrak{D}$ as

$$\tau_{\mathfrak{D}}(\varepsilon) := \inf\Big\{t \geq 0 : X_t^\varepsilon \notin \mathfrak{D}\Big\}.$$

Within classical SDE theory, there is no difference between the reflected and the non-reflected process since the exit domain $\mathfrak{D}$ is necessarily contained in the domain of constraint $\mathcal{D}$. This is not the case for McKean-Vlasov equations where the reflective term acts on the law to ensure it remains on the domain $\mathcal{D}$ and is thus different from the law of the non-reflected McKean-Vlasov. In the language of particle systems, see (5.1.3), each particle i is additionally affected by the reflections of all other particles $j \neq i$.

One of our contributions here is to rigorously argue that although the law of the reflected process and the law of the non-reflected process are different, the difference *does not* affect the distribution of the exit-time $\tau_{\mathfrak{D}}(\varepsilon)$. Further, we remark that the results of Sections 5.5.1, 5.5.2 and 5.5.3 typically hold under much broader conditions than those of Assumption 5.5.1. This not the case for the proof of Theorem 5.5.11 which relies on classical methods and so determines the scope of our results.

5.5.1 Control of the moments

In this section, we study the distance between the law of the process at time t and the Dirac measure at $\tilde{x}$.

Definition 5.5.6. Let $\mathcal{D}$ satisfy Assumption 5.2.5. Let W be a d-dimensional Brownian motion and let $r > 1$, b, f, x_0 and $\tilde{x}$ satisfy Assumption 5.5.1. Let X^ε be the solution to Equation (5.5.1). Define $\xi_\varepsilon^r : \mathbb{R}_+ \to \mathbb{R}_+$ to be

$$\xi_\varepsilon^r(t) := \mathbb{E}\Big[\|X_t^\varepsilon - \tilde{x}\|^r\Big].$$

For $\kappa > 0$, define

$$T^{\kappa,r}(\varepsilon) := \min\Big\{t \geq 0 : \xi_\varepsilon^r(t) \leq \kappa^r\Big\}.$$

Proposition 5.5.7. We have

$$\sup_{t\in\mathbb{R}^+} \xi_\varepsilon^r(t) \leq \max\Big\{\|x_0 - \tilde{x}\|^r, \Big(\tfrac{d\varepsilon(r-1)}{2L}\Big)^{r/2}\Big\}.$$

For $\varepsilon < \frac{\kappa^2 L}{d(r-1)}$, we have

$$T^{\kappa,r}(\varepsilon) \leq \tfrac{1}{rL}\log\Big(\tfrac{2\|x_0-\tilde{x}\|}{\kappa^2} - 1\Big).$$

Finally, for all $t \geq T^{\kappa,r}(\varepsilon)$ with $\varepsilon < \frac{\kappa^2 L}{2r-1}$ we have $\xi_\varepsilon(t) \leq \kappa^{2r}$.

Proof. Let $t \in \mathbb{R}_+$. We apply the Itô formula, integrate, take expectations and then the derivative in time. We obtain

$$\begin{aligned}
\xi_\varepsilon^r(t) =& \mathbb{E}\Big[\|x_0 - \tilde{x}\|^r\Big] \\
&+ \int_0^t r\mathbb{E}\Big[\|X_s^\varepsilon - \tilde{x}\|^{r-2}\Big\langle X_s^\varepsilon - \tilde{x}, b(X_s^\varepsilon)\Big\rangle\Big] + r\mathbb{E}\Big[\|X_s^\varepsilon - \tilde{x}\|^{r-2}\Big\langle X_s^\varepsilon - \tilde{x}, f * \mu_s^\varepsilon(X_s^\varepsilon)\Big\rangle\Big]ds \\
&+ \frac{dr(r-1)}{2}\varepsilon\int_0^t \mathbb{E}\Big[\|X_s^\varepsilon - \tilde{x}\|^{r-2}\Big]ds - r\mathbb{E}\Big[\int_0^t \|X_s^\varepsilon - \tilde{x}\|^{r-1}\Big\langle X_s^\varepsilon - \tilde{x}, dk_s^\varepsilon\Big\rangle\Big].
\end{aligned}$$

Using the uniform strict concavity of B, we get

$$r\int_0^t \mathbb{E}\Big[\|X_s^\varepsilon - \tilde{x}\|^{r-2}\Big\langle X_s^\varepsilon - \tilde{x}, b(X_s^\varepsilon)\Big\rangle\Big]ds \leq -rL\int_0^t \xi_\varepsilon^r(s)ds.$$

Next, denoting by $\overline{X_t^\varepsilon}$ an independent version of X_t^ε and G the concave even polynomial such that $F(x) = G(\|x\|)$, we get

$$\begin{aligned}
& r\int_0^t \mathbb{E}\left[\|X_s^\varepsilon - \tilde{x}\|^{r-2}\frac{G'\big(\|X_s^\varepsilon - \overline{X_s^\varepsilon}\|\big)}{\|X_s^\varepsilon - \overline{X_s^\varepsilon}\|}\Big\langle X_s^\varepsilon - \overline{X_s^\varepsilon}, X_s^\varepsilon - \tilde{x}\Big\rangle\right] \\
&= r\int_0^t \mathbb{E}\left[\frac{G'\big(\|X_s^\varepsilon - \overline{X_s^\varepsilon}\|\big)}{\|X_s^\varepsilon - \overline{X_s^\varepsilon}\|}\Big\langle \big(X_s^\varepsilon - \tilde{x}\big) - \big(\overline{X_s^\varepsilon} - \tilde{x}\big), \big(X_s^\varepsilon - \tilde{x}\big)\|X_s^\varepsilon - \tilde{x}\|^{r-2}\Big\rangle\right]ds \\
&= \frac{r}{2}\int_0^t \mathbb{E}\left[\frac{G'\big(\|X_s^\varepsilon - \overline{X_s^\varepsilon}\|\big)}{\|X_s^\varepsilon - \overline{X_s^\varepsilon}\|}\Big\langle \big(X_s^\varepsilon - \tilde{x}\big) - \big(\overline{X_s^\varepsilon} - \tilde{x}\big), \big(X_s^\varepsilon - \tilde{x}\big)\|X_s^\varepsilon - \tilde{x}\|^{r-2} - \big(\overline{X_s^\varepsilon} - \tilde{x}\big)\|\overline{X_s^\varepsilon} - \tilde{x}\|^{r-2}\Big\rangle\right]ds \\
&\leq 0,
\end{aligned}$$

since by Cauchy–Schwarz inequality, $\forall x, y \in \mathbb{R}^d$ (see alternatively [HIP08, Lemma 2.3 (d)])

$$\big\langle x\|x\|^{r-2} - y\|y\|^{r-2}, x - y\big\rangle \geq \big(\|x\|^{r-1} - \|y\|^{r-1}\big)\big(\|x\| - \|y\|\big) \geq 0.$$

We obtain

$$\frac{d}{dt}\xi_\varepsilon^r(t) \leq -rL\cdot\xi_\varepsilon^r(t)^{1-\frac{2}{r}}\Big(\xi_\varepsilon^r(t)^{\frac{2}{r}} - \frac{d(r-1)\varepsilon}{2L}\Big).$$

Thus we get the bound

$$|\xi_\varepsilon^r(t)|^{\frac{2}{r}} \leq \max\Big\{\tfrac{d(r-1)\varepsilon}{2L}, \|x_0-\tilde{x}\|^2\Big\}.$$

Choosing $\varepsilon < \frac{\kappa^2 L}{d(r-1)}$, we see $\sup_{t\in\mathbb{R}_+}|\xi_\varepsilon^r(t)|^{\frac{2}{r}} \leq \max\Big\{\frac{\kappa^2}{2}, \|x_0-\tilde{x}\|^2\Big\}$.

Now additionally suppose that $\|x_0-\tilde{x}\|^2 > \frac{\kappa^2}{2}$ then we get the upper bound

$$|\xi_\varepsilon^r(t)|^{\frac{2}{r}} \leq \tfrac{\kappa^2}{2} + \Big(\|x_0-\tilde{x}\|^2 - \tfrac{\kappa^2}{2}\Big)\exp\Big(-rLt\Big).$$

In this case

$$T^{\kappa,r}(\varepsilon) \leq \tfrac{1}{rL}\log\Big(\tfrac{2\|x_0-\tilde{x}\|}{\kappa^2} - 1\Big).$$

Conversely, if $\|x_0-\tilde{x}\|^2 \leq \frac{\kappa^2}{2}$ then $T^{\kappa,r}(\varepsilon) = 0$. □

5.5.2 Probability of exiting before converging

Recall that after time $T^{\kappa,r}(\varepsilon)$, the process X_t^ε is expected to remain close to $\tilde{x}$. Additionally, it also happens that before time $T^{\kappa,r}(\varepsilon)$ and in the small noise limit the process X_t^ε does not leave $\mathfrak{D}$. This can be argued from the fact that the dynamical system ψ_t introduced in Assumption 5.5.3 stays in the domain $\mathfrak{D}$.

Proposition 5.5.8. Let $\tau_{\mathfrak{D}}(\varepsilon)$ be the stopping time as defined in Definition 5.5.5. Let ξ_ε^r and $T^{\kappa,r}(\varepsilon)$ be as defined in Definition 5.5.6. Then for any $\kappa > 0$ we have that

$$\lim_{\varepsilon\to 0}\mathbb{P}\Big[\tau_{\mathfrak{D}}(\varepsilon) < T^{\kappa,r}(\varepsilon)\Big] = 0.$$

Proof. Let $t \in \mathbb{R}_+$. Then,

$$\begin{aligned}\mathbb{E}\Big[\|X_t^\varepsilon - \psi_t\|^2\Big] =& \varepsilon dt + 2\int_0^t \mathbb{E}\Big[\Big\langle X_s^\varepsilon - \psi_s, b(X_s^\varepsilon) - b(\psi_s)\Big\rangle\Big]ds \\ &+ 2\int_0^t \mathbb{E}\Big[\Big\langle X_s^\varepsilon - \psi_s, f*\mu_s^\varepsilon(X_s^\varepsilon)\Big\rangle\Big]ds - 2\int_0^t \mathbb{E}\Big[\Big\langle X_s^\varepsilon - \psi_s, dk_s^\varepsilon\Big\rangle\Big].\end{aligned}$$

Using standard methods, we get

$$\mathbb{E}\Big[\|X_t^\varepsilon - \psi_t\|^2\Big] \leq \tfrac{\varepsilon d}{2L}\Big(1 - \exp\Big(-2Lt\Big)\Big).$$

Then, for any $\delta > 0$ define

$$\tau_\delta(\varepsilon) := \inf\Big\{t > 0 : \|X_t^\varepsilon - \psi_t\| > \delta\Big\}.$$

Thus for any $T > 0$,

$$\lim_{\varepsilon\to 0}\mathbb{P}\Big[\tau_\delta(\varepsilon) < T\Big] = 0.$$

We are interested in the interval $[0, T^{\kappa,r}(\varepsilon)]$, which depends on ε but has a uniform bound. Thus by Proposition 5.5.7,

$$\mathbb{P}\Big[\tau_\delta(\varepsilon) < T^{\kappa,r}(\varepsilon)\Big] \leq \mathbb{P}\Big[\tau_\delta(\varepsilon) < \tfrac{1}{rL}\log\Big(\tfrac{2\|x_0-\tilde{x}\|}{\kappa^2} - 1\Big)\Big],$$

which we just argued, goes to 0 as $\varepsilon \to 0$.

Finally, from Assumption 5.5.3, we have $\big\{\psi_t \;:\; t > 0\big\} \subset \mathfrak{D}$ and consequently for any $\kappa > 0$ we obtain the limit

$$\lim_{\varepsilon\to 0}\mathbb{P}\Big[\tau_{\mathfrak{D}}(\varepsilon) < T^{\kappa,r}(\varepsilon)\Big] = 0.$$

□

5.5.3 The coupling result

Now, we study the exit of the diffusion from the domain after the time $T^{\kappa,r}(\varepsilon)$. To do so, we use the inequality

$$\sup_{t\geq T^{\kappa,r}(\varepsilon)} \xi_\varepsilon(t) \leq \kappa^r,$$

which holds for any $\kappa > 0$ provided $\varepsilon < \frac{\kappa^2 L}{d(r-1)}$.

From this we deduce that the drift $b(\cdot) + f * \mu_t^\varepsilon(\cdot)$ is close to the vector field $b(\cdot) + f(\cdot - \tilde{x})$. Let $\mathcal{K} \subset \mathfrak{D}$ be a compact set with non-zero Lebesgue measure interior such that $\tilde{x} \in \mathfrak{D}$. We consider the following diffusion defined for $t \geq T^{\kappa,r}(\varepsilon)$ as

$$\begin{aligned} Z_t^\varepsilon =& X_{T^{\kappa,r}(\varepsilon)} + \sqrt{\varepsilon}\big(W_t - W_{T^{\kappa,r}(\varepsilon)}\big) + \int_{T^{\kappa,r}(\varepsilon)}^t b(Z_s^\varepsilon)ds + \int_{T^{\kappa,r}(\varepsilon)}^t f\big(Z_s^\varepsilon - \tilde{x}\big)ds - k_t^{Z,\varepsilon}, \\ |k^{Z,\varepsilon}|_t =& \int_{T^{\kappa,r}(\varepsilon)}^t \mathbb{1}_{\partial\mathcal{D}}(Z_s^\varepsilon)d|k^{Z,\varepsilon}|_s, \quad k_t^{Z,\varepsilon} = \int_{T^{\kappa,r}(\varepsilon)}^t \mathbb{1}_{\partial\mathcal{D}}(Z_s^\varepsilon)\mathbf{n}(Z_s^\varepsilon)d|k^{Z,\varepsilon}|_s \qquad \text{when } X^\varepsilon_{T^{\kappa,r}(\varepsilon)} \in \mathcal{K} \\ Z_t^\varepsilon =& X_t^\varepsilon \qquad \text{if } X^\varepsilon_{T^{\kappa,r}(\varepsilon)} \notin \mathcal{K}. \end{aligned} \tag{5.5.2}$$

Definition 5.5.9. Let $\mathcal{D}$ satisfy Assumption 5.2.5. Let W be a d-dimensional Brownian motion and let $r > 1$, b, f x_0 and $\tilde{x}$ satisfy Assumption 5.5.1. Let $\mathcal{K}$ be a compact set with non-zero Lebesgue measure interior that $\tilde{x} \in \mathcal{K}$ and $\mathcal{K} \subset \mathfrak{D}$. Let X^ε be the solution to Equation (5.5.1) and let Z^ε be the solution to (5.5.2).

Define the stopping times

$$\tau_{\mathcal{K},\kappa}(\varepsilon) := \inf\Big\{t > T^{\kappa,r}(\varepsilon) : X_t^\varepsilon \notin \mathcal{K}\Big\}, \qquad \tau'_{\mathcal{K},\kappa}(\varepsilon) := \inf\Big\{t > T^{\kappa,r}(\varepsilon) : Z_t^\varepsilon \notin \mathcal{K}\Big\},$$

and $\mathcal{T}_{\mathcal{K},\kappa}(\varepsilon) := \min\Big\{\tau_{\mathcal{K},\kappa}(\varepsilon), \tau'_{\mathcal{K},\kappa}(\varepsilon)\Big\}$.

The following Proposition establishes a coupling between X^ε the reflected McKean-Vlasov SDE and Z^ε the reflected SDE. That is, in the time interval $[T^{\kappa,r}(\varepsilon), \mathcal{T}_{\mathcal{K},\kappa}(\varepsilon)]$ the processes remain close to each other with high probability when the noise is small enough.

Proposition 5.5.10. Let $\mathcal{T}_{\mathcal{K},\kappa}$ be as in Definition 5.5.9. Then $\exists \kappa_0 > 0$ such that $\forall \kappa < \kappa_0$ $\exists \varepsilon_0 > 0$ such that $\forall \varepsilon < \varepsilon_0$ we have

$$\mathbb{P}\left[\sup_{T^{\kappa,r}(\varepsilon)\leq t\leq \mathcal{T}_{\mathcal{K},\kappa}(\varepsilon)} \|Z_t^\varepsilon - X_t^\varepsilon\| \geq \eta(\kappa)\right] \leq \eta(\kappa),$$

where η is some positive, continuous and increasing function such that $\eta(0) = 0$.

Proof. Let $t \in \mathbb{R}_+$. If $X_{T^{\kappa,r}(\varepsilon)} \in \mathcal{K}$ then, for all $T^{\kappa,r}(\varepsilon) \leq t \leq \mathcal{T}_\kappa(\varepsilon)$, we have

$$\begin{aligned} \|Z_t^\varepsilon - X_t^\varepsilon\|^2 =& +2\int_{T^{\kappa,r}(\varepsilon)}^t \Big\langle Z_s^\varepsilon - X_s^\varepsilon, b(Z_s^\varepsilon) - b(X_s^\varepsilon)\Big\rangle ds \\ &+ 2\int_{T^{\kappa,r}(\varepsilon)}^t \Big\langle Z_s^\varepsilon - X_s^\varepsilon, f(Z_s^\varepsilon - \tilde{x}) - f * \mu_s^\varepsilon(X_s^\varepsilon)\Big\rangle ds - 2\int_{T^{\kappa,r}(\varepsilon)}^t \Big\langle Z_s^\varepsilon - X_s^\varepsilon, dk_s^{Z,\varepsilon} - dk_s^\varepsilon\Big\rangle. \end{aligned}$$

Set

$$\eta(\kappa) := \sup_{\nu\in\mathbb{B}_{\tilde{x}}^{\kappa,r}} \sup_{x\in\mathcal{K}} \Big(\frac{\|f * \nu(x) - f(x - \tilde{x})\|}{L}\Big)^{\frac{2}{3}},$$

where $\mathbb{B}_{\tilde{x}}^{\kappa,r}$ was introduced in Definition 5.5.4. Using Assumption 5.2.5 and Grönwall Inequality, we get

$$\sup_{T^{\kappa,r}(\varepsilon)\leq t\leq \mathcal{T}_{\mathcal{K},\kappa}(\varepsilon)} \|Z_t^\varepsilon - X_t^\varepsilon\|^2 \leq \eta(\kappa)^3 \quad \Rightarrow \quad \mathbb{E}\Big[\sup_{T^{\kappa,r}(\varepsilon)\leq t\leq \mathcal{T}_{\mathcal{K},\kappa}(\varepsilon)} \|Z_t^\varepsilon - X_t^\varepsilon\|^2\Big] \leq \eta(\kappa)^3.$$

Appealing to Markov's inequality yields the claim. □

5.5.4 The Exit-time result

Let $\tilde{Z}^\varepsilon$ evolve as Z^ε without reflection, that is for $t \in [T^{\kappa,r}(\varepsilon), \infty)$,

$$\tilde{Z}^\varepsilon_t = X_{T^{\kappa,r}(\varepsilon)} + \sqrt{\varepsilon}\big(W_t - W_{T^{\kappa,r}(\varepsilon)}\big) + \int_{T^{\kappa,r}(\varepsilon)}^t b(\tilde{Z}^\varepsilon_s)ds + \int_{T^{\kappa,r}(\varepsilon)}^t f(\tilde{Z}^\varepsilon_s - \tilde{x})ds.$$

As the closure of the domain $\mathfrak{D}$ from which the process exits is included into the domain $\mathcal{D}$ where there is reflection, we remark that $Z^\varepsilon_t = \tilde{Z}^\varepsilon_t$ whilst $t \le \tau'_{\mathfrak{D}}(\varepsilon)$, where

$$\tau'_{\mathfrak{D}}(\varepsilon) := \inf\Big\{t \ge T^{\kappa,r}(\varepsilon) : \tilde{Z}^\varepsilon_t \notin \mathfrak{D}\Big\}.$$

As a consequence, the first exit-time from $\mathfrak{D}$ of the diffusion $\tilde{Z}^\varepsilon$ is the same as the first exit-time from $\mathfrak{D}$ of the diffusion Z^ε. However, the latter exit-time is well understood thanks to the classical Freidlin-Wentzell theory.

The familiar reader will recognise Δ given as

$$\Delta := \inf_{z\in\partial\mathfrak{D}} \Big\{B(z) + F(z-\tilde{x}) - B(\tilde{x})\Big\},$$

to be the exit cost from the domain $\mathfrak{D}$, see [Tug10, Proposition B.4, Item 3].

Theorem 5.5.11. Let $\mathcal{D}$ satisfy Assumption 5.2.5. Let W be a d-dimensional Brownian motion and let $r > 1$, b, f, x_0 and $\tilde{x}$ satisfy Assumption 5.5.1. Let X^ε be the solution to Equation (5.5.1). Then for all $\delta > 0$ the following limit holds

$$\lim_{\varepsilon\to 0} \mathbb{P}\left[\tfrac{2}{\varepsilon}(\Delta-\delta) < \log\Big(\tau_{\mathfrak{D}}(\varepsilon)\Big) < \tfrac{2}{\varepsilon}(\Delta+\delta)\right] = 1.$$

Proof. The proof is inspired by [Tug12], we proceed in a stepwise fashion.

Step 1. Let $\kappa > 0$ and we introduce the usual least distance of $x \in \mathbb{R}^d$ to a (non-empty) set $A \subset \mathbb{R}^d$ as $d(x;A) := \inf\{\|x-a\| : a \in A\}$. We can prove (by proceeding like in [Tug12, Proposition 2.2]) that there exist two families of domains $(\mathfrak{D}_{i,\kappa})_{\kappa>0}$ and $(\mathfrak{D}_{e,\kappa})_{\kappa>0}$ such that

- $\mathfrak{D}_{i,\kappa} \subset \mathfrak{D} \subset \mathfrak{D}_{e,\kappa}$,
- $\mathfrak{D}_{i,\kappa}$ and $\mathfrak{D}_{e,\kappa}$ are stable by $b(s,\cdot) + f(\cdot - \tilde{x})$,
- $\sup_{z\in\partial\mathfrak{D}_{i,\kappa}} \mathrm{d}\,(z;\mathfrak{D}^c) + \sup_{z\in\partial\mathfrak{D}_{e,\kappa}} \mathrm{d}\,(z;\mathfrak{D})$ tends to 0 when κ goes to 0,
- $\inf_{z\in\partial\mathfrak{D}_{i,\kappa}} \mathrm{d}\,(z\,;\,\mathfrak{D}^c) = \inf_{z\in\partial\mathfrak{D}_{e,\kappa}} \mathrm{d}\,(z;\mathfrak{D}) = r(\kappa)$.

Step 2. By $\tau'_{i,\kappa}(\varepsilon)$ (resp. $\tau'_{e,\kappa}(\varepsilon)$), we denote the first exit-time of Z^ε from $\mathfrak{D}_{i,\kappa}$ (resp. $\mathfrak{D}_{e,\kappa}$).
Step 3. We prove here the upper bound:

$$\begin{aligned}\mathbb{P}\left[\tau_{\mathfrak{D}}(\varepsilon) \ge e^{\frac{2(\Delta+\delta)}{\varepsilon}}\right] &= \mathbb{P}\left[\tau_{\mathfrak{D}}(\varepsilon) \ge e^{\frac{2(\Delta+\delta)}{\varepsilon}}, \tau'_{e,\kappa}(\varepsilon) \ge e^{\frac{2(\Delta+\delta)}{\varepsilon}}\right] + \mathbb{P}\left[\tau_{\mathfrak{D}}(\varepsilon) \ge e^{\frac{2(\Delta+\delta)}{\varepsilon}}, \tau'_{e,\kappa}(\varepsilon) < e^{\frac{2(\Delta+\delta)}{\varepsilon}}\right]\\ &\le \mathbb{P}\left[\tau'_{e,\kappa}(\varepsilon) \ge e^{\frac{2(\Delta+\delta)}{\varepsilon}}\right] + \mathbb{P}\left[\tau_{\mathfrak{D}}(\varepsilon) \ge e^{\frac{2(\Delta+\delta)}{\varepsilon}}, \tau'_{e,\kappa}(\varepsilon) < e^{\frac{2(\Delta+\delta)}{\varepsilon}}\right]\\ &=: a_\kappa(\varepsilon) + b_\kappa(\varepsilon).\end{aligned}$$

Step 3.1. By classical results in Freidlin-Wentzell theory, [HIPP14, Theorem 2.42], there exists $\kappa_1 > 0$ such that for all $0 < \kappa < \kappa_1$, we have

$$\lim_{\varepsilon\to 0} \mathbb{P}\left[\tau'_{e,\kappa}(\varepsilon) < \exp\left(\frac{2}{\varepsilon}\,(\Delta+\delta)\right)\right] = 1.$$

Therefore, the first term $a_\kappa(\varepsilon)$ tends to 0 as ε goes to 0.
Step 3.2. For κ sufficiently small, we have $\mathfrak{D}_{e,\kappa} \subset \mathcal{K}$ and consequently we have

$$\begin{aligned}&\mathbb{P}\Big[\tau_{\mathfrak{D}}(\varepsilon) \ge e^{\frac{2(\Delta+\delta)}{\varepsilon}}, \tau'_{e,\kappa}(\varepsilon) \le e^{\frac{2(\Delta+\delta)}{\varepsilon}}\Big]\\ &\qquad \le \mathbb{P}\Big[\|X_{\tau'_{e,\kappa}(\varepsilon)} - Z_{\tau'_{e,\kappa}(\varepsilon)}\| \ge \eta(\kappa)\Big] \le \mathbb{P}\Big[\sup_{T^{\kappa,r}(\varepsilon)\le t\le \mathcal{T}_{\mathcal{K},\kappa}(\varepsilon)} \|X^\varepsilon_t - Z^\varepsilon_t\| \ge \eta(\kappa)\Big].\end{aligned}$$

According to Proposition 5.5.10, there exists $\varepsilon_0 > 0$ such that the previous term is less than $\eta(\kappa)$ for all $\varepsilon < \varepsilon_0$.

Step 3.3. Let $\delta > 0$. By taking κ arbitrarily small, we obtain the upper bound

$$\lim_{\varepsilon \to 0} \mathbb{P}\left[\tau_{\mathfrak{D}}(\varepsilon) \geq \exp\left(\frac{2(\Delta+\delta)}{\varepsilon}\right)\right] = 0.$$

Step 4. Analogous arguments show that $\lim_{\varepsilon\to 0} \mathbb{P}\left[T^{\kappa,r}(\varepsilon) \leq \tau_{\mathfrak{D}}(\varepsilon) \leq e^{\frac{2(\Delta-\delta)}{\varepsilon}}\right] = 0$. However, by Proposition 5.5.2 we have $\lim_{\varepsilon\to 0} \mathbb{P}\left[\tau_{\mathfrak{D}}(\varepsilon) \leq T^{\kappa,r}(\varepsilon)\right] = 0$.

This concludes the proof. $\square$

Appendix

5.A Large Deviations

Lemma 5.A.1. Let $z_0 \in \mathbb{R}^d$ be deterministic. For $t \geq 0$, let $b_t \in \mathbb{R}^d$, $\sigma_t \in \mathbb{R}^{d \times d'}$,$k_t \in \mathbb{R}^d$ be progressively measurable processes, with k having bounded variation. Let Z_t be the solution of

$$Z_t = z_0 + \int_0^t b_s ds + \sqrt{\varepsilon} \int_0^t \sigma_s dW_s + k_t,$$

where k is such that

$$\int_0^t \langle Z_s, dk_s \rangle \leq 0 \quad \text{a.s.} \quad \text{for all } t \geq 0. \tag{5.A.1}$$

Further assume that $\tau_1 \in [0,T]$ is a stopping time with respect the filtration generated by $\{W_t \ : t \in [0,T]\}$, and that

$$\|b_t\| \leq B(\rho^2 + \|Z_t\|^2)^{\frac{1}{2}} \qquad \text{and} \qquad \|\sigma_t\| \leq M(\rho^2 + \|Z_t\|^2)^{\frac{1}{2}}, \tag{5.A.2}$$

for some constants M, B, ρ. Then for any $\delta > 0$, $\varepsilon < 1$

$$\varepsilon \log\Big(\mathbb{P}(\sup_{t \in [0,\tau_1]} \|Z_t\|) \geq \delta)\Big) \leq 2B + M^2\Big(2 + d\Big) + \log\Big(\frac{\rho^2 + \|z_0\|^2}{\rho^2 + \delta^2}\Big). \tag{5.A.3}$$

Proof. The proof is a slight adaptation of [DZ98, Lemma 5.6.18]. Let $\varepsilon < 1$. Define $U_t = \phi(Z_t) = (\rho^2 + \|Z_t\|^2)^{\frac{1}{\varepsilon}}$, and note $\nabla\phi(Z_t) = \frac{2\phi(Z_t)}{\varepsilon(\rho^2 + \|Z_t\|^2)} Z_t$. By Itô we have

$$U_t = \phi(z_0) + \int_0^t \tilde{b}_s ds + \int_0^t \tilde{\sigma}_s dW_s + \int_0^t \langle \nabla\phi(Z_s), \alpha_s \rangle d|k|_s, \tag{5.A.4}$$

where

$$\tilde{\sigma}_t := \sqrt{\varepsilon}\nabla\phi(Z_t)'\sigma_t \quad \text{and} \quad \tilde{b}_t := \sqrt{\varepsilon}\nabla\phi(Z_t)'b_t + \frac{\varepsilon}{2}\text{Trace}\big[\sigma_t \nabla^2\phi(Z_t)\sigma_t'\big].$$

Note that for $t \in [0, \tau_1]$ we have,

$$\|\nabla\phi(Z_t)'b_t\| \leq \frac{2B\phi(Z_t)}{\varepsilon(\|Z_t\|^2)^{\frac{1}{2}}}\|Z_t\| = \frac{2BU_t}{\varepsilon},$$

and

$$\begin{aligned}\frac{\varepsilon}{2}\text{Trace}\big[\sigma_t \nabla^2\phi(Z_t)\sigma_t'\big] &\leq \frac{\varepsilon}{2}\|\sigma\|^2\|\nabla^2\phi(Z_t)\| \\ &\leq \frac{\varepsilon}{2}M^2(\rho^2 + \|Z_t\|^2)\|\nabla^2\phi(Z_t)\| \leq \frac{M^2(d+2)U_t}{\varepsilon},\end{aligned} \tag{5.A.5}$$

indeed we can directly compute and decompose

$$\nabla^2\phi(Z_t) = \frac{2}{\varepsilon}\frac{\phi(Z_t)}{(\rho^2 + \|Z_t\|^2)} I_d + 2\Big(\frac{1}{\varepsilon} - 1\Big)\frac{2}{\varepsilon}\frac{\phi(Z_t)}{(\rho^2 + \|Z_t\|^2)^2} Z_t Z_t' = AI_d + B(I_d Z_t)(I_d Z_t)',$$

with A and B two auxiliary variables representing the coefficients of I_d and $(I_dZ_t)(I_dZ_t)'$, for $Z_t \in \mathbb{R}^d$, $Z_tZ_t' \in \mathbb{R}^{d\times d}$ and I_d the d-dimensional identity matrix. Hence

$$\begin{aligned}\|\nabla^2\phi(Z_t)\| \leq A\cdot d + B\|Z_t\|^2 &= \frac{2}{\varepsilon}\frac{\phi(Z_t)}{\rho^2+\|Z_t\|^2}\Big(d\frac{\phi(Z_t)}{\rho^2+\|Z_t\|^2}\Big) + \frac{4}{\varepsilon}\Big(\frac{1}{\varepsilon}-1\Big)\frac{\phi(Z_t)}{\rho^2+\|Z_t\|^2}\frac{\|Z_t\|^2}{\rho^2+\|Z_t\|^2}\\ &\leq \Big[\frac{2d}{\varepsilon}+\frac{4}{\varepsilon^2}\Big]\frac{U_t}{\rho^2+\|Z_t\|^2},\end{aligned}$$

using this result on the 1st term in (5.A.5), yields the result.

Hence for any $t \in [0,\tau_1]$ we have

$$\tilde{b}_t \leq \frac{KU_t}{\varepsilon} \quad \text{with } K = 2B + M^2(d+2) < \infty. \tag{5.A.6}$$

Fix $\delta > 0$, define the stopping time $\tau_2 = \inf\{t \geq 0 : \|Z_t\| \geq \delta\} \wedge \tau_1$. Let $t \in [0,\tau_2]$, note that

$$\|\tilde{\sigma}_t\| \leq \|\nabla\phi(Z_t)\|\|\sigma_t\| \leq \frac{2M}{\varepsilon}\frac{(\rho^2+\|Z_t\|^2)^{\frac{1}{\varepsilon}}}{(\rho^2+\|Z_t\|^2)^{\frac12}}\|Z_t\| \leq \frac{\sqrt{2}M}{\sqrt{\rho}\varepsilon}\frac{(\rho^2+\|Z_t\|^2)^{\frac{1}{\varepsilon}}}{\|Z_t\|^{\frac12}}\|Z_t\| \leq \frac{\sqrt{2}M}{\sqrt{\rho}\varepsilon}(\rho^2+\delta^2)^{\frac{1}{\varepsilon}}\delta^{\frac12},$$

in other words $\|\tilde{\sigma}\|$ is uniformly bounded on $[0,\tau_2]$. Hence for $t \in [0,\tau_2]$

$$\int_0^t \tilde{\sigma}_s dW_s = U_t - \int_0^t \tilde{b}_s ds - \int_0^t \langle\nabla\phi(Z_s), dk_s\rangle,$$

is a Martingale. Therefore Doob's theorem implies

$$\mathbb{E}[U_{t\wedge\tau_2}] = \phi(z_0) + \mathbb{E}\Big[\int_0^{t\wedge\tau_2}\tilde{b}_s ds\Big] + \mathbb{E}\Big[\int_0^{t\wedge\tau_2}\langle\nabla\phi(Z_s), dk_s\rangle\Big].$$

Non-negativity of U and (5.A.2), and (5.A.1) imply that

$$\mathbb{E}[U_{t\wedge\tau_2}] \leq \phi(z_0) + \frac{K}{\epsilon}\mathbb{E}\Big[\int_0^{t\wedge\tau_2} U_s ds\Big].$$

From here one can conclude by proceeding identically to [DZ98, Lemma 5.6.18]. □

5.B Additional Existence & Uniqueness results

Theorem 5.B.1. Let $\mathcal{D}$ satisfy Assumption 5.2.5. Let $p \geq 2$. Let W be a d' dimensional Brownian motion. Let $\theta : \Omega \to \mathcal{D}$, $b : [0,T]\times\Omega\times\mathcal{D} \to \mathbb{R}^d$ and $\sigma : [0,T]\times\Omega\times\mathcal{D} \to \mathbb{R}^{d\times d'}$ be progressively measurable maps. Suppose that

- $\theta \in L^p(\mathcal{F}_0,\mathbb{P};\mathcal{D})$.
- $\exists x_0 \in \mathcal{D}$ such that b and σ satisfy the integrability conditions

$$\mathbb{E}\Big[\Big(\int_0^T \|b(s,x_0)\|ds\Big)^p\Big] \vee \mathbb{E}\Big[\Big(\int_0^T \|\sigma(s,x_0)\|^2 ds\Big)^{p/2}\Big] < \infty.$$

- b and σ satisfy a Lipschitz condition over $\mathcal{D}$, $\exists L > 0$ such that for almost all $(s,\omega) \in [0,T]\times\Omega$ and $\forall x,y \in \mathcal{D}$,

$$\|b(s,x)-b(s,y)\| \vee \|\sigma(s,x)-\sigma(s,y)\| \leq L\|x-y\|.$$

Then there exists a unique solution to the reflected Stochastic Differential Equation (5.3.1) in $\mathcal{S}^p([0,T])$ and

$$\mathbb{E}\Big[\|X-x_0\|^p_{\infty,[0,T]}\Big] \lesssim \mathbb{E}\Big[\|\theta-x_0\|^p\Big] + \mathbb{E}\Big[\Big(\int_0^T \|b(s,x_0)\|ds\Big)^p\Big] + \mathbb{E}\Big[\Big(\int_0^T \|\sigma(s,x_0)\|^2 ds\Big)^{p/2}\Big].$$

Proof. Let $n \in \mathbb{N}$, and for clarity we emphasise this is distinct from $\mathbf{n}$ as defined in Definition 5.2.6. We consider the following sequence of random processes defined recursively over the interval $[0, T]$:

- $X^{(0)} = \theta$,
- $Y_t^{(n+1)} := \theta + \int_0^t b(s, X_s^{(n)})ds + \int_0^t \sigma(s, X_s^{(n)})dW_s$,
- $(X^{(n)}, k^n)$ is the solution to the Skorokhod problem $(Y^{(n)}, \mathcal{D}, \mathbf{n})$.

The solution to the Skorokhod problem $(X^{(n+1)}, k^n)$ exists $\mathbb{P}$-almost surely by Theorem 5.2.7 since the process $Y^{(n)}$ is a semi-martingale. By taking an intersection of the sequence of $\mathbb{P}$-measure-1 sets, we obtain a $\mathbb{P}$-measure-1 set on which all such Skorokhod problems are solvable.

Thus $X^{(n+1)}$ is the recursively defined Itô process

$$\begin{aligned} X_t^{(n+1)} =& \theta + \int_0^t b(s, X_s^{(n)})ds + \int_0^t \sigma(s, X_s^{(n)})dW_s - k_t^n, \\ |k^n|_t =& \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^{(n+1)})d|k^n|_s \quad k_t^n = \int_0^t \mathbb{1}_{\partial\mathcal{D}}(X_s^{(n+1)})\mathbf{n}(X^{(n+1)})d|k^n|_s. \end{aligned}$$

It is immediate that $X^{(0)} \in \mathcal{S}^p([0, T])$. Now suppose that $X^{(n)} \in \mathcal{S}^p([0, T])$.

Next, we show that this sequence of Picard iterations converges. Firstly,

$$X_t^{(1)} - X_t^{(0)} = \int_0^t b(s, \theta)ds + \int_0^t \sigma(s, \theta)dW_s - k_t^0,$$

and hence $\mathbb{E}\Big[\|X_t^{(1)} - \theta\|_{\infty,[0,T]}^p\Big] \le \mathbb{E}\Big[\Big(\int_0^T |b(s, \theta)|ds\Big)^p\Big] + \mathbb{E}\Big[\Big(\int_0^T |\sigma(s, \theta)|^2 ds\Big)^{p/2}\Big]$.

Next consider

$$\begin{aligned} &\|X_t^{(n+1)} - X_t^{(n)}\|^p \\ &\quad= p\int_0^t \|X_s^{(n+1)} - X_s^{(n)}\|^{p-2}\Big\langle X_s^{(n+1)} - X_s^{(n)}, b(s, X_s^{(n)}) - b(s, X_s^{(n-1)})\Big\rangle ds \\ &\quad\quad + p\int_0^t \|X_s^{(n+1)} - X_s^{(n)}\|^{p-2}\Big\langle X_s^{(n+1)} - X_s^{(n)}, \Big(\sigma(s, X_s^{(n)}) - \sigma(s, X_s^{(n-1)})\Big)dW_s\Big\rangle \\ &\quad\quad + \tfrac{p}{2}\int_0^t \|X_s^{(n+1)} - X_s^{(n)}\|^{p-2}\Big\|\sigma(s, X_s^{(n)}) - \sigma(s, X_s^{(n-1)})\Big\|^2 ds \\ &\quad\quad + \tfrac{p(p-2)}{2}\int_0^t \|X_s^{(n+1)} - X_s^{(n)}\|^{p-4}\Big\|(X_s^{(n+1)} - X_s^{(n)})'\Big(\sigma(s, X_s^{(n)}) - \sigma(s, X_s^{(n-1)})\Big)\Big\|^2 ds \\ &\quad\quad - p\int_0^t \|X_s^{(n+1)} - X_s^{(n)}\|^{p-2}\Big\langle X_s^{(n+1)} - X_s^{(n)}, \mathbf{n}(X_s^{(n)})d|k^n|_s - \mathbf{n}(X_s^{(n-1)})d|k^{n-1}|_s\Big\rangle. \end{aligned}$$

Taking a supremum over the time interval $[0, T]$ and taking expectations yields

$$\begin{aligned} \mathbb{E}\Big[\|X^{(n+1)} - X^{(n)}\|_{\infty,[0,T]}^p\Big] \le& pL\mathbb{E}\Big[\|X^{(n+1)} - X^{(n)}\|_{\infty,[0,T]}^{p-1}\int_0^T \|X^{(n)} - X^{(n-1)}\|_{\infty,[0,s]}ds\Big] \\ &+ pC_1L\mathbb{E}\Big[\|X^{(n+1)} - X^{(n)}\|_{\infty,[0,T]}^{p-1}\Big(\int_0^T \|X^{(n)} - X^{(n-1)}\|_{\infty,[0,s]}^2 ds\Big)^{1/2}\Big] \\ &+ \tfrac{p(p-1)L^2}{2}\mathbb{E}\Big[\|X^{(n+1)} - X^{(n)}\|_{\infty,[0,T]}^{p-2}\int_0^T \|X^{(n)} - X^{(n-1)}\|_{\infty,[0,s]}^2 ds\Big], \end{aligned}$$

where the final term was dominated by 0 using Lemma 5.2.4. An application of Young's Inequality yields

$$\begin{aligned}\mathbb{E}\Big[\|X^{(n+1)}-X^{(n)}\|^p_{\infty,[0,T]}\Big] \leq&(p-1)^{p-1}\big(4L\big)^pT^{p-1}\int_0^T \mathbb{E}\Big[\|X^{(n)}-X^{(n-1)}\|^p_{\infty,[0,s]}\Big]ds\\ &+(p-1)^{p-1}\big(4LC_1\big)^pT^{(p-2)/2}\int_0^T \mathbb{E}\Big[\|X^{(n)}-X^{(n-1)}\|^p_{\infty,[0,s]}\Big]ds\\ &+2(p-1)^{p/2}(p-2)^{(p-2)/2}4^{p/2}T^{(p-2)/2}\int_0^T \mathbb{E}\Big[\|X^{(n)}-X^{(n-1)}\|^p_{\infty,[0,s]}\Big]ds\\ \leq& K\int_0^T \mathbb{E}\Big[\|X^{(n)}-X^{(n-1)}\|^p_{\infty,[0,s]}\Big]ds. \end{aligned} \tag{5.B.1}$$

Therefore, by inductively substituting in for preceding terms of the sequence and integrating, we get

$$\mathbb{E}\Big[\|X^{(n+1)}-X^{(n)}\|^p_{\infty,[0,T]}\Big] \leq \frac{K^n}{n!}T^n\mathbb{E}\Big[\|X^{(1)}-\theta\|^p_{\infty,[0,T]}\Big].$$

Thus

$$\mathbb{E}\Big[\|X^{(n)}-\theta\|^p_{\infty,[0,T]}\Big] \leq \mathbb{E}\Big[\|\theta\|^p\Big]+\sum_{i=1}^n \mathbb{E}\Big[\|X^{(i)}-X^{(i-1)}\|^p_{\infty,[0,T]}\Big] < \mathbb{E}\Big[\|\theta\|^p\Big]+\mathbb{E}\Big[\|X^{(1)}-\theta\|^p_{\infty,[0,T]}\Big]e^{KT}.$$

Therefore, there exists a limit of the sequence of random variables $X^{(n)}$ in the Banach space $\mathcal{S}^p([0,T])$.

Further, by Chebyshev's inequality we have

$$\mathbb{P}\Big[\Big\{\|X^{(n+1)}-X^{(n)}\|_{\infty,[0,T]}>2^{-n}\Big\}\Big] \leq \frac{(2K)^n}{n!},$$

so that by the Borel-Cantelli lemma

$$\mathbb{P}\Big[\limsup_{n\to\infty}\Big\{\|X^{(n+1)}-X^{(n)}\|_{\infty,[0,T]}>2^{-n}\Big\}\Big]=0,$$

so that the limit of the $X^{(n)}$ exists $\mathbb{P}$-almost surely. Denote this limit by the stochastic process X.

Finally, let

$$Y_t=\theta+\int_0^t b(s,X_s)ds+\int_0^t \sigma(s,X_s)dW_s,$$

and let (Z,k) be the solution to the Skorokhod problem $(Y,\mathcal{D},\mathbf{n})$. Thus Z satisfies the SDE

$$\begin{aligned} Z_t =&\theta+\int_0^t b(s,X_s)ds+\int_0^t \sigma(s,X_s)dW_s-k_t,\\ |k|_t =&\int_0^t \mathbb{1}_{\partial\mathcal{D}}(Z_s)d|k|_s, \quad k_t=\int_0^t \mathbb{1}_{\partial\mathcal{D}}(Z_s)\mathbf{n}(Z_s)d|k|_s. \end{aligned} \tag{5.B.2}$$

By similar estimates and Lemma 5.2.4 we show, as $n\to\infty$, that $\mathbb{E}[\,\|X^{(n)}-Z\|^p_\infty]\to 0$. We know that X is the unique limit of the random processes $X^{(n)}$, so X must satisfy the stochastic differential equation (5.B.2).

In light of the estimates above, uniqueness follows trivially and we sketch only the core argument. Assume X,Y are two solution to (5.3.1), then estimating $\mathbb{E}[\,\|X-Y\|^p_{\infty,[0,T]}]$ as in (5.B.1) leads to an inequality where Grönwall's inequality can be directly applied to yield $\mathbb{E}[\,\|X-Y\|^p_{\infty,[0,T]}]=0$ and hence delivering uniqueness. □

Proof of Theorem 5.3.2. Let $n\in\mathbb{N}$. Define the drift term

$$b_n(s,x):=\begin{cases} b(s,x), & \text{if } x\in\mathcal{D}_n,\\ b\Big(s,\arg\min_{y\in\mathcal{D}_n}\|x-y\|\Big), & \text{if } x\notin\mathcal{D}_n. \end{cases}$$

By the local Lipschitz condition of b, we have that b_n is a uniformly Lipschitz function. By Theorem 5.B.1, we know that for each $n \in \mathbb{N}$, there exists a unique solution to the SDE

$$X_t^n = \theta + \int_0^t b_n(s, X_s^n) ds + \int_0^t \sigma(s, X_s^n) dW_s - k_t^n,$$

with $|k^n|_t = \int_0^t \mathbb{1}_{\partial \mathcal{D}}(X_s^n) ds$ and $k_t^n = \int_0^t \mathbb{1}_{\partial \mathcal{D}}(X_s^n) \mathbf{n}(X_s^n) d|k^n|_s$ over the interval $[0,T]$. Next, define the sequence of stopping times $\tau_n := \inf\{t \in [0,T] : X_t \notin \mathcal{D}_n\}$, and $\tau_\infty := \lim_{n\to\infty} \tau_n$. Observe that on the interval $[0, \tau_n]$, we have $b_n(s, X_s^n) = b(s, X_s^n)$. Thus we can equivalently write that on the interval $[0, \tau_n]$ that

$$X_t^n = \theta + \int_0^t b(s, X_s^n) ds + \int_0^t \sigma(s, X_s^n) dW_s - k_t^n,$$

and so $X_t = X_t^n$. Applying the one-sided Lipschitz condition, we have

$$\begin{aligned}
\mathbb{E}\Big[\|X - x_0\|_{\infty,[0,T\wedge\tau_n]}^p\Big] \lesssim & \mathbb{E}\Big[\|\theta - x_0\|^p\Big] + \mathbb{E}\bigg[\Big(\int_0^{T\wedge\tau_n} \|b(s,x_0)\| ds\Big)^p\bigg] + \mathbb{E}\bigg[\Big(\int_0^{T\wedge\tau_n} \|\sigma(s,x_0)\|^2 ds\Big)^{p/2}\bigg] \\
\lesssim & \mathbb{E}\Big[\|\theta - x_0\|^p\Big] + \mathbb{E}\bigg[\Big(\int_0^{T} \|b(s,x_0)\| ds\Big)^p\bigg] + \mathbb{E}\bigg[\Big(\int_0^{T} \|\sigma(s,x_0)\|^2 ds\Big)^{p/2}\bigg].
\end{aligned}$$

As each $\tau_n < \tau_{n+1}$, we have that the sequence of random variables satisfies $\|X - x_0\|_{\infty,[0,T\wedge\tau_n]} \leq \|X - x_0\|_{\infty,[0,T\wedge\tau_{n+1}]}$, so we apply Beppo Levi to conclude that

$$\mathbb{E}\Big[\|X - x_0\|_{\infty,[0,T\wedge\tau_\infty]}^p\Big] \lesssim \mathbb{E}\Big[\|\theta - x_0\|^p\Big] + \mathbb{E}\bigg[\Big(\int_0^{T} \|b(s,x_0)\| ds\Big)^p\bigg] + \mathbb{E}\bigg[\Big(\int_0^{T} \|\sigma(s,x_0)\|^2 ds\Big)^{p/2}\bigg].$$

Note that the probability

$$\mathbb{P}\Big[\tau_n < T\Big] = \mathbb{P}\Big[\|X^n - x_0\|_{\infty,[0,T]} \geq n\Big] \leq \mathbb{P}\Big[\|X - x_0\|_{\infty,[0,T\wedge\tau_\infty]} \geq n\Big] \leq \frac{1}{n^p} \mathbb{E}\big[\, \|X - x_0\|_{\infty,[0,T\wedge\tau_\infty]}^p\big].$$

Thus by the Borel Cantelli lemma,

$$\mathbb{P}\big[\limsup_{n\to\infty} \big\{\tau_n < T\big\}\big] = 0.$$

□

By the Cauchy-Schwarz inequality and the polynomial growth of f, we obtain

$$\begin{aligned}
&\tfrac{1}{N} \sum_{j=1}^N \mathbb{E}\Big[\Big\langle X_s^{i,N} - X_s^i, f(X_s^i - X_s^j) - f * \mu_s(X_s^i)\Big\rangle\Big] \\
&\qquad \leq C \mathbb{E}\Big[\|X_s^{i,N} - X_s^i\|^2\Big]^{1/2} \Big(1 + \mathbb{E}\Big[\|X_s^i\|^{2r}\Big]\Big)^{1/2}
\end{aligned}$$

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