

# Gradient flows in spaces of probability measures for finite-volume schemes, metric graphs and non-reversible Markov chains

by

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# Abstract

This thesis is based on three main topics: In the first part, we study convergence of discrete gradient flow structures associated with regular finite-volume discretisations of Fokker-Planck equations. We show evolutionary  $\Gamma$ -convergence of the discrete gradient flows to the  $L^2$ -Wasserstein gradient flow corresponding to the solution of a Fokker-Planck equation in arbitrary dimension  $d \geq 1$ . Along the argument, we prove Mosco- and  $\Gamma$ -convergence results for discrete energy functionals, which are of independent interest for convergence of equivalent gradient flow structures in Hilbert spaces.

The second part investigates  $L^2$ -Wasserstein flows on metric graph. The starting point is a Benamou-Brenier formula for the  $L^2$ -Wasserstein distance, which is proved via a regularisation scheme for solutions of the continuity equation, adapted to the peculiar geometric structure of metric graphs. Based on those results, we show that the  $L^2$ -Wasserstein space over a metric graph admits a gradient flow which may be identified as a solution of a Fokker-Planck equation.

In the third part, we focus again on the discrete gradient flows, already encountered in the first part. We propose a variational structure which extends the gradient flow structure to Markov chains violating the detailed-balance conditions. Using this structure, we characterise contraction estimates for the discrete heat flow in terms of convexity of corresponding path-dependent energy functionals. In addition, we use this approach to derive several functional inequalities for said functionals.

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# Included Publications

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## CONTENTS

Introduction	1
1. Gradient flow structures for Wasserstein spaces and for finite-state Markov chains	1
1.1. Gradient flows on the metric space $(\mathcal{P}(X), W_2)$	1
1.2. Gradient flows for finite state Markov chains	2
2. Overview of results	3
2.1. Evolutionary $\Gamma$ -convergence of entropy gradient flow structures for Fokker-Planck equations	3
2.2. Gradient flows on Wasserstein spaces over metric graphs	7
2.3. A variational structure for non-reversible Markov chains	8
References	10
Evolutionary $\Gamma$ -Convergence of Entropy Gradient Flow Structures for Fokker-Planck Equations in Multiple Dimensions	13
1. Introduction	13
Notation	14
2. Gradient flows	14
Fokker-Planck equations as Wasserstein gradient flows	14
Onsager formalism for gradient flows	15
Discrete optimal transport and gradient flows	16
The discrete Fokker-Planck equation as gradient flow	16
3. Statement of the main results	17
4. Previous works and known results	20
The convergence of the discrete flows	20
The one-dimensional setting	20
Scaling limits for discrete optimal transport in any dimension.	21
Regularity of the discrete flows	22
5. Proof of the main result: the Wasserstein evolutionary $\Gamma$ -convergence	22
5.1. Compactness and space-time regularity	22
5.2. Asymptotic lower bounds for the functionals	24
5.3. Proof of the Wasserstein evolutionary $\Gamma$ -convergence	26
6. A look at gradient flow structures in Hilbert spaces	27
6.1. Gradient flows in Hilbert spaces: the $L^2$ and $H^{-1}$ distance	27
6.2. The $L^2$ - and $H^{-1}$ -gradient flow structures in the discrete setting	28
6.3. Convergence of $L^2$ -Gradient flows for Dirichlet forms	29
6.4. Convergence of $H^{-1}$ -gradient flows for the $L^2$ -energy functional	31
7. Mosco convergence of discrete energies: the statement	33
8. Mosco convergence of the localised functionals	35
8.1. Regularity of finite energy sequences	35
8.2. Sobolev bound and inner regularity	38
9. Representation and characterisation of the limit	42
9.1. Locality	43
9.2. Subadditivity	44
9.3. The characterization of the $\Gamma$ -limit	46
References	49
Parabolic Harnack Inequalities for Linear Diffusions with an Application to Markov Chains on Locally Finite Graphs	53

1. Introduction	53
2. Parabolic Harnack inequalities for linear diffusions on metric measure spaces	54
Application to Markov chains on infinite graphs	59
3. The finite volume framework	60
References	65
Gradient Flows for Metric Graphs	67
1. Introduction	67
Organisation of the Paper	69
2. Preliminaries on optimal transport	70
2.1. Absolutely continuous curves and gradient flows in metric spaces	70
2.2. Wasserstein spaces	71
3. Optimal transport on metric graphs	72
3.1. Metric graphs and function spaces on metric graphs	72
3.2. Geodesics in Wasserstein Spaces	73
3.3. The Monge problem for Wasserstein spaces over metric graphs	74
4. The continuity equation on a metric graph	80
4.1. Regularisation of solutions to the continuity equation	84
5. Geodesic convexity of the entropy and curvature in the sense of Alexandrov on $W_2(\mathfrak{G})$	93
6. Convergence of the JKO-scheme	95
6.1. Optimality conditions of the JKO-scheme at each time step	95
6.2. Interpolation between time steps	97
6.3. Passing to the limiting equation	101
7. Gradient Flows in Wasserstein Spaces over Metric Graphs	102
7.1. The Entropy-Fisher dissipation equality	103
7.2. The energy-dissipation equality for the lower semicontinuous envelope of the metric slope	107
7.3. The energy-dissipation equality for the metric slope	109
References	110
A Variational Structure for Non-Reversible Markov Chains	113
1. Introduction	113
Open problem	114
Organisation of the article	114
Notation	114
2. Non-reversible perturbations of continuous-time Markov chains	115
3. The modified Onsager operator for non-reversible Markov chains	118
4. Lower convexity bounds in terms of the infinitesimal generator	125
5. The complete geodesic space $(\mathcal{P}_N, \mathcal{W})$	128
6. Bounds for $\mathcal{W}$ in terms of Wasserstein distances	132
7. Functional inequalities	133
8. Appendix: Properties of the logarithmic mean	140
References	141

## INTRODUCTION

The central objects of this thesis are gradient flows for energy functionals on Wasserstein spaces and their counterparts on discrete spaces arising from continuous-time Markov chains.

### 1. GRADIENT FLOW STRUCTURES FOR WASSERSTEIN SPACES AND FOR FINITE-STATE MARKOV CHAINS

A Wasserstein space over a metric space  $(X, d)$  consists of the set  $\mathcal{P}(X)$  of all Borel probability measures on  $X$  endowed with a metric – the so-called  $L^p$ -Wasserstein distance. In case,  $X$  is a complete and connected Riemannian manifold, the  $L^p$ -Wasserstein distance may be introduced for  $p > 1$  by the Benamou-Brenier formula [BB00]

$$W_p^p(\mu_0, \mu_1) := \inf \left\{ \int_0^1 \|v_t\|_{L^p(\mu_t)}^p dt \right\}, \quad (1)$$

where the infimum is over all pairs  $(\mu_t, v_t)_{t \in [0,1]}$  of curves  $t \mapsto \mu_t$  joining  $\mu_0$  to  $\mu_1$  in the space of Borel probability measures on  $X$  and vectorfields  $t \mapsto v_t$  solving the continuity equation

$$\frac{d}{dt} \mu_t + \nabla \cdot (v_t \mu_t) = 0 \quad (2)$$

in the sense of distributions. More generally, the  $L^p$ -Wasserstein distance may be defined on metric spaces via the optimal transport problem going back to the works of Gaspard Monge [Mon81] and Leonid V Kantorovich [Kan42]; we omit the definitions and details of this approach.

Provided that  $X$  is compact, the  $L^p$ -Wasserstein distances metrises the topology of weak convergence on  $\mathcal{P}(X)$ .

**1.1. Gradient flows on the metric space  $(\mathcal{P}(X), W_2)$ .** There is a surprising relation between solutions for Fokker-Planck equations on Euclidean domains  $\Omega \subseteq \mathbb{R}^n$  with no-flux boundary conditions and gradient flows for entropy functionals in the  $L^2$ -Wasserstein space over  $(\Omega, |\cdot|_2)$ .

Recall that a gradient flow for a smooth functional  $F$  on Euclidean space or a Riemannian manifold takes the simple form of a curve  $(x_t)_{t \geq 0}$  solving

$$\frac{d}{dt} x_t = -\nabla F(x_t).$$

While this equation extends in a straightforward fashion to, say, lower semicontinuous functionals on Hilbert spaces via the notion of subdifferentials (see e.g. [BP70b], [BP70a], [Bré71]), a generalisation to metric spaces is more involved. One possible choice is to define a gradient flow  $(x_t)_{t \geq 0}$  for a functional  $F$  on a metric space  $(X, d)$  in terms of the energy dissipation inequality

$$F(x_t) + \frac{1}{2} \int_s^t |\dot{x}_r|_d^2 + |\partial_d F|^2(x_r) dr \leq F(x_s) \quad \forall s \geq t, \quad (\text{EDI})$$

which we assume to hold for times  $t = 0$  and a.e.  $t > 0$ . In this inequality, the expression  $|\dot{x}_r|_d$  denotes the so-called metric derivative of  $x_t$  and may be interpreted as the “modulus of the speed” for the curve  $t \mapsto x_t$ .

On the other hand,  $|\partial_d F|$  denotes the (local slope) of the functional  $F$  and may be seen as a generalisation for the gradient of  $F$ .

The key observation in the celebrated work [JKO98] is the following: Weak solutions for the heat equation with no-flux boundary conditions on a Euclidean domain  $\Omega \subseteq \mathbb{R}^n$  satisfy (2.5) for  $F$  corresponding to the logarithmic entropy  $\text{Ent}(\mu) := \int_{\Omega} \rho \log \rho dx$  whenever  $d\mu = \rho dx$  on  $(\mathcal{P}(\Omega), W_2)$ . Indeed, in this setting, there exists precisely one such curve satisfying (2.5) for a given initial condition  $\mu_0 = \bar{\mu} \in \mathcal{P}(\Omega)$  with finite entropy  $\text{Ent}(\bar{\mu}) < +\infty$ .

Since then, this metric notion of a gradient flow and its relatives have been successfully applied to several energy functionals on Wasserstein spaces over Euclidean domains, Riemannian manifolds and even metric measure spaces (see e.g. [Ott01], [CMV+03], [CMV06], [AGS08], [GST09], [AGS14]).

**1.2. Gradient flows for finite state Markov chains.** The situation is different however, in case of a discrete space  $\mathcal{X}$ . Then the  $L^p$ -Wasserstein space does not permit two disjoint points to be connected by a constant-speed geodesic, that is a curve  $(\mu_t)_{t \in [0,1]}$  in  $(\mathcal{P}(\mathcal{X}), W_p)$  satisfying the scaling relation

$$W_p(\mu_s, \mu_t) = |s - t| W_p(\mu_0, \mu_1) \quad \forall s, t \in [0, 1]. \quad (3)$$

Note that, up to parametrisation, constant speed geodesics in  $(\mathcal{P}(\mathcal{X}), W_p)$  are precisely the curves which (together with a corresponding vectorfield) achieve the infimum in (1). As a consequence, there is no hope for a Benamou-Brenier formula (1) to hold.

To overcome this issue, a different metric on the space of discrete probability measures on a finite space  $\mathcal{X}$  has been proposed independently in the works [Maa11], [Mie11], [CHLZ12]. This time the main ingredient is not a metric on  $\mathcal{X}$  but a continuous-time Markov chain on  $\mathcal{X}$  described by a infinitesimal generator  $Q \in \mathbb{R}^{\mathcal{X} \times \mathcal{X}}$ . It is assumed that the Markov chain is irreducible and satisfies the detailed balance conditions

$$\pi(x)Q(x, y) = \pi(y)Q(y, x) \quad \forall x, y \in \mathcal{X} \quad (4)$$

for a unique stationary distribution  $\pi$  of  $Q$ .

Then a metric  $\mathcal{W}$  on  $\mathcal{P}(\mathcal{X})$  is introduced by

$$\mathcal{W}^2(\mu_0, \mu_1) := \inf \left\{ \int_0^1 \langle \psi_t, \mathcal{K}(\mu_t) \psi_t \rangle dt \right\}, \quad (5)$$

where the infimum is over all pairs  $(\mu_t, \psi_t)_{t \in [0,1]}$  of smooth curves  $t \mapsto \mu_t$  connecting  $\mu_0$  to  $\mu_1$  in  $\mathcal{P}(\mathcal{X})$  and measurable “vectorfields”  $t \mapsto \psi_t$  in  $\mathbb{R}^{\mathcal{X}}$  satisfying the discrete continuity equation

$$\frac{d}{dt} \mu_t = \mathcal{K}(\mu_t) \psi_t \quad \text{a.e. } t \in [0, 1]. \quad (6)$$

Here  $\mathcal{K} : \mathcal{P}(\mathcal{X}) \rightarrow \mathbb{R}^{\mathcal{X} \times \mathcal{X}}$  denotes the Onsager operator given by

$$\mathcal{K}(\mu) := \sum_{x, y \in \mathcal{X}} \pi(x)Q(x, y) \theta \left( \frac{\mu(x)}{\pi(x)}, \frac{\mu(y)}{\pi(y)} \right) (e(x) - e(y)) \otimes (e(x) - e(y)), \quad (7)$$

where  $\theta : \mathbb{R}_0^+ \times \mathbb{R}_0^+ \rightarrow \mathbb{R}_0^+$  denotes a mean function – yet to be defined – and  $e(x)$  denotes the unit vector at  $x$ .

Apart from a definition which mimics the Benamou-Brenier formula (1), the metric  $\mathcal{W}$  shows properties similar to the  $L^2$ -Wasserstein distance over Euclidean domains. In particular, any two points in  $(\mathcal{P}(\mathcal{X}), \mathcal{W})$  may be joined by a constant-speed geodesic – even more, the interior of  $\mathcal{P}(\mathcal{X})$  (that is the set of all nowhere vanishing probability measures on  $\mathcal{X}$ ) admits a Riemannian structure which induces  $\mathcal{W}$ .

Besides geometric properties in common, we may identify the EDI gradient flow  $(\mu_t)_{t \geq 0}$  for the entropy Ent on  $(\mathcal{P}(\mathcal{X}), \mathcal{W})$  as a solution for

$$\frac{d}{dt} \mu_t = \mu_t Q, \quad (8)$$

provided that we fit the mean  $\theta$  in (7) to the energy functional; in case of the logarithmic entropy Ent, this is the logarithmic mean

$$\theta_{\log}(a, b) := \frac{a - b}{\log a - \log b} \quad \forall a, b > 0 : a \neq b.$$

## 2. OVERVIEW OF RESULTS

In this section we give a brief overview of the works [FMP20a], [FMP20b], [EFMM20] and [FM20] comprised in this thesis.

**2.1. Evolutionary  $\Gamma$ -convergence of entropy gradient flow structures for Fokker-Planck equations.** For the metric  $\mathcal{W}$  shares similarities with the  $L^2$ -Wasserstein distance, yet arises from a very different structure on the underlying space – namely a continuous-time Markov chain instead of a metric topology, it seems natural to ask how both distances are related. In the works [GM13], [GKM18], [GKMP19] Gromov-Hausdorff convergence of  $(\mathcal{P}(\mathcal{X}), \mathcal{W})$  to  $(\mathcal{P}(\Omega), W_2)$  is studied in the framework of finite volume schemes which means that the state spaces  $\mathcal{X} = \mathcal{T}$  consist of suitably regular meshes on an  $n$ -dimensional torus (as in [GM13]) or a compact domain in  $\mathbb{R}^n$  (as in [GKM18]) with mesh size  $[\mathcal{T}] \rightarrow 0$ .

The equation (8) may be related to a finite volume-scheme as follows: Consider a finite partition  $\mathcal{T}$  (called *mesh*) of a bounded domain  $\Omega \subset \mathbb{R}^n$  with non-empty convex interior as well as the linear drift-diffusion equation

$$\frac{d}{dt} \rho_t = \Delta \rho_t + \nabla \cdot (\rho_t \nabla V) = \nabla \cdot (\sigma \nabla (\frac{\rho_t}{\sigma})) \quad (9)$$

with a no-flux boundary conditions on  $\Omega$  and an equilibrium density  $\sigma = C e^{-V}$  for a potential function  $V \in C^1(\bar{\Omega})$  and a normalisation constant  $C > 0$ .

We recall that a so-called *two-point flux approximation finite-volume scheme* may be derived from (9) by integrating the left- and the right-hand side over a suitably regular element  $K \in \mathcal{T}$  (called *cell*) and applying the divergence theorem viz.

$$\frac{d}{dt} \int_K \rho_t dx = \sum_{\substack{L \in \mathcal{T} \\ L \sim K}} \int_{\Gamma_{KL}} \sigma \nabla (\frac{\rho_t}{\sigma}) \cdot \nu_K d\mathcal{H}^{n-1},$$

where  $L \sim K$  denotes neighbouring cells  $L$  and  $K$ ,  $\Gamma_{KL}$  the common interface between  $K$  and  $L$ , and  $\nu_K$  the outward-pointing normal on  $\partial K$ . Now the approximation of this equation takes the form

$$\frac{d}{dt} \mu_t(K) = \sum_{\substack{L \in \mathcal{T} \\ L \sim K}} S_{KL} \frac{1}{d_{KL}} \left( \frac{\mu_t(K)}{\pi_K} - \frac{\mu_t(L)}{\pi_L} \right) \mathcal{H}^{n-1}(\Gamma_{KL}). \quad (10)$$

We expect the expressions  $\mu_t(K)$ ,  $S_{KL}$ , and  $\frac{1}{d_{KL}} \left( \frac{\mu_t(K)}{\pi_K} - \frac{\mu_t(L)}{\pi_L} \right)$  to approximate the density  $\rho_t$  on  $K$ , the equilibrium density  $\sigma$  on the common interface  $\Gamma_{KL}$ , and the directional derivative  $\nabla (\frac{\rho_t}{\sigma}) \cdot \nu_K$ , respectively. In particular,  $\pi_K := \int_K \sigma dx$  takes over the role of a discretised equilibrium and  $d_{KL}$  denotes the Euclidean distance between reference points  $x_K$  and  $x_L$  interior of their respective cells  $K$  and  $L$ .

Note that (10) corresponds to the discrete heat equation (8), provided that we consider the infinitesimal generator

$$Q(K, L) = \frac{S_{KL}}{\pi_K d_{KL}} \mathcal{H}^{n-1}(\Gamma_{KL})$$

on the state space  $\mathcal{T}$ . Evidently, a pair  $(Q, \pi)$  defined this way satisfies the detailed balance conditions (4) and, hence, is admissible for the  $\mathcal{W}$ -gradient flow structure for the discrete entropy.

Convergence of this finite volume scheme as described in (10) is a well-studied subject (see e.g. [EGH00], [BHO18]). Nevertheless, in [FMP20a] we are concerned about convergence of gradient flows in  $(\mathcal{P}(\mathcal{T}), \mathcal{W})$  to corresponding gradient flows in  $(\mathcal{P}(\Omega), W_2)$  by purely variational methods. More precisely, we use an abstract notion of evolutionary  $\Gamma$ -convergence of EDI gradient flows introduced in [SS04], [Ser11]. To this end, consider a sequence of meshes  $(\mathcal{T}_N)_{N \in \mathbb{N}}$  on a fixed compact domain  $\Omega \subset \mathbb{R}^n$  with mesh size  $[\mathcal{T}_N] \searrow 0$  as well as (relative) logarithmic entropy functionals  $\text{Ent}_N$  and  $\text{Ent}_\Omega$  on  $\mathcal{P}(\mathcal{T}_N)$  and  $\mathcal{P}(\Omega)$ , respectively: The main-ingredients are a sequence of curves  $(\mu_t^N)_{N \in \mathbb{N}}$  of curves  $t \mapsto \mu_t$  satisfying (2.5) for entropies  $\text{Ent}_N$  on  $\mathcal{P}(\mathcal{T}_N)$  and a limit curve  $t \mapsto \mu_t$  in  $\mathcal{P}(\Omega)$  such that the following assumptions hold:

(i) *Well-preparedness of the initial conditions:*

The piecewise constant interpolants of  $\mu_0^N$  converge to  $\mu_0$  in  $(\mathcal{P}(\Omega), W_2)$  as  $N \rightarrow \infty$ .

(ii)  *$\Gamma$ -liminf bound on the entropies:*

$$\liminf_{N \rightarrow \infty} \text{Ent}_N(\mu_t^N) \geq \text{Ent}_\Omega(\mu_t) \quad \forall t \geq 0. \quad (11a)$$

(iii)  *$\Gamma$ -liminf bound on the metric derivatives:*

$$\liminf_{N \rightarrow \infty} \int_0^T |\dot{\mu}_t^N|_{\mathcal{W}}^2 dt \geq \int_0^T |\dot{\mu}_t|_{W_2}^2 dt \quad \forall T > 0. \quad (11b)$$

(iv)  *$\Gamma$ -liminf bound on the metric slopes:*

$$\liminf_{N \rightarrow \infty} \int_0^T |\partial_{\mathcal{W}} \mu_t^N|^2 dt \geq \int_0^T |\partial_{W_2} \mu_t|^2 dt \quad \forall T > 0. \quad (11c)$$

This approach of showing evolutionary  $\Gamma$ -convergence for curves satisfying (2.5) for the entropies on  $(\mathcal{P}(\mathcal{T}_N), \mathcal{W})$  to their continuous counterparts was already successfully implemented by [DL15] in a 1-dimensional setting, under an isotropy condition on the meshes, using interpolation techniques that seem to be limited to the real line.

The achievement of [FMP20a] is an evolutionary  $\Gamma$ -convergence result, valid for compact, convex domains in  $\mathbb{R}^n$  for arbitrary dimension  $n$  and mild assumptions on the regularity of the meshes.

Whereas the first bound (11a) on the limit inferior of the entropies  $(\text{Ent}_N)_{N \in \mathbb{N}}$  is a consequence of the well-known weak lower-semicontinuity of relative entropy functionals (see e.g. Lemma 9.4.3 in [AGS08]) together with Fatou's lemma, the  $\Gamma$ -liminf bounds on the metric derivatives and slopes in arbitrary dimension are based on the following crucial tool: namely, a Mosco-convergence result for energy functionals  $\mathcal{F}_{\mu_N}^N : L^2(\Omega) \rightarrow [0, +\infty]$  given by

$$\mathcal{F}_{\mu_N}^N(\varphi) := \frac{1}{2} \langle \varphi, \mathcal{K}(\mu_N) \varphi \rangle,$$

whenever  $\varphi$  is constant on every cell in the mesh  $\mathcal{T}_n$  and, hence, may be interpreted as a function on  $\mathcal{T}$ ; otherwise, put  $\mathcal{F}_{\mu_N}^N(\varphi) = +\infty$ .



Under the assumptions that the piecewise constant interpolation densities for  $\mu_N$  converge weakly to some limit measure  $\mu \in \mathcal{P}(\Omega)$  as  $N \rightarrow \infty$  and the  $(\mu_N)_{N \in \mathbb{N}}$  are uniformly bounded from above and away from zero, the functionals  $\mathcal{F}_{\mu_N}^N$  converge in Mosco-sense to the (continuous) Dirichlet form given by  $\mathbf{F}_\mu(\varphi) := \frac{1}{2} \int_\Omega |\nabla \varphi|^2 d\mu$ , i.e. we have the following bounds:

(i) For every sequence  $(\varphi_N)_{N \in \mathbb{N}}$ , weakly convergent to  $\varphi$  in  $L^2(\Omega)$ , it holds

$$\liminf_{N \rightarrow \infty} \mathcal{F}_{\mu_N}^N(\varphi_N) \geq \mathbf{F}_\mu(\varphi). \quad (12a)$$

(ii) For every  $\varphi \in L^2(\Omega)$ , there exists a sequence  $(\varphi_N)_{N \in \mathbb{N}}$  strongly convergent to  $\varphi$  in  $L^2(\Omega)$  such that

$$\limsup_{N \rightarrow \infty} \mathcal{F}_{\mu_N}^N(\varphi_N) \leq \mathbf{F}_\mu(\varphi). \quad (12b)$$

The proof of this result is based on a compactness and representation procedure, following ideas from [AC04] and [BFLM02].

In order to infer the  $\Gamma$ -liminf bound on the metric derivatives from the Mosco-convergence result above, we use the fact that both the metric derivatives  $|\dot{\mu}_t^N|_{\mathcal{W}}$  and  $|\dot{\mu}_t|_{W_2}$  may be expressed in terms of the Legendre duals of suitable Dirichlet forms viz.

$$\frac{1}{2} |\dot{\mu}_t^N|_{\mathcal{W}}^2 = \sup_{\varphi \in L^2(\Omega)} \left\{ \langle \varphi, \frac{d}{dt} \mu_t^N \rangle - \mathcal{F}_{\mu_t^N}^N(\varphi) \right\}, \quad (13)$$

where the pairing between  $\varphi$  and  $\frac{d}{dt} \mu_t^N$  is understood in the sense of

$$\langle \varphi, \frac{d}{dt} \mu_t^N \rangle = \sum_{K \in \mathcal{T}} \varphi(K) \frac{d}{dt} \mu_t^N(K),$$

whenever  $\varphi$  takes only a constant value on each cell in  $\mathcal{T}$ , as well as

$$\frac{1}{2} |\dot{\mu}_t|_{W_2}^2 = \sup_{\varphi \in C_c^\infty(\Omega)} \left\{ \langle \varphi, \frac{d}{dt} \mu_t \rangle - \mathbf{F}_{\mu_t}(\varphi) \right\} \quad (14)$$

with the canonical pairing

$$\langle \varphi, \frac{d}{dt} \mu_t \rangle = \frac{d}{dt} \int_\Omega \varphi d\mu_t.$$

Assuming enough regularity on the  $\mu_t^N$ , we may use (12b) for a sequence of piecewise constant interpolants  $\varphi_n \rightarrow \varphi$  in  $L^2(\Omega)$  as well as (13) to infer

$$\langle \varphi, \frac{d}{dt} \mu_t \rangle - \mathbf{F}_{\mu_t}(\varphi) \leq \liminf_{N \rightarrow \infty} \left( \langle \varphi, \frac{d}{dt} \mu_t^N \rangle - \mathcal{F}_{\mu_t^N}^N(\varphi) \right) \leq \frac{1}{2} |\dot{\mu}_t^N|_{\mathcal{W}}^2.$$

Now, taking the supremum over all  $\varphi \in C_c^\infty(\Omega)$  in this inequality, using (14) and integrating both sides over the interval  $(0, T)$  gives the  $\Gamma$ -liminf bound (11b).

The proof of the  $\Gamma$ -liminf bound on the metric slopes takes advantage of the Mosco-convergence of Dirichlet forms as well. Indeed, we have the relations

$$\frac{1}{2} |\partial_{\mathcal{W}} \mu_t^N|^2 = \mathcal{F}_{\mu_t^N}^N(\sqrt{\rho_t^N}) \quad \text{for } \rho_t^N := \frac{\mu_t^N}{\pi_N}$$

and

$$\frac{1}{2} |\partial_{W_2} \mu_t|^2 = \mathbf{F}_{\mu_t}(\sqrt{\rho_t}) \quad \text{for } \rho_t := \frac{d\mu_t}{dx}.$$

Thus, integrating both sides of (12a) over the time interval  $(0, T)$  for  $\varphi_N = \sqrt{\rho_t^N}$  and  $\varphi = \sqrt{\rho_t}$  translates directly into  $\Gamma$ -liminf bound (11c), provided that the  $\mu_t^N$  are again regular enough to invoke the Mosco-convergence of the Dirichlet forms  $\mathcal{F}_{\mu_t^N}^N$ .

In order to verify that the measures  $\mathcal{F}_{\mu_t^N}^N$  satisfy the regularity requirements for both Mosco-bounds in (12) to hold, we will make use of a careful analysis of parabolic Harnack inequalities for the discrete heat flow in (8), undertaken in the accompanying note [FMP20b].

Harnack inequalities for diffusions and jump processes are intensively studied both on locally finite graphs (e.g. [Del99], [BBK09]) and in metric measure spaces (e.g. [Stu96], [CKW17], [CKW18], [CKW19a], [CKW19b]).

Note that the framework for gradient flows for finite state Markov chains described above allows for an interpretation of the state space  $\mathcal{X}$  as a finite weighted graph, due to the detailed balance conditions (4): Two nodes  $x, y \in \mathcal{X}$  are connected by an edge  $\{x, y\}$  with edge weight  $j(x, y) = \pi(x)Q(x, y)$ , precisely, when  $Q(x, y) > 0$ . Endowed with a suitable metric (like for instance the usual graph metric) as well as the stationary distribution  $\pi$  of the Markov chain, we may further interpret this graph/Markov chain as a metric measure space.

Nonetheless, in case of the finite volume scheme as described above and employed in [FMP20a], none of the cited works above in the realms of Harnack inequalities is directly applicable out of the box to obtain regularity for the discrete measures  $\mathcal{F}_{\mu_t^N}^N$ . In particular, the main reference for quadratic diffusions on locally finite graphs [Del99], requires the stationary distribution to satisfy the normalisation condition  $\pi(x) = \sum_{y \in \mathcal{X}} j(x, y)$  to hold, which is not the case in our setting of [FMP20a].

Hence, the goal of [FMP20b] is to fill up the small gap in the existing literature and prove the validity of a parabolic Harnack inequality in the quadratic case for bounded-horizon jump processes as well as a Hölder regularity result for the corresponding discrete heat flow. The latter result allows for an application in the finite volume framework as we obtain the required regularity for on the curves  $(\mu_t^N)_{t \geq t_0}$  uniformly for all  $N \in \mathbb{N}$ , only in dependence of some time  $t_0 > 0$ .

Let us briefly describe the main results mentioned above in the particular case of our finite volume setting (see [FMP20b] for the general statements for jump processes on metric measure spaces and locally finite graphs).

Then a parabolic Harnack inequality holds as follows: For every time  $t_0 > 0$  there exist constants  $C_H, R > 0, N_n \in \mathbb{N}$ , and  $0 < \eta_0 < \eta_1 < \eta_2 < 1$  such that for every non-negative solution  $(\mu_t^N)_{t \geq 0}$  of the discrete heat equation  $\frac{dt}{dt} \mu_t = \mu_t Q_N$  with  $N \geq N_0$ , it holds

$$\sup_{\substack{t \in Q_s^- \\ K \in \mathcal{T}_N}} \mu_t(K) \leq C_H \inf_{\substack{t \in Q_s^+ \\ K \in \mathcal{T}_N}} \mu_t(K) \quad \forall s \geq t_0,$$

where

$$Q_s^- := [s - \eta_1 R^2, s - \eta_0 R^2] \quad \text{and} \quad Q_s^+ := [s, s + \eta_2 R^2].$$

As a consequence, this Harnack inequality implies the following regularity result, used in [FMP20a] to invoke the Mosco-bounds (12) for the discrete heat flow: For every time  $t_0 > 0$  there exist constants  $C, \lambda > 0$  and  $N_n \in \mathbb{N}$  such that every non-negative solution  $(\mu_t^N)_{t \geq 0}$  of the discrete heat equation  $\frac{dt}{dt} \mu_t = \mu_t Q_N$  with  $N \geq N_0$  satisfies

$$|\mu_t^N(K) - \mu_t^N(L)| \leq C |x_K - x_L|^\lambda \sup_{\substack{s \geq t/2 \\ K \in \mathcal{T}_N}} \mu_s(K) \quad \forall K, L \in \mathcal{T}_N, t \geq t_0. \quad (15)$$

In view of  $|x_K - x_L| = d_{KL}$  denoting the distance between reference points  $x_K$  and  $x_L$  in the interior of respective cells  $K$  and  $L$  in  $\mathcal{T}_N$ , one may see (15) as a discrete  $\lambda$ -Hölder bound on the meshes  $\mathcal{T}_N$ , stable in terms of constants as  $N \rightarrow \infty$ .

**2.2. Gradient flows on Wasserstein spaces over metric graphs.** As already mentioned above, the discrete heat flow (8) may be interpreted as a gradient flow with respect to the metric  $\mathcal{W}$  for probability measures on a finite weighted graph corresponding to a Markov chain generator  $Q$  satisfying the detailed balance conditions (4).

Yet, a connected weighted graph  $G = (V, E)$  gives rise to another gradient flow structure by following the more traditional approach of Wasserstein gradient flows on a geodesic space associated to  $G$ . This means that we require any two points in the associated space to be connected by a constant-speed geodesic. A natural geometric approach is to construct such a geodesic space by interpreting the edges of the graph  $G$  as line-segments glued together at corresponding nodes. The resulting space is then called a *metric graph* over  $G$ .

More formally, a metric edge space  $\bar{\mathfrak{E}}$  over a directed graph  $G$  with weight function  $m : E \rightarrow \mathbb{R}^+$  may be understood as the (topological) disjoint union of all intervals  $\{[0, m_e]\}_{e \in E}$ , each interval identified with an directed edge  $e \in E$  with edge weight  $m_e := m(e)$ . Then the metric graph  $\mathfrak{G}$  over  $G$  emerges as (topological) quotient space  $\mathfrak{G} := \bar{\mathfrak{E}} / \sim$ , where points  $x \sim y$  are identified, whenever they are (the canonical injections of) endpoints of intervals, corresponding to the same node in  $V$ .

Provided, that we ignore the orientation of  $G$ , the metric graph  $\mathfrak{G}$  may be endowed with a natural metric  $d$  which measures the total length of the shortest path between any two points. Under the assumption that the underlying graph  $G$  is finite and connected,  $(\mathfrak{G}, d)$  is a compact geodesic space – and so is every Wasserstein space  $(\mathcal{P}(\mathfrak{G}), W_p)$  for  $p \geq 1$ .

However, a characterisation of the  $L^p$ -Wasserstein distance in terms of a Benamou-Brenier formula (1) is not straightforward in  $\mathcal{P}(\mathfrak{G})$ . Indeed, we first have to adapt the continuity equation (c€) to the setting of a metric graph by imposing boundary conditions on each node in  $V$ , which preserve the total mass  $\mu_t$  on  $\mathfrak{G}$ , viz.

$$\sum_{e \in E_w^{\text{in}}} U_t(w_e) = \sum_{e \in E_w^{\text{out}}} U_t(w_e) \quad \forall w \in V, \quad (16)$$

where  $U_t$  denotes the density of the momentum field  $v_t \cdot \mu_t$  defined on  $\bar{\mathfrak{E}}$ ,  $w_e$  is the (canonical injection of the) endpoint of the interval  $[0, m_e]$  corresponding to a node  $w \in V$  with adjacent edge  $e \in E$ , as well as the sets  $E_w^{\text{out}}$  and  $E_w^{\text{in}}$  of all edges with  $w$  as tail and head, respectively.

Now following the classical proofs for the Benamou-Brenier formula (1), one runs into considerable obstacles caused by the particular geometry of metric graphs. In fact, a Wasserstein space over a typical metric graph is a so-called branching space, i.e. there exist constant-speed geodesics  $(\mu_t)_{t \in [0,1]}$ ,  $(\tilde{\mu}_t)_{t \in [0,1]}$  and  $t_0 \in (0, 1)$  such that the values of  $\mu_t$  and  $\tilde{\mu}_t$  agree at all times  $t < t_0$  but not at any time  $t > t_0$ .

In particular, this means that a constant-speed geodesic in  $(\mathcal{P}(\mathfrak{G}), W_p)$  is uniquely defined as a solution of the continuity equation (c€) and node conditions (16) in terms of the pair of initial values  $(\mu_0, v_t)$ , no matter the regularity of  $\mu_0$ . Hence, techniques which rely on describing solutions of (c€) in terms of a flow are not at our disposal for the proof of a Benamou-Brenier formula (1) for Wasserstein spaces over metric graphs.

Instead, our approach in [EFMM20] is inspired by [GH15] where a notion for the continuity equation is studied in a setting of metric measure spaces, thus, using proof techniques not relying on flows.

On the other hand, in [GH15] only curves of probability measures with bounded densities are considered. In particular, under this restriction a Benamou-Brenier formula (1) in  $(\mathcal{P}(\mathfrak{G}), W_2)$  may only be inferred between any two measures  $\mu_0$  and  $\mu_1$  that can be connected by a geodesic  $\mu_t$  possessing a density in  $L^\infty(\mathfrak{G})$  for all times  $t \in [0, 1]$ .

In order to remove this restrictive assumption, we employ a regularisation for distributional solutions of the continuity equation (c€). On Euclidean domains the pair  $(\mu_t, v_t)_{t \in [0, 1]}$  may be regularised by means of an even and compact convolution kernel, which preserves the no-flux-boundary conditions accompanying (c€) on a neighbourhood of the domain.

In contrast, on a metric graph we have to employ a more delicate regularisation scheme which results in regularised curves solving not only (c€) but also satisfying the node conditions (16). As a result, we show in [EFMM20] that the Benamou-Brenier formula (1) is valid between any two probability measures in  $(\mathcal{P}(\mathfrak{G}), W_2)$ .

Furthermore, we use the regularisation scheme for solutions of the continuity equation on metric graphs to prove a *chain-rule* for relative entropy functionals along suitably regular curves  $(\mu_t)_{t \in [0, T]}$  in  $(\mathcal{P}(\mathfrak{G}), W_2)$ . In particular, for the logarithmic entropy we obtain

$$\frac{d}{dt} \text{Ent}(\mu_t) = \int_{\bar{\mathfrak{E}}} \langle \nabla \log \rho_t, U_t \rangle dx \quad \text{a.e. } t \in (0, T), \quad (17)$$

whenever the pair  $(\mu_t, v_t)_{t \in [0, T]}$  solves the continuity equation (c€) with node conditions (16) such that

- (i) the curve  $t \mapsto \mu_t$  is 2-absolutely continuous,
- (ii)  $d\mu_t = \rho_t dx$  and  $U_t = v_t \rho_t$  with  $(t, x) \mapsto \sqrt{\rho_t(x)}$  belonging to  $L^1(0, T; W^{1,2}(\bar{\mathfrak{E}}))$ .

Hölder's and Young's inequality allow us to estimate the right-hand side of (64) as

$$\int_{\bar{\mathfrak{E}}} \langle \nabla \log \rho_t, U_t \rangle dx \leq \int_{\bar{\mathfrak{E}}} |\nabla \log \rho_t| \cdot |U_t| dx \leq \frac{1}{2} \int_{\bar{\mathfrak{E}}} |\nabla \log \rho_t|^2 + |U_t|^2 dx. \quad (18)$$

Note that we have equality in (18), precisely, when  $U_t = -\nabla \log \rho_t$  for a.e.  $t \in [0, T]$ . In this case, the continuity equation (c€) simplifies to the heat equation

$$\frac{d}{dt} \rho_t = \nabla \rho_t, \quad (19a)$$

together with node conditions

$$\sum_{e \in E_w^{\text{in}}} \nabla \rho_t(w_e) = \sum_{e \in E_w^{\text{out}}} \nabla \rho_t(w_e) \quad \forall w \in V. \quad (19b)$$

In particular,  $(\rho_t)_{t \in [0, T]}$  solves (19) if and only if the corresponding curve of probability measures  $d\mu_t = \rho_t dx$  satisfies a energy dissipation equality

$$\frac{d}{dt} \text{Ent}(\mu_t) = \frac{1}{2} |\dot{\mu}_t|_{W_2}^2 + \frac{1}{2} |\partial_{W_2} \text{Ent}|^2(\mu_t) dx \quad \text{a.e. } t \in (0, T), \quad (20)$$

where we identified  $\int_{\bar{\mathfrak{E}}} |U_t| dx$  with the metric derivative  $|\dot{\mu}_t|_{W_2}$  and  $\int_{\bar{\mathfrak{E}}} |\nabla \log \rho_t| dx$  with the metric slope  $|\partial_{W_2} \text{Ent}|$ .

**2.3. A variational structure for non-reversible Markov chains.** Finally, in [FM20] we turn our attention back to the gradient flow structure for finite-state Markov chains. We investigate the role of the detailed balance conditions (4) for the gradient flow structure accompanying (22) as introduced above.

To this aim, note that violating the detailed balance conditions (4) breaks the symmetry of the Onsager operator (7). As a consequence, (5) need not define a metric on  $\mathcal{P}(\mathcal{X})$  anymore.

Given a non-reversible Markov chain, i.e. the corresponding infinitesimal generator  $A$  violates the detailed balance conditions (4), and an equilibrium distribution  $\pi$  for  $A$ , we propose the use of the following symmetric Onsager operator instead:

$$\check{\mathcal{K}}(\mu) := \sum_{x,y \in \mathcal{X}} \theta_{\log}(A(x,y)\mu(x), A(y,x)\mu(y)) (e(x) - e(y)) \otimes (e(x) - e(y)). \quad (21)$$

Whenever  $A$  agrees with an infinitesimal generator  $Q$  satisfying the detailed balance conditions (4), the Onsager operator  $\check{\mathcal{K}}$  agrees with the usual one in (7).

Provided that one replaces  $\mathcal{K}$  by  $\check{\mathcal{K}}$ , the formula (5) gives rise to a metric  $\mathcal{W}$  on  $\mathcal{P}(\mathcal{X})$ , no matter the validity of the detailed balance conditions.

It is well-known from numerical investigations (see e.g. [RBS16] [CLP99], [DHN00], [LP17]) that a perturbation of a Markov chain generator, which breaks the detailed balance conditions (4), may improve the rate of convergence to equilibrium in terms of spectral gap.

On a more rigorous level, it is known that the  $L^2$ -energy production along a curve  $t \mapsto \mu_t$  solving

$$\frac{d}{dt} \mu_t = \mu_t A \quad (22)$$

depends only on the reversible part of  $A$ , given by

$$Q = \text{diag}(\pi)^{-1} \text{Sym}(\text{diag}(\pi)A). \quad (23)$$

Note that  $Q$  is an infinitesimal generator with the same equilibrium distribution  $\pi$  satisfying the detailed balance conditions (4).

Such a result is not known to hold, when the  $L^2$ -energy is replaced by a logarithmic entropy. Indeed, in [FM20] we present a simple numerical example showing that the rate of convergence in terms of the entropy relative to the equilibrium distribution may actually decrease, when a non-reversible perturbation is performed as above.

Nevertheless, we may use the variational structure introduced above via the Onsager operator  $\check{\mathcal{K}}$  to relate geodesic convexity of a modified entropy functional to contraction estimates for solutions of (22) in terms of the metric  $\mathcal{W}$ . To this aim, we introduce a family of functionals  $\{V_t\}_{t \in [0,1]}$  on the space of constant-speed geodesics in  $(\mathcal{P}(\mathcal{X}), \mathcal{W})$  by setting

$$V_t(g) := \int_0^t \sum_{x,y \in \mathcal{X}} \psi_r(x) \check{\mathcal{K}}(g_t)(x,y) L(x,y) dr$$

where  $g : [0,1] \rightarrow \mathcal{P}(\mathcal{X})$  denotes a constant-speed geodesic and the matrix  $L$  satisfies the element-wise relation  $A(x,y) = e^{L(x,y)} Q(x,y)$  for all  $x,y \in \mathcal{X}$  and  $Q$  as in (23).

Note that, whenever  $A$  satisfies the detailed balance conditions (4), one may choose  $L \equiv 0$  and the functionals  $V_t$  vanish.

Now any two solutions  $(\mu_t)_{t \in [0,T]}$ ,  $(\tilde{\mu}_t)_{t \in [0,T]}$  of the discrete heat equation (22), staying in a small enough geodesic ball, satisfy the contraction estimate

$$\mathcal{W}(\mu_t, \tilde{\mu}_t) \leq e^{\lambda t} \mathcal{W}(\mu_0, \tilde{\mu}_0) \quad (24)$$

for a constant  $\lambda \in \mathbb{R}$ , precisely, when  $t \mapsto \text{Ent}(g_t) + V_t(g)$  is  $\lambda$ -convex for all constant speed geodesics  $g : [0,1] \rightarrow \mathcal{P}(\mathcal{X})$ .

This result may be seen as a discrete counterpart to a contraction result in [Ket16] for non-reversible diffusions in terms of the  $L^2$ -Wasserstein distance.

As seen above in our Markov chain setting, reversibility of the diffusion operator implies that the contraction constant  $\lambda$  is related to  $\lambda$ -convexity of just the logarithmic entropy along constant-speed geodesics in the Wasserstein space. As shown in the celebrated works [S<sup>+</sup>06] and [LV09], the convexity constant  $\lambda$  then represents a *synthetic lower Ricci curvature bound*.

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# EVOLUTIONARY $\Gamma$ -CONVERGENCE OF ENTROPY GRADIENT FLOW STRUCTURES FOR FOKKER-PLANCK EQUATIONS IN MULTIPLE DIMENSIONS

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## 1. INTRODUCTION

This paper deals with the convergence of discrete gradient flow structures arising from finite volume discretizations of Fokker-Planck equations on convex domains in  $\mathbb{R}^d$ . For a given potential  $V \in C(\overline{\Omega})$ , we consider the Fokker-Planck equation

$$\partial_t \mu = \Delta \mu + \nabla \cdot (\mu \nabla V) \quad \text{on } (0, T) \times \Omega, \quad (1.1)$$

where  $\Omega$  is a convex, open and bounded subset of  $\mathbb{R}^d$  and  $T \in (0, +\infty)$ . Since the seminal works of Jordan, Kinderlehrer and Otto [JKO98, Ott01], it is known that (1.1) can be formulated as a gradient flow in the space of probability measures  $\mathcal{P}(\overline{\Omega})$  endowed with the 2-Wasserstein distance  $\mathbf{W}_2$  from optimal transport. The driving functional is the relative entropy with respect to the invariant measure  $\overline{\mathbf{m}}(dx) := \frac{1}{Z_V} \exp(-V(x)) dx$ , where  $Z_V$  is a normalising constant.

Here we consider spatial discretisations of (1.1) obtained by finite volume methods for a general class of admissible meshes. In this setting it is very well known that solutions to the discrete equations converge to solutions of (1.1); see, e.g. [EGH00], [BHO18] for results in dimension 2 and 3 and [DEG<sup>+</sup>18] for more general situations.

In this paper we exploit the fact that the discretised Fokker-Planck equations can also be formulated as gradient flow with respect to a suitable discrete dynamical transport distance  $\mathcal{W}_{\mathcal{T}}$ ; see the independent works [CHLZ12, Maa11, Mie11]. This gradient flow structure has been intensively studied in relation to curvature bounds and functional inequalities [EM12, CHLZ12, EM14, EMT15, EMR15, EMW19].

In this paper we prove *evolutionary  $\Gamma$ -convergence* of the discrete gradient flow structures to the Wasserstein gradient flow structure; i.e. rather than directly passing to the limit at the level of the gradient flow equation, we pass to the limit in the *energy-dissipation inequality* that characterises the gradient flow structure.

This yields a new proof of convergence for the associated gradient flow equations, which does not rely on specific properties such as linearity or second order. Instead, the method is based on properties of functionals and tools such as  $\Gamma$ - and Mosco convergence.

The method of evolutionary  $\Gamma$ -convergence was pioneered by Sandier and Serfaty [SS04]; see [Mie16] for a survey on the topic. This method has recently been applied in various situations such as gradient systems with a wiggly energy; see [DFM19].

For Fokker-Planck equations in dimension  $d = 1$ , evolutionary  $\Gamma$ -convergence was proved by Disser and Liero [DL15]. Their proof relies on interpolation techniques which do not easily extend to multiple dimensions. Our proof is different and relies on compactness and representation theorems, in particular [BFLM02, Theorem 2],

adapting ideas from [AC04]. Our variational proof suggests the possibility of extending those techniques to more general settings (e.g. higher order and/or nonlinear PDE).

The fact that the method of evolutionary  $\Gamma$ -convergence works on arbitrary admissible meshes is remarkable in view of recent work on the limiting behaviour of the associated transport distances; in fact, it was shown in [GKM18] that the convergence of  $\mathcal{W}_{\mathcal{T}}$  to  $\mathbf{W}_2$  (in the limit of vanishing mesh size of  $\mathcal{T}$ ) requires a restrictive isotropy condition on the meshes; see [GKMP19] for explicit examples. This discrepancy in convergence behaviour can be explained by regularity: to prove evolutionary  $\Gamma$ -convergence one may impose spatial smoothness assumptions on the discrete dynamics (in view of regularity results for the discrete gradient flows); by contrast, the transport costs on anisotropic meshes are minimised along highly oscillatory curves.

**Organisation of the paper.** In Section 2 we present the general gradient flow picture linked to the Fokker-Planck equation in  $\mathbb{R}^d$ , both at the continuous and at the discrete level in a finite volume framework.

In Section 3 we present our main contributions of this work, namely the energy bounds of Theorem 3.3 and evolutionary  $\Gamma$ -convergence of the Wasserstein discrete gradient structures to the continuous one, reproving the convergence of the discrete scheme, in Theorem 3.6. In Section 4 we sum up the previous and known results, discussing different point of views and limitations.

In Section 5 we prove our main results, namely Theorem 3.3 and Theorem 3.6. In Section 6 we give a short discussion about possible different gradient flow structures for the Fokker-Planck equation on Hilbert spaces.

We then move to Section 7 and Section 8, where we present and prove the Mosco convergence of some discrete functionals to their continuous counterparts, including the one of certain Dirichlet forms.

**Notation.** Throughout the paper we use the notation  $a \lesssim b$  (or  $b \gtrsim a$ ) if  $a \leq Cb$  with  $C < \infty$  depending only on  $\Omega$ ,  $\zeta$  and  $\bar{\mathbf{m}}$ . We write  $a \approx b$  if  $a \lesssim b$  and  $a \gtrsim b$ .

## 2. GRADIENT FLOWS

In this section we describe the formulation of the Fokker-Planck equations as Wasserstein gradient flows of functionals on the space of probabilities, both at the continuous and at the discrete level. For the sake of clarity, our discussion will be somewhat informal. We refer to Section 3 below for rigorous statements of the main results.

**Fokker-Planck equations as Wasserstein gradient flows.** On a bounded convex domain  $\Omega \subset \mathbb{R}^d$ , we consider the Fokker-Planck equation

$$\partial_t \mu_t = \Delta \mu_t + \nabla \cdot (\mu_t \nabla V) \quad (2.1)$$

with a driving potential  $V \in C(\bar{\Omega}) \cap C^1(\Omega)$ . This equation describes the time-evolution of the distribution of a Brownian particle in a potential field. The steady state is given by the probability measure

$$\bar{\mathbf{m}} \in \mathcal{P}(\Omega) \quad \text{with density} \quad \sigma(x) = \frac{d\bar{\mathbf{m}}}{dx} = \frac{1}{Z_V} e^{-V(x)}, \quad (2.2)$$

where  $Z_V > 0$  is a normalising constant.

Since the seminal work of Jordan, Kinderlehrer and Otto [JKO98], it is known that (2.1) is a gradient flow with respect to the Wasserstein distance  $\mathbf{W}_2$  from optimal transport. In its dynamical formulation,  $\mathbf{W}_2$  is given by the *Benamou–Brenier formula*

$$\mathbf{W}_2(\mu_0, \mu_1)^2 = \inf \left\{ \int_0^1 \int_{\Omega} |v_t(x)|^2 d\mu_t(x) dt \right\}, \quad (2.3)$$

where the infimum runs over all curves  $(\mu_t)_t$  in the space of probability measures and all vectorfields  $(v_t)_t$  satisfying the continuity equation

$$\partial_t \mu_t + \nabla \cdot (\mu_t v_t) = 0 \quad (2.4)$$

in the sense of distributions, with boundary conditions  $\mu_t|_{t=0} = \mu_0$  and  $\mu_t|_{t=1} = \mu_1$ . The driving functional in this gradient flow formulation is the relative entropy  $\mathbf{H} : \mathcal{P}(\bar{\Omega}) \rightarrow [0, +\infty]$  given by

$$\mathbf{H}(\mu) := \begin{cases} \int_{\mathbb{R}^d} \rho(x) \log \rho(x) d\bar{\mathbf{m}} & \text{if } d\mu = \rho d\bar{\mathbf{m}}, \\ +\infty & \text{otherwise.} \end{cases}$$

The gradient flow structure can be interpreted at various levels: the original formulation in [JKO98] was given in terms of a time-discrete minimising movement scheme. Another interpretation is in terms of Otto's formal infinite-dimensional Riemannian calculus on the Wasserstein space [Ott01]. Yet another approach relies on the metric formulation of gradient flows in terms of the *energy dissipation inequality* (EDI)

$$\mathbf{H}(\mu_t) + \frac{1}{2} \int_0^T |\dot{\mu}_t|_{\mathbf{W}_2}^2 + |\partial_{\mathbf{W}_2} \mathbf{H}(\mu_t)|^2 dt \leq \mathbf{H}(\mu_0), \quad (2.5)$$

where  $|\dot{\mu}_t|_{\mathbf{W}_2}$  denotes the  $\mathbf{W}_2$ -metric derivative of the curve  $\mu_t$  and  $\partial_{\mathbf{W}_2} \mathbf{H}$  the slope of the entropy functional, namely

$$|\dot{\mu}_t|_{\mathbf{W}_2} := \lim_{h \rightarrow 0} \frac{1}{h} \mathbf{W}_2(\mu_{t+h}, \mu_t), \quad |\partial_{\mathbf{W}_2} \mathbf{H}(\mu)| := \limsup_{\nu \rightarrow \mu} \frac{[\mathbf{H}(\mu) - \mathbf{H}(\nu)]_-}{\mathbf{W}_2(\mu, \nu)},$$

where  $[a]_- = \max\{0, -a\}$ . Writing  $\rho = \frac{d\mu}{d\bar{\mathbf{m}}}$ , we have the identity

$$|\partial_{\mathbf{W}_2} \mathbf{H}(\mu)|^2 = \mathbf{I}(\mu), \quad \text{where} \quad \mathbf{I}(\mu) := \int_{\Omega} |\nabla \log \rho|^2 \rho d\bar{\mathbf{m}} = 4 \int_{\Omega} |\nabla \sqrt{\rho}|^2 d\bar{\mathbf{m}} \quad (2.6)$$

is the *relative Fisher information* with respect to  $\bar{\mathbf{m}}$ .

**Onsager formalism for gradient flows.** Let us formulate (2.5) in terms of a suitable energy  $\mathbf{A}$  and its Legendre transform  $\mathbf{A}^*$ . Consider the energy functional

$$\mathbf{A}(\mu, \varphi) := \frac{1}{2} \int_{\Omega} |\nabla \varphi|^2 d\mu, \quad \varphi \in C_c^\infty(\mathbb{R}^d), \mu \in \mathcal{P}(\Omega), \quad (2.7)$$

and its Legendre dual of  $\mathbf{A}$  with respect to the second variable

$$\mathbf{A}^*(\mu, \eta) = \sup_{\varphi \in C_c^\infty(\Omega)} \{ \langle \varphi, \eta \rangle - \mathbf{A}(\mu, \varphi) \}$$

for any distribution  $\eta \in \mathcal{D}'(\Omega)$ . Note that

$$\mathbf{A}^*(\mu, w) = \mathbf{A}(\mu, \varphi) \quad (2.8)$$

whenever  $w = -\nabla \cdot (\mu \nabla \varphi)$ . The connection to Wasserstein geometry is given by the infinitesimal Benamou–Brenier formula

$$\frac{1}{2} |\dot{\mu}_t|_{\mathbf{W}_2}^2 = \mathbf{A}^*(\mu_t, \partial_t \mu_t).$$

Moreover, the relative Fisher information can then be written as

$$\frac{1}{2} |\partial_{\mathbf{W}_2} \mathbf{H}(\mu)|^2 = \mathbf{A}(\mu, -D\mathbf{H}(\mu)), \quad (2.9)$$

where  $D\mathbf{H}(\mu) = \log \rho$  is the  $L^2(\bar{\mathbf{m}})$ -differential of  $\mathbf{H}$ . Hence, it follows from (2.8) and (2.9) that (2.5) can be equivalently stated as

$$\mathbf{H}(\mu_T) + \int_0^T \mathbf{A}^*(\mu_t, \dot{\mu}_t) + \mathbf{A}(\mu_t, -D\mathbf{H}(\mu_t)) dt \leq \mathbf{H}(\mu_0). \quad (2.10)$$

This formulation is particularly convenient to relate the continuous framework to the continuous one, as we discuss in the next subsection.

**Discrete optimal transport and gradient flows.** Since the works of [Maa11] and [Mie11], entropy gradient flows have been widely investigated in discrete settings as well. The connection between a novel discrete optimal transport distance and some evolution equations, such as heat flow on finite graphs, have been analysed and many properties of such metric structures have been studied (see e.g. [EM12], [Mie13], [EM14], [MPR14], [FM16]). In this work we focus on discrete spaces arising from finite volume discretisations.

**The discrete Fokker-Planck equation as gradient flow.** We consider a finite partition  $\mathcal{T}$  of  $\bar{\Omega}$  into sets (called cells) with nonempty and convex interior. We assume that  $\mathcal{T}$  is *admissible*, in the sense that each of the cells  $K \in \mathcal{T}$  contains a point  $x_K \in \bar{K}$  such that  $x_K - x_L$  is orthogonal to  $\Gamma_{KL} := \partial K \cap \partial L$  for any neighbouring cell  $L$  of  $K$ . Furthermore, we assume that the mesh is  $\zeta$ -regular for  $\zeta \in (0, 1]$ , which means that the following conditions hold:

$$\begin{aligned} (\text{inner ball}) \quad & B(x_K, \zeta[\mathcal{T}]) \subseteq K && \text{for all } K \in \mathcal{T}, \\ (\text{area bound}) \quad & \mathcal{H}^{d-1}(\Gamma_{KL}) \geq \zeta[\mathcal{T}]^{d-1} && \text{for all } K, L \in \mathcal{T} \text{ with } K \sim L, \end{aligned} \quad (2.11)$$

where  $[\mathcal{T}] := \max\{\text{diam}(K) : K \in \mathcal{T}\}$  denotes the size of the mesh.

We consider a reversible continuous-time random walk on  $\mathcal{T}$  with invariant measure  $\pi$  and edge weights  $w_{KL}$  given by

$$\pi(\{K\}) := \bar{\mathbf{m}}(K), \quad w_{KL} := \frac{\mathcal{H}^{d-1}(\Gamma_{KL})}{d_{KL}} S_{KL} \quad \text{for } K \sim L. \quad (2.12)$$

Here we write  $d_{KL} := |x_K - x_L|$  and  $S_{KL}$  is a suitable average of the density on  $K$  and  $L$  viz.

$$S_{KL} := \theta(\sigma(x_K), \sigma(x_L)) \quad (2.13)$$

for some fixed function  $\theta : \mathbb{R}_+ \times \mathbb{R}_+ \rightarrow \mathbb{R}_+$  satisfying

$$\min\{a, b\} \leq \theta(a, b) \leq \max\{a, b\}.$$

The associated Kolmogorov forward equation is a discrete approximation of (2.1), given by

$$\frac{d}{dt} m_t(K) = \sum_{L \sim K} w_{KL} \left( \frac{m_t(L)}{\pi_L} - \frac{m_t(K)}{\pi_K} \right). \quad (2.14)$$

It was shown in [Maa11] and [Mie11] that this equation is the gradient flow of the discrete relative entropy

$$\mathcal{H}_{\mathcal{T}}(m) := \sum_{K \in \mathcal{T}} m(K) \log \frac{m(K)}{\pi_K^{\mathcal{T}}}.$$

Thus (2.14) can be written as  $\frac{dm}{dt} = -\mathcal{K}_{\mathcal{T}}(m)D\mathcal{H}_{\mathcal{T}}(m)$ , with an Onsager operator  $\mathcal{K}_{\mathcal{T}} : \mathcal{P}(\mathcal{T}) \times L^2(\mathcal{T}, \pi) \rightarrow L^2(\mathcal{T}, \pi)$  given by

$$(\mathcal{K}_{\mathcal{T}}(m)f)(K) = \sum_{L \in \mathcal{T}} w_{KL} \theta_{\log} \left( \frac{m_K}{\pi_K^{\mathcal{T}}}, \frac{m_L}{\pi_L^{\mathcal{T}}} \right) (f(L) - f(K)). \quad (2.15)$$

The discrete analogue of (2.7) is given by the operator  $\mathcal{A}_{\mathcal{T}} : \mathcal{P}(\mathcal{T}) \times L^2(\mathcal{T}, \pi) \rightarrow \mathbb{R}_+$  defined by

$$\mathcal{A}_{\mathcal{T}}(m, f) = \frac{1}{4} \sum_{K, L \in \mathcal{T}} (f(K) - f(L))^2 \theta_{\log} \left( \frac{m_K}{\pi_K^{\mathcal{T}}}, \frac{m_L}{\pi_L^{\mathcal{T}}} \right) w_{KL}, \quad (2.16)$$

where  $w$  is defined in (2.12). As in the continuous setting,

$$\mathcal{A}_{\mathcal{T}}^*(m_t, \dot{m}_t) = \frac{1}{2} |\dot{m}_t|_{\mathcal{W}_{\mathcal{T}}}^2.$$

Written in the metric EDI-formulation, (2.14) is equivalent to

$$\mathcal{H}_{\mathcal{T}}(m_t) + \int_0^T \mathcal{A}_{\mathcal{T}}^*(m_t, \dot{m}_t) + \mathcal{A}_{\mathcal{T}}(m_t, -D\mathcal{H}_{\mathcal{T}}(m_t)) dt \leq \mathcal{H}_{\mathcal{T}}(m_0). \quad (2.17)$$

On the other hand, in the finite dimensional setting of  $\mathcal{P}(\mathcal{T})$  we simply have

$$\begin{aligned} \mathcal{A}_{\mathcal{T}}(m_t, -D\mathcal{H}_{\mathcal{T}}(m_t)) &= \frac{1}{2} \langle \mathcal{K}_{\mathcal{T}}^{-1}(m_t) \nabla_{\mathcal{W}_{\mathcal{T}}} \mathcal{H}_{\mathcal{T}}(m_t), \nabla_{\mathcal{W}_{\mathcal{T}}} \mathcal{H}_{\mathcal{T}}(m_t) \rangle \\ &= \frac{1}{2} |\nabla_{\mathcal{W}_{\mathcal{T}}} \mathcal{H}_{\mathcal{T}}(m_t)|_{\mathcal{W}_{\mathcal{T}}}^2, \end{aligned}$$

which is the finite-dimensional counterpart of (2.6). As in the continuous setting, the *discrete Fisher information* relative to  $\mathcal{H}_{\mathcal{T}}$  is given by

$$\mathcal{I}_{\mathcal{T}}(m) := 2\mathcal{A}_{\mathcal{T}}(m, -D\mathcal{H}_{\mathcal{T}}(m)) \quad \text{for } m \in \mathcal{P}(\mathcal{T}). \quad (2.18)$$

### 3. STATEMENT OF THE MAIN RESULTS

In this section we present our main result, the evolutionary  $\Gamma$ -convergence of the discrete to continuous gradient flow structures. The proof of this result in Section 5 is based on regularity results for discrete flows [FMP20] and on a Mosco convergence result for discrete energies (cf. Section 5) of independent interest.

We consider a sequence of admissible,  $\zeta$ -regular meshes  $\mathcal{T}_N$  with vanishing mesh size  $[\mathcal{T}_N] \rightarrow 0$  as  $N \rightarrow +\infty$ . To avoid towers of subscripts, we simply write  $\mathcal{A}_N := \mathcal{A}_{\mathcal{T}_N}$ ,  $\mathcal{W}_N := \mathcal{W}_{\mathcal{T}_N}$ , etc.

We introduce the canonical embedding  $\iota_{\mathcal{T}} : \mathcal{P}(\mathcal{T}) \rightarrow \mathcal{P}(\Omega)$  defined by

$$\iota_{\mathcal{T}} m = \sum_{K \in \mathcal{T}} m(K) \mathcal{U}_K \quad \text{for } m \in \mathcal{P}(\mathcal{T}), \quad (3.1)$$

where  $\mathcal{U}_K$  denotes the uniform probability measure on  $K \subset \Omega$ .

The corresponding projection operator  $P_{\mathcal{T}} : \mathcal{P}(\Omega) \rightarrow \mathcal{P}(\mathcal{T})$  is given by

$$(P_{\mathcal{T}} \mu)(K) = \mu(K) \quad (3.2)$$

for  $K \in \mathcal{T}$ . In particular,  $\iota_{\mathcal{T}}$  is a right-inverse of  $P_{\mathcal{T}}$ . By construction we then have  $\pi_{\mathcal{T}} := P_{\mathcal{T}}\bar{m}$ .

We denote by  $r$  the density of  $m \in \mathcal{P}(\mathcal{T})$  with respect to  $\pi_{\mathcal{T}}$ , namely

$$dm = r d\pi_{\mathcal{T}} \iff r(K) = \frac{m(K)}{\pi_{\mathcal{T}}(K)} \quad \forall K \in \mathcal{T}.$$

**Definition 3.1** (Assumptions on approximating sequences). *Let  $(\mathcal{T}_N)_N$  be a vanishing sequence of  $\zeta$ -regular meshes and let  $m_N \in \mathcal{P}(\mathcal{T}_N)$  for  $N \geq 1$ . Write  $r_N = \frac{m_N}{\pi_N}$ . We consider the following conditions:*

(i) *The density lower bound holds if for some  $\underline{k} > 0$ ,*

$$\inf_{K \in \mathcal{T}_N} r_N(K) \geq \underline{k} > 0 \quad \forall N \in \mathbb{N}. \quad (\text{lb})$$

(ii) *The upper bound holds if for some  $\bar{k} < \infty$ ,*

$$\sup_{K \in \mathcal{T}_N} r_N(K) \leq \bar{k} < +\infty \quad \forall N \in \mathbb{N}. \quad (\text{ub})$$

(iii) *The neighbour continuity bound holds if*

$$\lim_{N \rightarrow \infty} \sup_{K \sim L \in \mathcal{T}_N} |r_N(K) - r_N(L)| = 0. \quad (\text{nc})$$

(iv) *The pointwise condition holds if  $\mu_N := \iota_N m_N \rightharpoonup \mu$  for some  $\mu \in \mathcal{P}(\bar{\Omega})$  with density  $\rho = \frac{d\mu}{d\bar{m}}$  and the following inequalities hold:*

$$\lim_{\varepsilon \rightarrow 0} \liminf_{N \rightarrow \infty} \sup_{x \in Q_\varepsilon(x_0)} \rho_N(x) \leq \rho(x_0) \leq \lim_{\varepsilon \rightarrow 0} \limsup_{N \rightarrow \infty} \inf_{x \in Q_\varepsilon(x_0)} \rho_N(x) \quad (\text{pc})$$

for a.e.  $x_0 \in \Omega$ , where  $Q_\varepsilon(x_0)$  denotes the open cube of size  $\varepsilon > 0$  centred in  $x_0$  and  $\rho_N(x) := r_N(K)$  for  $x \in K$ .

*Remark 3.2.* Clearly, the pointwise condition holds if there is pointwise convergence  $\rho_N(x) \rightarrow \rho(x)$  for all  $x \in \bar{\Omega}$ .

We first present a  $\liminf$ - $\Gamma$  convergence result. Then we apply it to the case of solutions of the discrete flows to obtain the evolutionary  $\Gamma$ -convergence results. Note that in fact the lower bound condition (lb) is not needed to obtain the first and the third bound in the theorem below.

**Theorem 3.3** (Lower bounds). *Let  $(\mathcal{T}_N)_N$  be a vanishing sequence of  $\zeta$ -regular meshes. Let  $\mu \in \mathcal{P}(\bar{\Omega})$  and  $m_N \in \mathcal{P}(\mathcal{T}_N)$  be such that  $\mu_N := \iota_N m_N \rightharpoonup \mu$  as  $N \rightarrow \infty$ . Then the following assertions hold:*

(i) *We have the following lower semicontinuity estimate for the entropies:*

$$\liminf_{N \rightarrow \infty} \mathcal{H}_N(m_N) \geq \mathbf{H}(\mu). \quad (3.3)$$

(ii) *Assume (lb), (ub) and (pc). Then*

$$\liminf_{N \rightarrow \infty} \mathcal{A}_N^*(m_N, e_N) \geq \mathbf{A}^*(\mu, \eta) \quad (3.4)$$

for every sequence  $(e_N)_N$  such that  $\iota_N e_N \rightharpoonup \eta$  in  $L^2(\Omega)$ . The same bound also holds without assuming (lb) if  $(e_N)_N$  satisfies

$$\limsup_{N \rightarrow \infty} \mathcal{A}_N^*(m_N, e_N) < +\infty. \quad (3.5)$$

(iii) Assume (nc). Then we have the following estimate for the Fisher information (as defined in (2.18) and (2.9), respectively):

$$\liminf_{N \rightarrow \infty} \mathcal{I}_N(m_N) \geq \mathbf{I}(\mu). \quad (3.6)$$

*Remark 3.4.* The bound in (3.4) can be obtained without assuming (ub) and (pc) if the mesh satisfies the so-called asymptotic isotropy condition (4.3) see Definition 4.1 and Proposition 4.3.

*Remark 3.5.* If  $m_N = P_N(\rho dx)$  for some continuous density  $\rho$ , the same result as in (ii) can be proved more generally for all  $e_N \in \mathcal{M}(\mathcal{T}_N)$ ,  $\eta \in \mathcal{M}(\Omega)$  and  $\iota_N e_N \rightharpoonup \eta$  in  $\mathcal{D}'(\Omega)$ . This is a consequence of an explicit construction of the recovery sequence for the action  $\mathcal{A}_N(m_N, \cdot)$  as in the isotropic case in Proposition 4.3; see Remark 8.7.

As a consequence of the previous result, we are able to obtain the evolutionary  $\Gamma$ -convergence of the discrete Wasserstein gradient structures.

Pick an initial measure  $\mu_0 \in \mathcal{P}(\bar{\Omega})$  such that  $\mathbf{H}(\mu_0) < +\infty$  and a sequence of approximating measures  $m_0^N \in \mathcal{P}(\mathcal{T}_N)$  satisfying  $\iota_N m_0^N \rightharpoonup \mu_0$ . For every  $N$  we consider the solution to the discrete Fokker-Planck equation  $m_t^N$  (2.14) with initial datum  $m_0^N$ .

Taking (2.17) into account, this equivalently reads

$$\mathcal{H}_N(m_t^N) + \int_0^T \mathcal{A}_N^*(m_t^N, \dot{m}_t^N) + \mathcal{A}_N(m_t^N, -D\mathcal{H}_N(m_t^N)) dt \leq \mathcal{H}_N(m_0^N).$$

Our main result shows that one can pass to the limit at the level of the discrete gradient flow formulation (2.17) in each of its parts and, as a consequence, recover the gradient flow structure in the limit as  $N \rightarrow \infty$ .

**Theorem 3.6** (Evolutionary  $\Gamma$ -convergence, Wasserstein case). *Let  $T > 0$  and consider a sequence of  $\zeta$ -admissible meshes  $(\mathcal{T}_N)_N$ . Fix an initial measure  $\mu_0 \in \mathcal{P}(\bar{\Omega})$  such that  $\mathbf{H}(\mu_0) < +\infty$ , together with measures  $m_0^N \in \mathcal{P}(\mathcal{T}_N)$  for  $N \geq 1$ , that are well-prepared in the sense that*

$$\iota_N m_0^N \rightharpoonup \mu_0 \quad \text{and} \quad \lim_{N \rightarrow +\infty} \mathcal{H}_N(m_0^N) = \mathbf{H}(\mu_0).$$

*Then the sequence of curves  $(\mu^N)_N$  defined by  $\mu_t^N := \iota_N m_t^N$  is compact in the space  $C([0, T]; (\mathcal{P}(\bar{\Omega}), \mathbf{W}_2))$ . Thus, up to a subsequence, we have for every  $t \in [0, T]$ ,*

$$\iota_N m_t^N \xrightarrow{\mathbf{W}_2} \mu_t \quad \text{as } N \rightarrow \infty. \quad (3.7)$$

*Moreover, the following estimates hold:*

$$\liminf_{N \rightarrow \infty} \mathcal{H}_N(m_t^N) \geq \mathbf{H}(\mu_t) \quad \forall t \in [0, T] \quad (\text{Entropy})$$

$$\liminf_{N \rightarrow \infty} \int_0^T \mathcal{A}_N^*(m_t^N, \dot{m}_t^N) dt \geq \int_0^T \mathbf{A}^*(\mu_t, \dot{\mu}_t) dt, \quad (\text{Metric derivative})$$

$$\liminf_{N \rightarrow \infty} \int_0^T \mathcal{A}_N(m_t^N, -D\mathcal{H}_N(m_t^N)) dt \geq \int_0^T \mathbf{A}(\mu_t, -D\mathbf{H}(\mu_t)) dt. \quad (\text{Fisher info})$$

*Moreover,  $(\mu_t)_t$  solves (2.5) and (equivalently) the continuous Fokker-Planck equation (1.1).*

*Remark 3.7.* The well-preparedness assumption holds in the special case where the discrete measures are defined by  $m_0^N := P_N \mu_0$  as in (3.2). Indeed, in that case we have  $\mathcal{H}_N(m_0^N) = \mathbf{H}(\iota_N P_N \mu_0)$  and the well-preparedness follows from Jensen's inequality.

Finally, in the last section of this work we also show that the result obtained in Section 7 can be used to prove the evolutionary  $\Gamma$ -convergence of some Hilbertian gradient flow structures which are an equivalent representation of the Fokker-Planck equations.

#### 4. PREVIOUS WORKS AND KNOWN RESULTS

In this section we discuss the general state of the art about convergence results of discrete Fokker-Planck structures to continuous ones.

**The convergence of the discrete flows.** It is well known [EGH00], [BHO18] (for dimension  $d = 2, 3$  at least) that the discrete heat flow converges in an appropriate sense to the continuous one, whenever one takes a vanishing sequence of admissible meshes. The authors in [EGH00], [BHO18] do not rely on a precise analysis of the flow and work mainly at the level of the equation. In particular, they exploit classical Sobolev a priori estimates and pass to the limit in a weak formulation directly at the level of the Laplacian (see e.g. [BHO18, Lemma 8]). The idea of the current work (as well as [DL15]) is to approach the problem of the convergence of discrete flows to the continuous one with a thorough analysis of different gradient flow structures as introduced in Section 2. Henceforth, the analysis itself does not rely on an application of semigroup theory and does not require a linear structure of the equation, leaving doors open for possible generalizations of such methods to non-linear settings.

**The one-dimensional setting.** The evolutionary  $\Gamma$ -convergence result has been obtained in the one-dimensional setting under additional geometric conditions using methods that do not extend in a straightforward fashion to higher dimensions.

First of all, in [DL15] a sequence of meshes that satisfies the center of mass condition

$$\int_{\partial K \cap \partial L} x \, d\mathcal{H}^{d-1} = \frac{x_K + x_L}{2}, \quad \text{for all } K \sim L \in \mathcal{T} \quad (4.1)$$

is used. Such a condition is sufficient, for example, to obtain the convergence of the discrete transport distance  $\mathcal{W}_N$  to the continuous one  $\mathbf{W}_2$ . Indeed, it is possible to show that (4.1) implies an isotropy condition of the mesh, which has been proved in [GKM18] to be sufficient (and essentially necessary) for the convergence of the distances; see also Definition 4.1 for more details.

More substantially, the one dimensional setting allows for an easier correspondence between the discrete setting and the continuous one, not only at the level of the measures (which is always possible via the maps  $\iota_{\mathcal{T}}$  and  $P_{\mathcal{T}}$ ) but also at the level of the vectorfields. In particular, given a solution  $(m_t, V_t)$  to the discrete continuity equation

$$\dot{m}_t = \mathcal{K}_{\mathcal{T}}(m_t)V_t, \quad (4.2)$$

with an Onsager operator  $\mathcal{K}_{\mathcal{T}}$  as given in (2.15), it is possible to define, just by linear interpolation on the points  $x_K$ , a continuous vectorfield  $v_t$  which is suitably close to



$V_t$  in the sense that  $(\iota_{\mathcal{T}}m_t, v_t)$  solves the continuity equation at the continuous level (2.4).

Such an explicit construction breaks down as soon as one considers dimensions  $d \geq 2$ . In particular, it is not clear how to define such an interpolation between a discrete vectorfield  $V_t(K, L)$  and a continuous one  $v_t(x)$ , which retains compatibility with the continuity equation as well.

In this work we drastically change both perspective and approach. Indeed, we do not rely on any explicit extension but rather attack the problem from a more variational point of view.

**Scaling limits for discrete optimal transport in any dimension.** In this short section we recall the key result obtained in [GKM18] about the convergence of the discrete transport distances. The authors proved that admissibility of the meshes is not sufficient to ensure the convergence of  $\mathcal{W}_{\mathcal{T}}$  to  $\mathbf{W}_2$ ; see also [GKMP19] for the study of discrete distances for general periodic partitions.

Nonetheless, the center of mass condition used in [DL15] can be weakened, in any dimension, by the so-called *asymptotic isotropy condition* [GKM18, Definition 1.3].

Below,  $[\mathcal{T}]$  denotes again the maximum diameter of a mesh.

**Definition 4.1** (Asymptotic isotropy). *A vanishing sequence of meshes  $(\mathcal{T}_N)_N$  is said to satisfy the asymptotic isotropy condition if for every  $N \in \mathbb{N}$  it holds*

$$\frac{1}{2} \sum_{L \in \mathcal{T}} w_{KL} (x_K - x_L) \otimes (x_K - x_L) \leq \pi(K) (I_d + \eta_{\mathcal{T}}(K)) \quad \forall K \in \mathcal{T}_N, \quad (4.3)$$

where  $\sup_{K \in \mathcal{T}_N} \|\eta_{\mathcal{T}}(K)\| \rightarrow 0$  as  $N \rightarrow \infty$ .

In the sequel  $(H_{\varepsilon})_{\varepsilon \geq 0}$  denotes the heat semigroup in  $\mathbb{R}^d$  and  $\mathcal{M}_0(\mathcal{T})$  the space of signed measure on  $\mathcal{T}$  with zero mass. The following coarse bound is taken from [GKM18, Lemma 3.4].

**Lemma 4.2** (Coarse energy bound). *Let  $\mathcal{T}$  be a  $\zeta$ -regular mesh. There exists a constant  $C < \infty$  such that for any  $m \in \mathcal{P}(\mathcal{T})$  and  $\sigma \in \mathcal{M}_0(\mathcal{T})$  we have*

$$\mathbf{A}^*(H_{[\mathcal{T}]} \iota_{\mathcal{T}} m, H_{[\mathcal{T}]} \iota_{\mathcal{T}} \sigma) \leq C \mathcal{A}_{\mathcal{T}}^*(m, \sigma). \quad (4.4)$$

Let us stress that the previous result holds without any isotropy assumption on the mesh. On the contrary, the next result instead relies on this condition.

**Proposition 4.3** (Action bounds). *Let  $(\mathcal{T}_N)_N$  be a sequence of meshes satisfying the asymptotic isotropy condition (4.3). Suppose  $m_N \in \mathcal{P}(\mathcal{T}_N)$  are such that  $\iota_N m_N \rightarrow \mu$  as  $N \rightarrow \infty$  for some  $\mu \in \mathcal{P}(\overline{\Omega})$ .*

(i) *Pick any  $\phi \in C^1(\overline{\Omega})$  and define  $f_N : \mathcal{T}_N \rightarrow \mathbb{R}$  by  $f_N(K) := \phi(x_K)$ . Then we have the upper bound*

$$\limsup_{N \rightarrow \infty} \mathcal{A}_{\mathcal{T}_N}(m_N, f_N) \leq \mathbf{A}(\mu, \phi). \quad (4.5)$$

(ii) *Let  $e_N \in \mathcal{M}_0(\mathcal{T}_N)$  and suppose that there exists  $\eta \in \mathcal{M}_0(\overline{\Omega})$  such that  $\iota_N e_N \rightarrow \eta$  as  $N \rightarrow \infty$ . Then we have the lower bound*

$$\mathbf{A}^*(\mu, \eta) \leq \liminf_{N \rightarrow \infty} \mathcal{A}_{\mathcal{T}_N}^*(m_N, e_N). \quad (4.6)$$

*Proof.* The proof is a straightforward modification of the one of [GKM18, Proposition 6.6], taking into account that  $\bar{\mathbf{m}}$  has a continuous and bounded density, both from below and above.  $\square$

Assuming the isotropy condition, the previous theorem shows that the same bound can be used to prove the lower bound for the metric derivative in (2.8); see also Remark 3.4.

*Remark 4.4.* The proof in [GKM18, Proposition 6.6] shows that whenever (4.5) holds for some sequence  $(f_N)_N$  such that  $\iota_N f_N \rightarrow \phi$  in  $L^2(\Omega)$ , then (ii) holds for every  $\iota_N e_N \rightarrow \eta$  in  $L^2(\Omega)$ , even if one a priori does not assume any local isotropy (4.3) of the meshes.

**Regularity of the discrete flows.** A key ingredient in the proof of our main result, Theorem 3.6, is a regularity result for the discrete Fokker-Planck equation that can be derived from a Harnack inequality [CKW19]; see also [FMP20].

**Proposition 4.5** (Regularity of discrete flows). *Let  $\mathcal{T}$  be a  $\zeta$ -regular mesh, let  $(m_t)_t$  be a solution to the discrete Fokker-Planck equation, and set  $r_t := \frac{dm_t}{d\pi}$ .*

- (i) *For any  $t > 0$ , there exist  $C = C(\Omega, \bar{\mathbf{m}}, \zeta, t) < +\infty$  and  $\lambda = \lambda(\Omega, \bar{\mathbf{m}}, \zeta) > 0$  such that the following Hölder estimate holds:*

$$|r_t(K) - r_t(L)| \leq C |x_K - x_L|^\lambda \sup_{K' \in \mathcal{T}} |r_{t/2}(K')| \quad \forall K, L \in \mathcal{T}. \quad (4.7)$$

- (ii) *For any  $t > 0$  the ultracontractivity estimate*

$$\|r_t\|_{L^\infty} \leq C t^{-\frac{d}{2}} \|r_0\|_{L^1(\pi)} \quad (4.8)$$

*holds for a constant  $C = C(\Omega, \bar{\mathbf{m}}, \zeta) < +\infty$ .*

We stress that the constants depend only on the aforementioned parameters.

## 5. PROOF OF THE MAIN RESULT: THE WASSERSTEIN EVOLUTIONARY $\Gamma$ -CONVERGENCE

In this section we prove our main result, the evolutionary  $\Gamma$ -convergence of the discrete gradient flow structures (Theorem 3.6). The section is divided into three parts: The first subsection contains a proof of compactness for the continuously embedded discrete solutions and some *a priori* estimates at first order in time (Proposition 5.2). The second subsection concerns the proof of Theorem 3.3, which relies on Theorem 7.2. In the third and final part we complete the proof of Theorem 3.6.

**5.1. Compactness and space-time regularity.** In this section we prove the compactness of the family of curves  $(t \mapsto \mu_t^N)_N$  in the space  $C([0, T]; (\mathcal{P}(\bar{\Omega}), \mathbf{W}_2))$ . We follow the strategy employed in [LMPR17, Theorem 3.1], which is based on a metric Arzelà-Ascoli theorem.

The corresponding one-dimensional result has been obtained in [DL15] using explicit interpolation formulas that are not available in the multi-dimensional setting. Our proof is based on the coarse bounds obtained in Lemma 4.2.

**Lemma 5.1** ( $\mathbf{W}_2$ -Equi-continuity). *Let  $\{\mathcal{T}_N\}_N$  be a family of admissible and  $\zeta$ -regular meshes. For each  $N \in \mathbb{N}$ , let  $(m_t^N)_{t \in [0, T]}$  be a continuous curve in  $\mathcal{P}(\mathcal{T}_N)$*

and suppose that the following uniform energy bound holds:

$$A := \sup_N \int_0^T \mathcal{A}_N^*(m_t^N, \dot{m}_t^N) dt < +\infty. \quad (5.1)$$

Then the curves  $\tilde{\mu}^N : [0, T] \rightarrow (\mathcal{P}(\bar{\Omega}), \mathbf{W}_2)$  defined by  $\tilde{\mu}_t^N := H_{[\mathcal{T}_N]} \iota_N m_t^N$  are equi- $\frac{1}{2}$ -Hölder continuous, i.e. for all  $0 \leq s < t \leq T$  we have

$$\mathbf{W}_2(\tilde{\mu}_t^N, \tilde{\mu}_s^N) \lesssim \sqrt{A(t-s)}. \quad (5.2)$$

*Proof.* For  $0 \leq s \leq t \leq T$  we invoke the Benamou-Brenier formula (2.3) and Lemma 4.2 to obtain

$$\begin{aligned} \mathbf{W}_2^2(\tilde{\mu}_t^N, \tilde{\mu}_s^N) &\leq (t-s) \int_s^t \mathbf{A}^*(\tilde{\mu}_h^N, \partial_h \tilde{\mu}_h^N) dh \\ &\lesssim (t-s) \sup_N \int_0^T \mathcal{A}_N^*(m_h^N, \partial_h m_h^N) dh \leq A(t-s), \end{aligned}$$

which concludes the proof.  $\square$

An immediate corollary of Lemma 5.1 is the following compactness result. We also obtain a regularity result that will be used in Section 5.3 below to pass to the limit at the level of the metric derivative.

**Proposition 5.2** (Compactness and regularity). *For  $t \in [0, T]$  and  $N \geq 1$  let  $\mu_t^N := \iota_N m_t^N \in \mathcal{P}(\bar{\Omega})$  be defined as in Theorem 3.6.*

(i) *There exists a  $\mathbf{W}_2$ -continuous curve  $t \mapsto \mu_t \in \mathcal{P}(\bar{\Omega})$  satisfying, up to a subsequence,*

$$\sup_{t \in [0, T]} \mathbf{W}_2(\mu_t^N, \mu_t) \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

(ii) *The density  $\rho_t := \frac{d\mu_t}{d\mathfrak{m}}$  exists for a.e.  $t > 0$ . Moreover, for each  $\delta \in (0, T)$ , the curve  $t \mapsto \rho_t$  belongs to  $H^1((\delta, T); L^2(\Omega))$ , and the sequence  $(\dot{\rho}^N)_N$  has a subsequence converging weakly in  $L^2((\delta, T); L^2(\Omega))$  to a curve  $t \mapsto \dot{\rho}_t$ .*

*Proof.* (i) We apply Lemma 5.1 to the family of discrete gradient flow solutions  $(t \mapsto m_t^N)_N$ . In this case, the required estimate (5.1) follows directly from the discrete EDI in (2.17) and the well-preparedness of the initial conditions  $(m_0^N)_N$ . Thus, Lemma 5.1 implies the  $\mathbf{W}_2$ -equi-continuity of the curves  $(\mu^N)_N$  defined by  $\tilde{\mu}_t^N := H_{\varepsilon_N} \iota_N m_t^N$ , where  $\varepsilon_N := [\mathcal{T}_N]$ .

The metric Arzelá-Ascoli Theorem [AGS08, Lemma 9.4.3] yields the existence of a limiting curve  $t \mapsto \mu_t$  satisfying  $\sup_t \mathbf{W}_2(\tilde{\mu}_t^N, \mu_t) \rightarrow 0$ . Using the well-known heat flow bound  $\mathbf{W}_2(\tilde{\mu}_t^N, \mu_t^N) \leq C\sqrt{\varepsilon_N}$  (see e.g. [GKM18, Lemma 2.2(iii)] for a proof), we obtain the desired result.

(ii) Fix  $0 < \delta < T$ . By self-adjointness of the discrete generator  $\mathcal{L}_N$  in  $L^2(\mathcal{T}_N, \pi_N)$  we have

$$\|\dot{r}_t^N\|_{L^2(\mathcal{T}_N, \pi_N)} = \|\mathcal{L}_N r_t^N\|_{L^2(\mathcal{T}_N, \pi_N)} \leq (t - \delta/2)^{-1} \|r_{\delta/2}^N\|_{L^2(\mathcal{T}_N, \pi_N)}$$

for any  $t > \delta/2$ ; see e.g. [Bre10, Theorem 7.7]. Moreover, from (4.8) we infer that

$$\|r_t^N\|_{L^\infty(\mathcal{T}_N, \pi_N)} \lesssim t^{-\frac{d}{2}}$$

for  $t > 0$ . It follows from those bounds that

$$\int_{\delta}^T \|\rho_t^N\|_{L^2(\Omega)}^2 dt \lesssim T\delta^{-d} \quad \text{and} \quad \int_{\delta}^T \|\dot{\rho}_t^N\|_{L^2(\Omega)}^2 dt \lesssim \delta^{-(d+1)}.$$

The Banach-Alaoglu theorem implies that there exists a subsequence such that  $(\rho^N)_N$  and  $(\dot{\rho}^N)_N$  converge weakly in  $L^2((\delta, T); L^2(\Omega))$  to limit curves  $\bar{\rho}^\delta$  and  $\bar{\sigma}^\delta$ , respectively. In view of (i) we infer that  $\bar{\rho}_t^\delta$  coincides with  $\rho_t := \frac{d\mu_t}{d\bar{\mathbf{m}}}$  for any  $\delta$ . Integration by parts yields for any  $\phi \in C_c^1((\delta, T); L^2(\Omega))$ ,

$$\int_{\delta}^T \langle \dot{\rho}_t^N, \phi_t \rangle_{L^2(\Omega)} dt = - \int_{\delta}^T \langle \rho_t^N, \dot{\phi}_t \rangle_{L^2(\Omega)} dt.$$

As both  $(\rho^N)_N$  and  $(\dot{\rho}^N)_N$  converge weakly in  $L^2((2\delta, T); L^2(\Omega))$ , we may pass to the limit to arrive at

$$\int_{\delta}^T \langle \bar{\sigma}^\delta, \phi_t \rangle_{L^2(\Omega)} dt = - \int_{\delta}^T \langle \rho_t, \dot{\phi}_t \rangle_{L^2(\Omega)} dt,$$

which shows that  $\bar{\sigma}_t^\delta$  is the weak derivative of  $\rho_t$  on  $(\delta, T)$ .  $\square$

*Remark 5.3.* Under stronger assumptions on the initial data (namely, well-preparedness of the Dirichlet energies) it is possible to deduce the weak compactness in the Sobolev space  $H^1((0, T); L^2(\Omega, \bar{\mathbf{m}}))$  directly from the EDI formulation in  $L^2(\Omega, \bar{\mathbf{m}})$  (6.2), as done in [Mie16, Theorem 3.3].

**5.2. Asymptotic lower bounds for the functionals.** We now have all the tools needed to prove Theorem 3.3.

*Proof of Theorem 3.3.* Let  $\mu$  and  $m_N$  be as in the statement of the theorem.

(i) *Lower bound for the entropy.* Note that  $\mathcal{H}_N(m_N) = \text{Ent}(\mu_N | \iota_N \pi_N)$  and  $\mathbf{H}(\mu) = \text{Ent}(\mu | \bar{\mathbf{m}})$ , where  $\text{Ent}(\cdot | \cdot)$  denotes the relative entropy. Since  $\mu_N \rightarrow \mu$  and  $\iota_N \pi_N \rightarrow \bar{\mathbf{m}}$ , the result follows immediately from the joint weak lower semicontinuity of  $\text{Ent}(\cdot | \cdot)$ , see e.g. [AGS08, Lemma 9.4.3].

(ii) *Lower bound for  $\mathcal{A}_N^*$ .* Assume first that (lb), (ub) and (pc) hold. Theorem 7.2 (in particular, the existence of a recovery sequence) implies that for every  $\phi \in C(\bar{\Omega})$  there exist  $f_N \in L^2(\mathcal{T}_N, \pi_N)$  such that  $\iota_N f_N \rightarrow \phi$  in  $L^2(\Omega, \bar{\mathbf{m}})$  and

$$\limsup_{N \rightarrow \infty} \mathcal{A}_N(m_N, f_N) \leq \mathbf{A}(\mu, \phi).$$

Since  $\iota_N e_N \rightarrow \eta$  in  $L^2(\Omega, \bar{\mathbf{m}})$ , it follows that  $\langle e_N, f_N \rangle_{L^2(\mathcal{T}_N, \pi_N)} \rightarrow \langle \eta, \phi \rangle_{L^2(\Omega, \bar{\mathbf{m}})}$  and

$$\begin{aligned} \langle \eta, \phi \rangle_{L^2(\Omega, \bar{\mathbf{m}})} - \mathbf{A}(\mu, \phi) &\leq \liminf_{N \rightarrow \infty} \langle e_N, f_N \rangle_{L^2(\mathcal{T}_N, \pi_N)} - \mathcal{A}_N(m_N, f_N) \\ &\leq \liminf_{N \rightarrow \infty} \mathcal{A}_N^*(m_N, e_N). \end{aligned}$$

Taking the supremum over  $\phi$ , we infer that  $\mathbf{A}^*(\mu, \eta) \leq \liminf_{N \rightarrow \infty} \mathcal{A}_N^*(m_N, e_N)$ , as desired.

Assume now that only (ub), (pc) hold, and that (3.5) holds in addition, i.e. we assume that  $E := \limsup_{N \rightarrow \infty} \mathcal{A}_N^*(\pi_N, e_N) < +\infty$ . The key observation is that the map  $m_N \mapsto \mathcal{A}_N^*(m_N, e_N)$  is convex. Indeed, the concavity of  $\theta_{\log}$  implies the concavity of  $m_N \mapsto \mathcal{A}(m_N, f_N)$ , and thus the convexity of its Legendre dual as a supremum of convex maps. To take advantage of this fact, we define  $m_N^\delta := (1 - \delta)m_N + \delta\pi_N$  for  $\delta \in [0, 1]$  and obtain

$$(1 - \delta)\mathcal{A}_N^*(m_N, e_N) \geq \mathcal{A}_N^*(m_N^\delta, e_N) - \delta\mathcal{A}_N^*(\pi_N, e_N).$$

Using (3.5) we obtain

$$(1 - \delta) \liminf_{N \rightarrow \infty} \mathcal{A}_N^*(m_N, e_N) \geq \liminf_{N \rightarrow \infty} \mathcal{A}_N^*(m_N^\delta, e_N) - \delta E$$

for every  $\delta \in [0, 1]$ . Note that  $\iota_N m_N^\delta \rightharpoonup \mu^\delta := (1 - \delta)\mu + \delta \bar{\mathbf{m}}$  and  $m_N^\delta$  satisfies (lb) with  $k = \delta$ . We may apply the first part of the result to  $m_N^\delta$  to deduce

$$(1 - \delta) \liminf_{N \rightarrow \infty} \mathcal{A}_N^*(m_N, e_N) \geq \mathbf{A}^*(\mu^\delta, \eta) - \delta E$$

for every  $\delta \in (0, 1]$ . Passing to the limit  $\delta \rightarrow 0$  and using the weak lower semicontinuity of  $\mathbf{A}^*(\cdot, \eta)$  we infer that

$$\liminf_{N \rightarrow \infty} \mathcal{A}_N^*(m_N, e_N) \geq \liminf_{\delta \rightarrow 0} \mathbf{A}^*(\mu^\delta, \eta) \geq \mathbf{A}^*(\mu, \eta),$$

which concludes the proof.

(iii) *Lower bound for the Fisher information.* Assume that (nc) holds. We first prove the lower bound (3.6) under the additional assumption (lb). This assumption will be removed at the end of the proof. Take  $m_N \in \mathcal{P}(\mathcal{T}_N)$  and write  $r_N = \frac{dm_N}{d\pi_N}$  as usual. The key identity relating the Fisher information to the Dirichlet form is

$$\mathcal{F}_N(\sqrt{r_N}) = \tilde{\mathcal{A}}_N(m_N, -D\mathcal{H}_N(m_N)), \quad (5.3)$$

where  $\tilde{\mathcal{A}}_N$  is defined by replacing the logarithmic mean  $\theta_{\log}$  in the definition of  $\mathcal{A}_N$  by  $\tilde{\theta}(a, b) := \theta_{\log}(\sqrt{a}, \sqrt{b})^2$ . Since  $\min\{a, b\} \leq \tilde{\theta}(a, b) \leq \theta_{\log}(a, b) \leq \max\{a, b\}$ , we have

$$|\theta_{\log}(a, b) - \tilde{\theta}(a, b)| \leq |a - b| \leq \frac{|a - b|}{\min\{a, b\}} \tilde{\theta}(a, b).$$

The assumptions (3.6) and (lb) yield

$$\varepsilon_N := \sup_{K \sim L \in \mathcal{T}_N} |r_N(K) - r_N(L)| \rightarrow 0 \quad \text{and} \quad \inf_{K \in \mathcal{T}_N} r_N(K) \geq k_{\min}. \quad (5.4)$$

Combining these estimates, we infer that

$$|\mathcal{I}_N(m_N) - \mathcal{F}_N(\sqrt{r_N})| = |(\mathcal{A}_N - \tilde{\mathcal{A}}_N)(m_N, -D\mathcal{H}_N(m_N))| \leq \frac{\varepsilon_N}{k_{\min}} \mathcal{F}_N(\sqrt{r_N}). \quad (5.5)$$

Let us now assume that  $\sup_N \mathcal{I}_N(m_N) < +\infty$  along some subsequence. (If this were not the case, the result would hold trivially.) The previous bound implies that also  $\sup_N \mathcal{E}_N(\sqrt{r_N}) < +\infty$ . Hence,  $(\sqrt{\rho_N})_N$  has a subsequence that converges strongly in  $L^2(\Omega)$  by Proposition 8.5. Let  $g \in L^2(\Omega)$  be its limit.

Since  $\|\rho_N - g^2\|_{L^1} \leq \|\sqrt{\rho_N} - g\|_{L^2} \|\sqrt{\rho_N} + g\|_{L^2}$ , we infer that  $\rho_N \rightarrow g^2$  in  $L^1(\Omega)$ . As  $\mu_N := \rho_N \mathcal{L}^d \rightharpoonup \mu$  in  $\mathcal{P}(\Omega)$  by assumption, we infer that  $\mu$  is absolutely continuous with density  $\rho := g^2$ .

Now we apply (5.5) and the Mosco convergence result  $\tilde{\mathbf{F}}_N \xrightarrow{\text{M}} \mathbf{F}$  from Theorem 7.2 to obtain

$$\liminf_{N \rightarrow \infty} \mathcal{I}_N(m_N) \geq \liminf_{N \rightarrow \infty} \mathcal{E}_N(\sqrt{r_N}) \geq \mathbf{F}(\sqrt{\rho}) = \mathbf{I}(\mu),$$

which concludes this part of the proof.

Let us now show how to remove the assumption (lb) as in the proof of (ii). The argument is based on the convexity of  $m \mapsto \mathcal{I}_N(m)$ , which is a consequence of the joint convexity of the map  $(a, b) \mapsto (a - b)(\log a - \log b)$  on  $(0, \infty) \times (0, \infty)$ .

Pick  $\delta \in (0, 1)$  and set  $m_N^\delta := (1 - \delta)m_N + \delta\pi_N$ . Note that  $m_N^\delta$  satisfies (lb) with  $k_{\min} = \delta$ . Moreover,  $\iota_N m_N^\delta \rightharpoonup \mu^\delta := (1 - \delta)\mu + \delta\bar{\mathbf{m}}$ . Applying the first part of the result we obtain

$$\mathbf{I}(\mu^\delta) \leq \liminf_{N \rightarrow \infty} \mathcal{I}_N(m_N^\delta) \leq (1 - \delta) \liminf_{N \rightarrow \infty} \mathcal{I}_N(m_N)$$

for every  $\delta \in (0, 1]$ , where the last inequality uses the convexity of  $\mathcal{I}_N$  and the fact that  $\mathcal{I}_N(\pi_N) = 0$ .

Since  $\mu^\delta \rightharpoonup \mu$ , the result follows from the lower semicontinuity of  $\mathbf{I}$  with respect to the weak convergence in  $\mathcal{P}(\Omega)$ .  $\square$

**5.3. Proof of the Wasserstein evolutionary  $\Gamma$ -convergence.** We are finally ready to prove Theorem 3.6. The compactness is given by Proposition 5.2, whereas the lower bound in (Entropy) follows from Theorem 3.3, together with (3.3) and an application of Fatou's lemma. We are left with the proof of the evolutionary lower bounds for the metric derivative and the Fisher information.

The next auxiliary result can be found in [Ste08, Corollary 4.4].

**Proposition 5.4** (Evolutionary  $\Gamma$ -liminf estimate). *Let  $X$  be a separable Hilbert space and let  $g_N, g_\infty : (0, T) \times X \rightarrow [0, +\infty]$  be convex and lower semicontinuous in space for a.e. time such that*

$$g_\infty(t, \varphi) \leq \inf \left\{ \liminf_{N \rightarrow \infty} g_N(t, \varphi_N) : \varphi_N \rightharpoonup \varphi \text{ in } X \right\} \quad (5.6)$$

for all  $\varphi \in X$  and for a.e.  $t \in (0, T)$ . Then, whenever  $\varphi_N \rightharpoonup \varphi$  in  $L^2(0, T; X)$ , we have

$$\int_0^T g_\infty(t, \varphi(t)) dt \leq \liminf_{N \rightarrow \infty} \int_0^T g_N(t, \varphi_N(t)) dt. \quad (5.7)$$

In the following, we combine the results obtained in Theorem 3.3 together with Proposition 5.4 in order to prove Theorem 3.6.

*Proof of the evolutionary lower bound for the metric derivative.* Fix  $0 < \delta < T$  and define  $g_N : (\delta, T) \times L^2(\Omega) \rightarrow [0, +\infty]$  by

$$g_N(t, \varphi) := \begin{cases} \mathcal{A}_N^*(m_t^N, \varphi), & \text{if } \varphi \in PC_N, \\ +\infty, & \text{otherwise.} \end{cases}$$

The maps  $g_N$  are convex and lower semicontinuous in  $L^2(\Omega)$  for every time  $t \in (0, T)$ . Set  $\varphi_N(t) := \iota_N \dot{m}_t^N$ . By Proposition 5.2, we can assume that  $\varphi_N \rightharpoonup \varphi := \dot{\rho}_t$  in  $L^2(\delta, T; L^2(\Omega))$  as  $N \rightarrow \infty$ .

Define  $g_\infty(t, \varphi) := \mathbf{A}^*(\mu_t, \varphi)$ . We apply Proposition 4.5 to deduce that  $m_t^N$  satisfies (ub) and (pc). Moreover, if we set  $e_N := \dot{m}_t^N$ , using that  $\mathcal{L}_N$  is self-adjoint in the discrete Sobolev space  $\mathcal{H}^{-1}$  (see also Appendix 6), we deduce that (3.5) is satisfied. Therefore we can apply Theorem 3.3 and (3.4) to infer that (5.7) is satisfied as well. We then apply Proposition 5.4 to the sequences  $g_N, g_\infty, \varphi_N, \varphi$  and deduce that

$$\liminf_{N \rightarrow \infty} \int_0^T \mathcal{A}_N^*(m_t^N, \dot{m}_t^N) dt \geq \int_\delta^T \mathbf{A}^*(\mu_t, \dot{\mu}_t) dt.$$

Passing to the limit  $\delta \rightarrow 0$  yields the result.  $\square$

*Proof of the evolutionary lower bound for the Fisher information.* We follow the same strategy as above; namely, we make use of a suitable application of Proposition 5.4. Once again, set  $X = L^2(\Omega)$ , but this time define

$$g_N(t, \varphi) := \begin{cases} \mathcal{A}_N(m_t^N, -D\mathcal{H}_N(P_N\varphi d\pi_N)), & \text{if } \varphi \in PC_N, \\ +\infty, & \text{otherwise.} \end{cases}$$

The maps  $g_N$  are convex (see also the proof of (3.6) in Theorem 3.3) and lower semicontinuous in  $X$  for every time  $t \in (0, T)$ . Consider the sequence  $\varphi_N(t) := \iota_N r_t^N$  where  $r_t^N = dm_t^N/d\pi_N$ , which we know to be weakly convergent in  $L^2(0, T; X)$  to  $\varphi(t) := \rho_t$ , by means of Proposition 5.2 and  $L^2(\Omega)$ -bounds, due to the monotonicity of the  $\mathcal{L}_N$ .

As another application of Proposition 4.5, we also have that (nc) is satisfied. Therefore, we may apply Theorem 3.3 to deduce from (3.6) that (5.7) is satisfied. This allows us to apply Proposition 5.4 to  $g_N, g_\infty, \varphi_N, \varphi$ , as defined above, and conclude the proof.

## 6. A LOOK AT GRADIENT FLOW STRUCTURES IN HILBERT SPACES

The role of this section is to make some connections between the Mosco convergence  $\mathbf{E}_N \xrightarrow{M} \mathbf{E}$  and equivalent gradient flow formulations of the same diffusion equation. In particular, we discuss evolutionary  $\Gamma$ -convergence of some gradient flow structures in Hilbert spaces, which are available for the description of Fokker-Planck equations. We are largely inspired by the abstract convergence results for gradient flows in reflexive Banach spaces obtained in [Mie16] (see also [Att84, Theorem 3.74] for an earlier result in Hilbert spaces).

In the first two subsections below we present two classical gradient flows in the respective Hilbert spaces  $L^2(\Omega, \bar{\mathbf{m}})$  and  $H^{-1}(\Omega)$ , followed by an introduction of their counterparts in a discrete setting. The final two subsections deal with corresponding evolutionary  $\Gamma$ -convergence results for the gradient flow structures discussed in this section.

**6.1. Gradient flows in Hilbert spaces: the  $L^2$  and  $H^{-1}$  distance.** The Wasserstein setting is not the only one in which one can interpret the solution of the Fokker-Planck equation as gradient flows of a suitable functional. In this section we describe two more possibilities of this kind, both in Hilbert spaces.

The first one is to work in the Hilbert space  $L^2(\Omega, \bar{\mathbf{m}})$  and with the Dirichlet form

$$\mathbf{E}(\varphi) := \begin{cases} \frac{1}{2} \int_{\Omega, \bar{\mathbf{m}}} |\nabla \varphi|^2 d\bar{\mathbf{m}}, & \text{if } \varphi \in H^1(\Omega) \subset L^2(\Omega, \bar{\mathbf{m}}), \\ +\infty, & \text{otherwise.} \end{cases} \quad (6.1)$$

In particular, the subdifferential of  $\mathbf{E}$  in  $\varphi$  is not empty if and only if  $\varphi \in D(\mathbf{L})$  for  $\mathbf{L}\varphi := \nabla \cdot (\sigma \nabla (\frac{\varphi}{\sigma}))$  and in this case

$$\partial_{L^2} \mathbf{E}(\varphi) = \{-\mathbf{L}\varphi\}, \quad \mathbf{L}\varphi \in L^2(\Omega, \bar{\mathbf{m}}).$$

On the other hand, the metric derivative is given by the  $L^2$ -norm of the time derivative. Thus, the EDI formulation of the gradient flow of the energy  $\mathbf{E}$  in  $L^2(\Omega, \bar{\mathbf{m}})$  reads

$$\mathbf{E}(\rho_T) + \frac{1}{2} \int_0^T \|\dot{\rho}_t\|_{L^2}^2 + \|\mathbf{L}\rho_t\|_{L^2}^2 dt \leq \mathbf{E}(\rho_0), \quad (6.2)$$

where we assume  $\rho_0 \in H^1(\Omega)$  (see Remark 5.3 for a related discussion).

A second possibility is to consider the Hilbert space  $H^{-1}(\Omega, \bar{\mathbf{m}})$  (i.e. the dual of the weighted Sobolev space  $H^1(\Omega, \bar{\mathbf{m}})$ ) and the functional

$$\mathbf{F}(L) := \begin{cases} \frac{1}{2} \int_{\Omega} \varphi^2 d\bar{\mathbf{m}} & \text{if } L = L_{\varphi}, \\ +\infty & \text{otherwise,} \end{cases} \quad (6.3)$$

where  $L_{\varphi} \in H^{-1}(\Omega, \bar{\mathbf{m}})$  is defined for  $\varphi \in L^2(\Omega, \bar{\mathbf{m}})$  by

$$L_{\varphi}(\psi) := \int_{\Omega} \varphi \psi d\bar{\mathbf{m}}, \quad \forall \psi \in H^1(\Omega, \bar{\mathbf{m}}).$$

Let us denote by  $\Delta_{\bar{\mathbf{m}}}\varphi$  the distributional  $\bar{\mathbf{m}}$ -Laplacian of  $\varphi \in H^1(\Omega, \bar{\mathbf{m}})$  as an element of  $H^{-1}(\Omega, \bar{\mathbf{m}})$ , namely

$$(-\Delta_{\bar{\mathbf{m}}}\varphi, \psi) := \int_{\Omega} \langle \nabla \varphi, \nabla \psi \rangle d\bar{\mathbf{m}} \quad \forall \psi \in H^1(\Omega, \bar{\mathbf{m}}).$$

It is then possible to prove that the subdifferential of  $\mathbf{F}$  is not empty only on  $L = L_{\varphi}$  with  $\varphi \in D(\mathbf{L})$  and in this case

$$\partial_{H^{-1}}\mathbf{F}(L_{\varphi}) = \{-\Delta_{\bar{\mathbf{m}}}\varphi\} \quad \text{for } \varphi \in D(\mathbf{L}).$$

In a fashion similar to the previous setting, the metric derivative is given by the  $H^{-1}(\Omega, \bar{\mathbf{m}})$ -norm of the time derivative. Altogether, the EDI formulation of the gradient flow of the energy  $\mathbf{F}$  in  $H^{-1}(\Omega, \bar{\mathbf{m}})$  reads

$$\mathbf{F}(L_{\rho_T}) + \frac{1}{2} \int_0^T \|\dot{\rho}_t\|_{H^{-1}}^2 + \|\Delta_{\bar{\mathbf{m}}}\rho_t\|_{H^{-1}}^2 dt \leq \mathbf{F}(L_{\rho_0}) \quad (6.4)$$

for  $\rho_0 \in L^2(\Omega, \bar{\mathbf{m}})$ .

**6.2. The  $L^2$ - and  $H^{-1}$ -gradient flow structures in the discrete setting.** In this section, we will recall two separate Hilbert space gradient flows which provide solutions to the discrete heat equation  $\dot{u}_t = \Delta_{\mathcal{T}}u_t$  in  $\mathcal{P}(\mathcal{T})$ . As done in the continuous setting above, one possibility is to consider the  $L^2$ -gradient flow with respect to the Dirichlet form

$$\mathcal{E}_{\mathcal{T}}(u) := \begin{cases} \frac{1}{4} \sum_{K,L \in \mathcal{T}} (u(K) - u(L))^2 w_{KL} & \text{if } dm = u d\pi_{\mathcal{T}} \text{ for } m \in \mathcal{P}(\mathcal{T}), \\ +\infty & \text{otherwise.} \end{cases}$$

For any smooth curve  $t \mapsto u_t$  of probability densities with respect to  $\pi_{\mathcal{T}}$ , the computation

$$\frac{d}{dt} \mathcal{E}_{\mathcal{T}}(u_t) = \frac{1}{2} \sum_{K,L \in \mathcal{T}} (u_t(K) - u_t(L))(\dot{u}_t(K) - \dot{u}_t(L))w_{KL} = -\langle \Delta_{\mathcal{T}}u_t, \dot{u}_t \rangle_{L^2(\pi_{\mathcal{T}})}$$

shows that  $-\Delta_{\mathcal{T}}u$  is indeed the  $L^2(\pi_{\mathcal{T}})$ -gradient of  $\mathcal{E}_{\mathcal{T}}(u)$ . Hence, The energy dissipation inequality (EDI) to the corresponding gradient flow reads

$$\mathcal{E}_{\mathcal{T}}(u_t) + \frac{1}{2} \int_s^t \|\dot{u}_r\|_{L^2(\pi_{\mathcal{T}})}^2 + \|\Delta_{\mathcal{T}}u_r\|_{L^2(\pi_{\mathcal{T}})}^2 dr \leq \mathcal{E}_{\mathcal{T}}(u_s) \quad \text{a.e. } s \geq 0, \forall t \geq s. \quad (6.5)$$

It is possible to endow a discrete function spaces with a Markov chain induced norm, in order to mimic the structure of an  $H^{-1}$ -space. In the setting of admissible,  $\zeta$ -regular meshes over a convex domain  $\Omega \subset \mathbb{R}^d$  this may be done, using a suitable



$\mathcal{H}^1$ -norm on  $L^2(\mathcal{T}, \pi_{\mathcal{T}})$  given by  $\frac{1}{2} \|\cdot\|_{\mathcal{H}^1}^2 := \mathcal{E}_{\mathcal{T}}$ . Thus, we may define  $\|\cdot\|_{\mathcal{H}^{-1}}$  on (the dual space of)  $L^2(\mathcal{T}, \pi_{\mathcal{T}})$  by means of

$$\|f\|_{\mathcal{H}^{-1}} := \sup_{\substack{g \in L^2(\pi_{\mathcal{T}}) \\ g \neq 0}} \frac{\langle f, g \rangle_{L^2(\pi_{\mathcal{T}})}}{\|g\|_{\mathcal{H}^1}} \quad \forall f \in L^2(\mathcal{T}, \pi_{\mathcal{T}}), \quad (6.6)$$

where we identified  $L^2(\mathcal{T}, \pi_{\mathcal{T}})$  with its dual.

Recall that the Laplacian acts as isometric isomorphism between  $H^1(\Omega)$  and  $H^{-1}(\Omega)$ . Such an identification is also possible in the discrete setting as done for instance in Section 3.1 of [EM12]. Indeed, note that  $\Delta_{\mathcal{T}}$  is a selfadjoint operator on  $L^2(\mathcal{T}, \pi_{\mathcal{T}})$ , which implies that  $\Delta_{\mathcal{T}}$  is bijective on the linear subspace  $\text{ran } \Delta_{\mathcal{T}} = \{f : \mathcal{T} : \mathbb{R} : \sum_{K \in \mathcal{T}} f_K \pi_K = 0\}$ . Hence, one may introduce the inner product

$$\langle f, g \rangle_{\mathcal{H}^{-1}} := -\langle \Delta_{\mathcal{T}}^{-1} f, g \rangle_{L^2(\pi)} \quad \forall f, g \in \text{ran } \Delta_{\mathcal{T}}.$$

The induced norm takes the form

$$\|f\|_{\mathcal{H}^{-1}}^2 = \frac{1}{2} \sum_{K, L \in \mathcal{T}} (\Delta_{\mathcal{T}}^{-1} f_L - \Delta_{\mathcal{T}}^{-1} f_K)^2 w_{KL} \quad \forall f \in \text{ran } \Delta_{\mathcal{T}},$$

which may be easily verified to agree with the definition given in (6.6) on the linear subspace  $\text{ran } \Delta_{\mathcal{T}}$ .

Now consider the functional

$$\mathcal{F}_{\mathcal{T}}(u) := \begin{cases} \frac{1}{2} \sum_{K \in \mathcal{T}} |u_K|^2 \pi_K & \text{if } dm = u \, d\pi \text{ for } m \in \mathcal{P}(\mathcal{T}), \\ +\infty & \text{otherwise.} \end{cases}$$

Then the EDI gradient flow for the functional  $\mathcal{F}_{\mathcal{T}}$  in the finite dimensional Hilbert space  $\mathcal{H}^{-1}$  is given as solution to

$$\mathcal{F}_{\mathcal{T}}(u_t) + \frac{1}{2} \int_s^t \|\dot{u}_r\|_{\mathcal{H}^{-1}}^2 + \|\Delta_{\mathcal{T}} u_r\|_{\mathcal{H}^{-1}}^2 \, dr \leq \mathcal{F}_{\mathcal{T}}(u_s) \quad \text{a.e. } s \geq 0, \forall t \geq s. \quad (6.7)$$

**6.3. Convergence of  $L^2$ -Gradient flows for Dirichlet forms.** We follow roughly the approach sketched in [Mie16, Section 3.2]. A crucial ingredient is the Mosco convergence  $\mathbf{E}_N \xrightarrow{M} \mathbf{E}$  for the Dirichlet form  $\mathbf{E}$  as defined in (6.1) and the embedded functionals  $\mathbf{E}_N$  corresponding to their discrete counterparts  $\mathcal{E}_{\mathcal{T}_N}$ .

In addition, we make use on the following result, the so-called strong weak-closedness of the graphs of the subdifferentials for the Dirichlet forms (see [Mie16, Proposition 2.9] or [Att84, Theorem 3.66] for a proof).

**Lemma 6.1.** *Consider a sequence of proper, lower semi-continuous, convex functionals  $J_N : X \rightarrow \mathbb{R} \cup \{+\infty\}$  on some reflexive Banach space  $X$  such that  $E_N \xrightarrow{M} E_0$ . Then for every sequence  $u^N \rightharpoonup u$  such that  $E_N(u^N) \rightarrow \eta \in \mathbb{R}$  and  $\partial E_\varepsilon(u^N) \ni \xi^N \rightarrow \xi$ , we have  $E_0(u) = \eta$  and  $\xi \in \partial E_N(u)$ .*

The strong-weak closedness result above and the Mosco convergence of the discrete Dirichlet forms allow us to prove the following convergence result.

**Proposition 6.2.** *Let  $T > 0$  and consider a sequence of  $\zeta$ -admissible meshes  $(\mathcal{T}_N)_N$ . Fix an initial value  $\rho_0 \in L^2(\Omega, \bar{\mathbf{m}})$  such that  $\mathbf{E}(\rho_0) < +\infty$ , together with a sequence of approximating functions  $u_0^N \in L^2(\mathcal{T}_N, \pi_N)$ , well-prepared in the sense that*

$$\iota_N u_0^N \rightharpoonup \rho_0 \quad \text{and} \quad \lim_{N \rightarrow \infty} \mathcal{E}_N(u_0^N) = \mathbf{E}(\rho_0).$$

Write  $\rho_t^N := \iota_N u_t^N$ ; then the sequence  $(\rho^N)_N$ , corresponding to curves  $(u_t^N)_{t \in [0, T]}$  satisfying the energy dissipation inequality (6.5) with initial values  $u_0^N$ , is weakly sequentially compact in  $H^1(0, T; L^2(\Omega, \bar{\mathbf{m}}))$ .

Up to a (non-relabelled) subsequence, we have  $\rho_t^N \rightarrow \rho_t$  in  $L^2(\Omega, \bar{\mathbf{m}})$  for every time  $t \in [0, T]$ .

Moreover, we have the following lower bounds at the energy and dissipation level:

$$\liminf_{N \rightarrow \infty} \mathcal{E}_N(u_t^N) \geq \mathbf{E}(\rho_t), \quad \forall t \in [0, T] \quad (\text{energy})$$

$$\liminf_{N \rightarrow \infty} \int_0^T \|\dot{u}_t^N\|_{L^2(\pi_N)}^2 dt \geq \int_0^T \|\dot{\rho}_t\|_{L^2(\bar{\mathbf{m}})}^2 dt, \quad (\text{metric derivative})$$

$$\liminf_{N \rightarrow \infty} \int_0^T \|D\mathcal{E}_N(u_t^N)\|_{L^2(\pi_N)}^2 dt \geq \int_0^T \|D\mathbf{E}(\rho_t)\|_{L^2(\bar{\mathbf{m}})}^2 dt. \quad (\text{metric slope})$$

In particular, the curve  $(\rho_t)_t$  solves the energy dissipation inequality (6.2) or, equivalently, the continuous Fokker-Planck equation (9).

*Proof.* As the initial condition is well prepared, we may assume that the discrete Dirichlet forms satisfy the uniform bound  $\mathcal{E}(u_0^N) \leq C$  for all  $N \in \mathbb{N}$ . Combined with the EDI in (6.7), this allows us to find uniform bound in terms of

$$\mathcal{E}(u_t^N) \leq C_0, \quad \int_0^t \|\iota_N \Delta_N u_r^N\|_{L^2(\bar{\mathbf{m}})}^2 dr \leq C_0, \quad \int_0^t \|\rho_r^N\|_{L^2(\bar{\mathbf{m}})}^2 dr \leq C_0 \quad (6.8)$$

for all times  $t \geq 0$ .

By means of weak compactness, the second and third bound in (6.8) allow us to extract (non-relabelled) subsequences  $\rho^N$  and  $\xi^N := \iota_N \Delta_N u^N$  such that  $\rho^N \rightharpoonup \rho$  in  $H^1(0, T; L^2(\Omega, \bar{\mathbf{m}}))$  and  $\xi^N \rightharpoonup \xi$  in  $L^2(0, T; L^2(\Omega, \bar{\mathbf{m}}))$ .

Using the uniform bound on the discrete Dirichlet forms, we may appeal to Proposition 8.5, in order to obtain a time-dependent subsequence of  $(\rho_t^N)_{N \in \mathbb{N}}$  converging to  $\rho_t$  in  $L^2(\Omega, \bar{\mathbf{m}})$ , together with the uniform bound  $\|\nabla \rho_t\|_{L^2(\bar{\mathbf{m}})} \leq C_0$  for each time  $t \geq 0$ .

As Theorem 7.2 establishes the Mosco convergence  $\mathbf{E}_N \xrightarrow{M} \mathbf{E}$ , we infer the estimate

$$\liminf_{N \rightarrow \infty} \mathcal{E}_N(u_t^N) = \liminf_{N \rightarrow \infty} \mathbf{E}_N(\rho_t^N) \geq \mathbf{E}(\rho_t) \quad \forall t \geq 0.$$

Turning to the metric differential and the metric slope, Fatou's lemma, together with the weak lower semicontinuity of the  $L^2$ -norm, yields

$$\int_0^T \|\dot{\rho}_r\|_{L^2(\bar{\mathbf{m}})}^2 dr \leq \liminf_{N \rightarrow \infty} \int_0^T \|\dot{\rho}_r^N\|_{L^2(\bar{\mathbf{m}})}^2 dr$$

and

$$\int_0^T \|\xi_r\|_{L^2(\bar{\mathbf{m}})}^2 dr \leq \liminf_{N \rightarrow \infty} \int_0^T \|\xi_r^N\|_{L^2(\bar{\mathbf{m}})}^2 dr. \quad (6.9)$$

In order to identify the expression  $\|\xi_r\|_{L^2(\bar{\mathbf{m}})}^2$  with the metric slope  $\|\partial \mathbf{E}(\rho_r)\|_{L^2(\bar{\mathbf{m}})}^2$ , we appeal to the fundamental theorem of Young measures adapted to strong-weak

topologies (cf. [MRS13, Theorem A.3]), which yields another subsequence (also denoted by  $\xi^N$ ) and a family of Young measures  $(\mu_t)_{t \in (0, T)}$  on  $L^2(\Omega, \bar{\mathbf{m}})$  such that for a.e. time  $t \in (0, T)$  the identity

$$\xi_t = \int_{L^2(\bar{\mathbf{m}})} w \, d\mu_t(w) \quad (6.10)$$

holds with the property that  $\mu_t$  is concentrated on the set of cluster points for  $(\xi_t^N)_{N \in \mathbb{N}}$  with respect to the weak topology on  $L^2(\Omega, \bar{\mathbf{m}})$ . Taking into account Lemma 6.1 for suitable (time-dependent) subsequences of  $(\rho_t^N)_{N \in \mathbb{N}}$  and  $(\xi_t^N)_{N \in \mathbb{N}}$ , we infer that  $\mu_t$  is concentrated on  $\partial \mathbf{E}(\rho_t)$  for a.e.  $t \in (0, T)$ . Since  $\partial \mathbf{E}(\rho_t)$  is single-valued for a.e.  $t$ , we infer from (6.10) that  $\xi_t = \partial \mathbf{E}(\rho_t)$ . As a result, (6.9) implies the required bound on the metric slope.  $\square$

*Remark 6.3.* An alternative proof of Proposition 6.2 may be established by means of gradient flow stability tools as found in [Ste08]. Indeed, it suffices to combine the characterisation results of gradient flows via the so-called Brezis-Ekeland principle in Section 1 of the same article with [Ste08, Lemma 6.1]; we omit the details.

**6.4. Convergence of  $H^{-1}$ -gradient flows for the  $L^2$ -energy functional.** In this last subsection we prove the evolutionary  $\Gamma$ -convergence of the  $H^{-1}$ -gradient flow structures.

**Proposition 6.4.** *Let  $T > 0$  and consider a sequence of admissible  $\zeta$ -meshes  $(\mathcal{T}_N)_N$ . Fix an initial value  $\rho_0 \in L^2(\Omega, \bar{\mathbf{m}})$ , together with a sequence of approximating functions  $u_0^N \in L^2(\mathcal{T}_N, \pi_N)$ , well-prepared in the sense that*

$$\lim_{N \rightarrow \infty} \mathcal{F}_N(u_0^N) = \mathbf{F}(\rho_0) < +\infty.$$

Write  $\rho_t^N := \iota_N u_t^N$ ; then the sequence  $(\rho_t^N)$  corresponding to curves  $(u_t^N)_{t \in [0, T]}$  satisfying the energy dissipation inequality (6.7) with initial values  $u_0^N$ , is weakly sequentially compact in  $H^1(0, T; L^2(\Omega, \bar{\mathbf{m}}))$

Up to a (non-relabelled) subsequence, we have  $\rho_t^N \rightharpoonup \rho_t$  in  $L^2(\Omega, \bar{\mathbf{m}})$  for every time  $t \in [0, T]$ .

Moreover, we have the following lower bounds at the energy and dissipation level:

$$\liminf_{N \rightarrow \infty} \mathcal{F}_N(u_t^N) \geq \mathbf{F}(\rho_t), \quad \forall t \in [0, T] \quad (\text{energy})$$

$$\liminf_{N \rightarrow \infty} \int_0^T \|\dot{u}_t^N\|_{\mathcal{H}^{-1}}^2 \, dt \geq \int_0^T \|\dot{\rho}_t\|_{H^{-1}(\bar{\mathbf{m}})}^2 \, dt, \quad (\text{metric derivative})$$

$$\liminf_{N \rightarrow \infty} \int_0^T \|D\mathcal{F}_N(u_t^N)\|_{\mathcal{H}^{-1}}^2 \, dt \geq \int_0^T \|D\mathbf{F}(\rho_t)\|_{H^{-1}(\bar{\mathbf{m}})}^2 \, dt. \quad (\text{metric slope})$$

In particular, the curve  $(\rho_t)_t$  solves the energy dissipation inequality (6.4) or, equivalently, the continuous Fokker-Planck equation (9).

*Proof.* The well-preparedness of the initial value implies

$$\lim_{N \rightarrow \infty} \|\rho_0^N\|_{L^2(\bar{\mathbf{m}})} = \|\rho_0\|_{L^2(\bar{\mathbf{m}})}.$$

In particular, we have the uniform bound  $\|\rho_0^N\|_{L^2(\bar{\mathbf{m}})} \leq C$  for all meshes  $N$  and some constant  $C > 0$ . Combined with the EDI in (6.7), this implies the a priori bound

$\|\rho^N\|_{L^\infty(0,T;L^2(\bar{\mathbf{m}}))} \leq C$ . Recalling

$$\frac{1}{2} \|\dot{u}_t^N\|_{\mathcal{H}^{-1}}^2 = \frac{1}{2} \|\Delta_N u_t^N\|_{\mathcal{H}^{-1}}^2 = \mathcal{E}_N(u_t^N), \quad (6.11)$$

we may also deduce the estimate on the discrete Dirichlet forms  $\int_0^T \mathcal{E}_N(u_t^N) dt \leq C$  along the same lines.

A uniform  $L^2(\bar{\mathbf{m}})$ -bound for the time-derivative of  $u_t^N$  is deduced from the well-preparedness of the initial condition and maximal monotone operator bounds on  $\dot{\rho}_t^N$  (see e.g. [Bre10, Theorem 7.7]) for every  $\delta > 0$  in terms of

$$\|\dot{\rho}_t^N\|_{L^2(\bar{\mathbf{m}})} = \|\dot{u}_t^N\|_{L^2(\pi)} \leq C_\delta \quad \forall t \in [\delta, T]$$

for a constant  $C_\delta > 0$  not depending on the mesh size. Hence, we may extract a subsequence  $(\rho^{N_N, \delta})_{N \in \mathbb{N}}$  weakly converging to  $\rho_t$  in  $H^1(\delta, T; L^2(\Omega, \bar{\mathbf{m}}))$ . Setting  $\rho^N := \rho^{N_N, \delta_N}$  for some sequence  $\delta_N \searrow 0$ , we infer  $\rho^N \rightharpoonup \rho$  in  $H^1(0, T; L^2(\Omega, \bar{\mathbf{m}}))$ . Thanks to the  $L^\infty$ -a priori estimate established above, we may also infer from weak compactness the existence of a further sub-sequence, also denoted by  $(\rho_t^N)_{N \in \mathbb{N}}$ , such that  $\rho_t^N \rightharpoonup \rho_t$  in  $L^2(\Omega, \bar{\mathbf{m}})$  for all  $t \in [0, T]$ .

Now the energy bound follows immediately, using that the norm  $\|\cdot\|_{L^2(\bar{\mathbf{m}})}$ . Therefore,  $\mathbf{F}$  is weakly lower semicontinuous in  $L^2(\Omega, \bar{\mathbf{m}})$  as well.

Using [Mie16, Theorem 2.8], one infers that the Mosco convergence  $\mathbf{E}_N \xrightarrow{\text{M}} \mathbf{E}$  (see Theorem 7.2 below) is actually equivalent to  $\mathbf{E}_N^* \xrightarrow{\text{M}} \mathbf{E}^*$ , where  $\mathbf{E}_N^*$  and  $\mathbf{E}^*$  denote the convex conjugates of the respective functionals  $\mathbf{E}_N$  and  $\mathbf{E}$  in  $L^2(\Omega)$ . In particular, we may invoke Proposition 5.4 for the family of time-independent functionals  $\mathbf{E}_N^*$  to obtain the desired bound on the metric derivative

$$\int_0^t \|\dot{\rho}_r\|_{H^{-1}(\Omega, \bar{\mathbf{m}})}^2 dr \leq \liminf_{N \rightarrow \infty} \int_0^t \|\dot{u}_r^N\|_{\mathcal{H}^{-1}}^2 dr \quad \forall t \leq T,$$

where we used the identities

$$\mathbf{E}^*(\dot{\rho}_t) = \frac{1}{2} \|\dot{\rho}_t\|_{H^{-1}(\Omega, \bar{\mathbf{m}})}^2 \quad \text{and} \quad \mathbf{E}_N^*(\dot{\rho}_t^N) = \mathcal{E}_N^*(\dot{u}_t^N) = \frac{1}{2} \|\dot{u}_t^N\|_{\mathcal{H}^{-1}}^2.$$

Due to Proposition 8.5, we have  $\|\nabla \rho_t\|_{L^2}^2 \lesssim \sup_N \mathcal{E}_N(u_t^N)$ . Thus, the bound on time integral over the discrete Dirichlet forms implies that  $\rho$  may be identified as an element of  $L^2(0, T; H^1(\Omega))$  with  $\int_0^T \|\nabla \rho_t\|_{L^2(\bar{\mathbf{m}})}^2 dt \lesssim C$ . In particular, we have the identity

$$\frac{1}{2} \|\Delta_{\bar{\mathbf{m}}} \rho_t\|_{H^{-1}(\Omega, \bar{\mathbf{m}})}^2 = \frac{1}{2} \|\nabla \rho_t\|_{L^2(\Omega, \bar{\mathbf{m}})}^2 = \mathbf{E}(\rho_t) \quad \text{a.e. } t \in [0, T]. \quad (6.12)$$

Moreover,  $\mathbf{E}_N \xrightarrow{\text{M}} \mathbf{E}$  implies  $\mathbf{E}(\rho_t) \leq \liminf_{N \rightarrow \infty} \mathcal{E}_{N_N}(\rho_t^{N_N})$  for every  $t \in [0, T]$ . Hence, both the identities in (6.11) and (6.12), together with Fatou's lemma, imply

$$\int_0^t \|\Delta_{\bar{\mathbf{m}}} \rho_r\|_{H^{-1}(\Omega, \bar{\mathbf{m}})}^2 dr \leq \liminf_{n \rightarrow \infty} \int_0^t \|\Delta_N u_t^N\|_{\mathcal{H}^{-1}}^2 dr \quad \forall t \leq T. \quad (6.13)$$

Identifying both  $\|\Delta_{\bar{\mathbf{m}}} \rho_r\|_{H^{-1}(\Omega, \bar{\mathbf{m}})}$  and  $\|\Delta_N u_t^N\|_{\mathcal{H}^{-1}}$  with the respective metric slopes  $\|D\mathbf{F}(\mu_t)\|_{H^{-1}(\bar{\mathbf{m}})}$  and  $\|D\mathcal{F}_N(u_t^N)\|_{\mathcal{H}^{-1}}$ , we conclude.  $\square$

## 7. MOSCO CONVERGENCE OF DISCRETE ENERGIES: THE STATEMENT

In this section we present a Mosco convergence result for sequences of discrete energies to the corresponding continuous energy. This result is a key tool to prove evolutionary  $\Gamma$ -convergence in Section 5. Let us first recall the definition of  $\Gamma$ - and Mosco convergence.

**Definition 7.1** ( $\Gamma$ - and Mosco convergence). *Let  $\mathcal{F}, \mathcal{F}_N : X \rightarrow \mathbb{R} \cup \{+\infty\}$  be functionals defined on a topological vector space  $X$ .*

(1) *The sequence  $(\mathcal{F}_N)_N$  is said to be  $\Gamma$ -convergent to  $\mathcal{F}$  if the following conditions hold:*

(i) **liminf inequality:** *for every sequence  $(x_N)_N \subseteq X$  strongly converging to  $x \in X$  we have*

$$\liminf_{N \rightarrow \infty} \mathcal{F}_N(x_N) \geq \mathcal{F}(x).$$

(ii) **limsup inequality:** *for every  $x \in X$  there exists a sequence (called recovery sequence)  $(x_N)_N \subseteq X$  strongly converging to  $x$  and such that*

$$\limsup_{N \rightarrow \infty} \mathcal{F}_N(x_N) \leq \mathcal{F}(x).$$

(2) *The sequence  $(\mathcal{F}_N)_N$  is said to be Mosco convergent to  $\mathcal{F}$  if the same conditions hold, with the modification that weakly convergent sequences are considered in (i).*

We use the notations  $\mathcal{F}_N \xrightarrow{\Gamma} \mathcal{F}$  and  $\mathcal{F}_N \xrightarrow{M} \mathcal{F}$  to indicate the respective  $\Gamma$ - and Mosco convergence.

Let us now fix the setup, which remains in force throughout Sections 7, 8 and 9. Consider a family of  $\zeta$ -regular meshes  $(\mathcal{T}_N)_N$  with  $[\mathcal{T}_N] \rightarrow 0$  as  $N \rightarrow \infty$ . We fix a reference measure  $\bar{\mathbf{m}} \in \mathcal{P}(\bar{\Omega})$  as in (2.2) and define  $\pi_N \in \mathcal{P}(\mathcal{T}_N)$  by  $\pi_N := P_N \bar{\mathbf{m}}$  as before.

We consider a measure  $\mu \in \mathcal{P}(\bar{\Omega})$  with density  $\rho = \frac{d\mu}{d\bar{\mathbf{m}}} \in L^2(\Omega)$ , together with discrete measures  $m_N \in \mathcal{P}(\mathcal{T}_N)$  with densities  $r_N = \frac{dm_N}{d\pi_N}$ .

We define the *discrete Dirichlet energy*  $\mathcal{F}_N : L^2(\mathcal{T}_N, \pi_N) \rightarrow \mathbb{R}_+$  by

$$\mathcal{F}_N(f) := \mathcal{A}_N(m_N, f), \quad (7.1)$$

where  $\mathcal{A}_N := \mathcal{A}_{\mathcal{T}_N}$  is defined as in (2.16). Observe that

$$\mathcal{F}_N(f) = \frac{1}{4} \sum_{K, L \in \mathcal{T}_N} \left( \frac{f(K) - f(L)}{d_{KL}} \right)^2 \theta_{\log}(r_N(K), r_N(L)) d_{KL} |\Gamma_{KL}| S_{KL}, \quad (7.2)$$

where  $S_{KL}$  has been defined in (2.13). This formula illuminates the role of  $\mathcal{F}_N$  as a natural discrete counterpart to the *continuous Dirichlet energy*  $\mathbf{F}_\rho : L^2(\Omega) \rightarrow \mathbb{R}_+ \cup \{+\infty\}$  given by

$$\mathbf{F}_\rho(\varphi) := \mathbf{A}(\mu, \varphi) = \begin{cases} \frac{1}{2} \int_{\Omega} |\nabla \varphi|^2 d\mu & \text{if } \varphi \in H^1(\Omega, \mu), \\ +\infty & \text{otherwise,} \end{cases} \quad (7.3)$$

where  $\mathbf{A}$  is defined in (2.7). Due to our assumptions on  $\mu$ , the weighted Sobolev space  $H^1(\Omega, \mu)$  coincides with the classical Sobolev space  $H^1(\Omega)$ .

To compare the discrete and the continuous functionals, we introduce  $\tilde{\mathbf{F}}_N : L^2(\Omega) \rightarrow \mathbb{R}_+ \cup \{+\infty\}$  by

$$\tilde{\mathbf{F}}_N(\varphi) := \begin{cases} \mathcal{F}_N(P_{\mathcal{T}}\varphi) & \text{if } \varphi \in PC_N \\ +\infty & \text{otherwise,} \end{cases} \quad (7.4)$$

where  $PC_N \subset L^2(\Omega)$  denotes the space of all functions on the partition  $\mathcal{T}_N$  that are constant on each cell  $K \in \mathcal{T}$  and  $P_{\mathcal{T}}\varphi(K) = \varphi(x_K)$  for  $\varphi \in PC_N$ .

The main result of this section reads as follows.

**Theorem 7.2** (Mosco convergence). *Let  $(\mathcal{T}_N)_N$  be a vanishing sequence of  $\zeta$ -regular meshes and suppose that  $\mu$  and  $(m_N)_N$  satisfy (1b), (ub) and (pc). Then we have Mosco convergence  $\tilde{\mathbf{F}}_N \xrightarrow{M} \mathbf{F}_\rho$  with respect to the  $L^2(\Omega)$ -topology.*

In the following, we give a sketch of the proof of Theorem 7.2. Our strategy is based on a compactness and representation procedure, following ideas from [AC04] and [BFLM02]. In particular, the paper [AC04] contains similar  $\Gamma$ -convergence results on a particular discrete lattice (the cartesian grid) for a more general class of functionals. These authors do not characterize the limiting functional explicitly, except in special situations, such as the periodic setting. For our application to evolutionary  $\Gamma$ -convergence, a characterisation of the limiting functional is crucial.

A key ingredient in the proof is a representation result from [BFLM02, Theorem 2]. To be able to apply this result, we need to perform a localisation procedure. In the following,  $\mathcal{O}(\Omega)$  denotes the class of all the open subsets of  $\Omega$ . For every  $A \in \mathcal{O}(\Omega)$  we then introduce the functionals  $\mathcal{F}_N : L^2(\mathcal{T}_N, \pi_N) \times \mathcal{O}(\Omega) \rightarrow \mathbb{R}$  by

$$\mathcal{F}_N(f, A) := \frac{1}{2} \sum_{\substack{K, L \in \mathcal{T}_N \setminus A \\ K \sim L}} (f(K) - f(L))^2 w_{KL} \theta_{\log}(r_N(K), r_N(L)),$$

where for any subset  $A \subseteq \Omega$ ,

$$\mathcal{T}|_A := \{K \in \mathcal{T} : \bar{K} \cap A \neq \emptyset\}. \quad (7.5)$$

The corresponding embedded functional  $\tilde{\mathbf{F}}_N : L^2(\Omega, \bar{\mathbf{m}}) \times \mathcal{O}(\Omega) \rightarrow [0, +\infty]$  is given by

$$\tilde{\mathbf{F}}_N(\varphi, A) := \begin{cases} \mathcal{F}_N(P_{\mathcal{T}}\varphi, A) & \text{if } \varphi \in PC_N, \\ +\infty & \text{otherwise.} \end{cases}$$

The proof of Theorem 7.2 consists of the following steps:

- (Step 1) We show first, as in [AC04, Proposition 3.4], that any subsequential  $\Gamma$ -limit point  $\mathbf{F}_{0,\rho}(\cdot, A)$  of the sequence  $(\tilde{\mathbf{F}}_N(\cdot, A))_N$  is only finite on  $H^1(\Omega)$ . This result is a prerequisite for performing Step 3. We also show that  $\Gamma$ -convergence implies Mosco convergence in this situation.
- (Step 2) Using a compactness argument [Bra02], we infer that, up to a subsequence, the functionals  $(\tilde{\mathbf{F}}_N(\cdot, A))_N$   $\Gamma$ -converge to a limiting functional  $\mathbf{F}_{0,\rho}(\cdot, A)$  for any  $A \in \mathcal{O}(\Omega)$ .
- (Step 3) We prove the applicability of a suitable representation theorem [BFLM02, Theorem 2], which allows us to deduce the following expression

$$\mathbf{F}_{0,\rho}(\varphi) = \int_{\Omega} f(x, \varphi, \nabla \varphi) dx = \int_{\Omega} \langle A(x) \nabla \varphi, \nabla \varphi \rangle dx; \quad (7.6)$$

see also [AC04, Theorem 2.2 and Remark 3.2].

(Step 4) In view of the previous steps, it remains to show that  $A(x) = \rho(x)\sigma(x)\text{Id}$ .

Steps 1 and 2 will be carried out in Section 8, while Steps 3 and 4 will be performed in Section 9.

*Remark 7.3.* Mosco convergence of Dirichlet forms is equivalent to strong convergence of the associated semigroups [Mos94]; see also [KS03] for a generalisation to Dirichlet forms defined on different spaces.

## 8. MOSCO CONVERGENCE OF THE LOCALISED FUNCTIONALS

In this section we perform Steps 1 and 2 of the proof strategy described above, i.e. we prove the following results.

**Theorem 8.1** (Regularity of  $\Gamma$ -limits). *Assume (lb). For  $A \in \mathcal{O}(\Omega)$ , let  $\mathbf{F}_{0,\rho}(\cdot, A)$  be a subsequential  $\Gamma$ -limit of the sequence  $(\tilde{\mathbf{F}}_N(\cdot, A))_N$  in  $L^2(\Omega)$ -topology. Then  $\mathbf{F}_{0,\rho}(\varphi, A) = +\infty$  for any  $\varphi \notin H^1(\Omega)$ . Moreover, the subsequence is also convergent in the Mosco sense.*

The proof of this result is contained in Section 8.1 and relies on an  $L^2$ -Hölder continuity result (Proposition 8.5).

**Theorem 8.2** (Localised Mosco compactness). *Assume (lb) and (ub). Then there exists a subsequence of  $(\tilde{\mathbf{F}}_N)_N$  such that for any  $A \in \mathcal{O}(\Omega)$ , the sequence  $(\tilde{\mathbf{F}}_N(\cdot, A))_N$  is Mosco convergent in the  $L^2(\Omega)$ -topology.*

The proof of this result is contained in Section 8.2 and relies on an inner regularity result (Proposition 8.8) which is based on a Sobolev upper bound (Proposition 8.6).

**8.1. Regularity of finite energy sequences.** In this subsection we prove that any  $\Gamma$ -limit  $\mathbf{F}_{0,\rho}$  is only finite on Sobolev maps, which allows us to work with Theorem 9.3. The proof of the corresponding result in [AC04] relies strongly on the symmetric structure of the cartesian grid (where affine interpolation of vectorfields can be used; see [AC04, Proposition 3.4]).

For any  $x, y \in \mathbb{R}$  we write  $x \lesssim y$  (or equivalently,  $y \gtrsim x$ ) if there exists a constant  $C = C(\zeta, d) \in \mathbb{R}_+$  such that  $x \leq Cy$ . For  $h \in \mathbb{R}^d$  we write  $\tau_h(x) := x + h$  and

$$K \stackrel{h}{\sim} L \quad \text{if} \quad \bar{L} \cap \tau_h \bar{K} \neq \emptyset.$$

**Lemma 8.3** (Existence of good paths). *Let  $\mathcal{T}$  be a  $\zeta$ -regular mesh. Then there exists a family of paths  $\{\gamma_{KL}\}_{K,L \in \mathcal{T}}$ , where*

$$\gamma_{KL} = \{\gamma_{KL}(i) : i = 0, \dots, n_{KL}\}, \quad K = \gamma_{KL}(0) \sim \gamma_{KL}(1) \sim \dots \sim \gamma_{KL}(n_{KL}) = L,$$

such that the following properties hold:

(1) for all  $K, L \in \mathcal{T}$  we have

$$n_{KL} \lesssim \frac{d_{KL}}{|\mathcal{T}|} \quad \text{and} \quad \sum_{i=0}^{n_{KL}} d_{\gamma_{KL}(i), \gamma_{KL}(i+1)} \lesssim d_{KL}; \quad (8.1)$$

(2) for any  $h \in \mathbb{R}^d$  and  $M, N \in \mathcal{T}$  with  $M \sim N$  we have

$$\# \left\{ (K, L) \in \mathcal{T}^2 : K \stackrel{h}{\sim} L, \{M, N\} \subset \gamma_{KL} \right\} \lesssim 1 \vee \frac{|h|}{|\mathcal{T}|}. \quad (8.2)$$

*Proof.* Part (1) has been proved in [GKM18, Lemma 2.12], so we focus on (2) and write  $S$  for the set whose cardinality we would like to bound. For  $r, l > 0$ , we consider the cylinder  $\text{Cyl}(r, l)$  of radius  $r$  and height  $2l$  given by

$$\text{Cyl}(r, l) := \{v = (v_1, v^*) \in \mathbb{R}^d : v_1 \in B_r^{d-1}, v^* \in [-l, l]\},$$

where  $B_r^{d-1}$  denotes the ball in  $\mathbb{R}^{d-1}$  of radius  $r$  centred in the origin. Without loss of generality we may assume that  $x_M = 0$ . Let  $S_1 \subset \mathbb{R}^d$  be the union of all  $K \in \mathcal{T}$  such that  $(K, L) \in S$  for some  $L \in \mathcal{T}$ .

We claim that

$$S_1 \subset \text{Cyl}(\bar{r}, \bar{l}) \tag{8.3}$$

for some  $\bar{r} \lesssim [\mathcal{T}]$  and  $\bar{l} \lesssim |h| + [\mathcal{T}]$ . Indeed, for all cells  $K, L \in \mathcal{T}$  with  $(K, L) \in S$ , the construction in [GKM18] yields that  $M \cup N$  is contained in the cylinder  $\bar{C}$  of radius  $2[\mathcal{T}]$ , whose central axis is obtained by extending the line segment between  $x_K$  and  $x_L$  by a distance  $[\mathcal{T}]$  in both directions. Hence, we can set  $\bar{r} := 2[\mathcal{T}]$ . Moreover, in order to conclude the proof of (8.3) it suffices to show that

$$|x| \lesssim [\mathcal{T}] + |h| \quad \forall K \in S_1, x \in K. \tag{8.4}$$

Observe that  $0 \in M \subset \bar{C}$  implies that there exists  $y \in \mathbb{R}^d$  belonging to the axis of  $\bar{C}$  with  $|y| \leq 2[\mathcal{T}]$ . This shows that one has

$$\bar{C} \subset B_{r_0}(y)$$

for  $r_0 := 4[\mathcal{T}] + d_{KL}$ .

Pick now any  $x \in K \in S_1$ . In particular  $x \in B_{r_0}(y)$ . Henceforth, we have

$$\begin{aligned} |x| &\leq |x - y| + |y| \leq r_0 + 2[\mathcal{T}] \leq 6[\mathcal{T}] + d_{KL} \\ &\leq 6[\mathcal{T}] + |x_K - x_L + h| + |h| \leq 8[\mathcal{T}] + |h|, \end{aligned}$$

where in the latter inequality we used that  $|x_K - x_L + h| \leq 2[\mathcal{T}]$  whenever  $K \stackrel{h}{\sim} L$ . This shows (8.4) and, thus, (8.3) as well.

Now we conclude the proof by a simply volume comparison argument: On one hand, the volume of the cylinder is given by

$$\mathcal{L}^d(\text{Cyl}(\bar{w}, \bar{r})) \lesssim [\mathcal{T}]^{d-1}([\mathcal{T}] + |h|) \lesssim [\mathcal{T}]^{d-1}([\mathcal{T}] \vee |h|). \tag{8.5}$$

On the other hand,  $S_1$  can be written as a disjoint union of cells. Let us denote by  $N_1 \in \mathbb{N}$  the number of such cells and by  $K_i$  the cells in  $S_1$ .

Moreover, by regularity we know that there exists a  $\delta \lesssim [\mathcal{T}]$  such that  $B_\delta(x_K) \subset K$  for every  $K \in \mathcal{T}$ . It follows that

$$\mathcal{L}^d(S_1) = \sum_{i=1}^{N_1} \mathcal{L}^d(K_i) \geq \sum_{i=1}^{N_1} \mathcal{L}^d(B_\delta(x_{K_i})) = N_1 \delta^d \gtrsim N_1 [\mathcal{T}]^d. \tag{8.6}$$

Putting (8.3), (8.5) and (8.6) together we infer that

$$N_1 \lesssim 1 \vee \frac{|h|}{[\mathcal{T}]}$$

We conclude the proof observing that regularity implies  $\#S \lesssim N_1$ . Indeed, for every  $K \in \mathcal{T}$ ,  $K \subset S_1$ , there exists a (universally) bounded number of cells  $L \in \mathcal{T}$



such that  $(K, L) \in S$ . This is due to the fact that, whenever  $L, L' \in \mathcal{T}$  are such that  $(K, L), (K, L') \in S$ , then by the triangle inequality we deduce that

$$d_{L, L'} \lesssim [\mathcal{T}].$$

As a result, regularity implies the claim, which allows us to conclude the proof.  $\square$

The following lemma provides a crucial estimate needed to deduce  $L^2$ -strong compactness of sequences with bounded energy. A similar result has been obtained in dimension  $d = 2, 3$  in [EGH00, Lemma 3.3] with bounds in terms of discrete Sobolev norms.

**Lemma 8.4** ( $L^2$ -Hölder continuity). *Assume (lb). Fix  $A \in \mathcal{O}(\Omega)$  and set  $A_\delta := \{x \in A : \text{dist}(x, \partial\Omega) > \delta\}$  for  $\delta > 0$ . Let  $\mathcal{T}$  be a  $\zeta$ -regular mesh, let  $f \in L^2(\mathcal{T}|_A)$  and define  $\varphi := \iota_{\mathcal{T}} f \in L^2(A)$ . For any  $h \in \mathbb{R}^d$  we have the  $L^2$ -bound*

$$\|\tau_h \varphi - \varphi\|_{L^2(A_{|h|})}^2 \lesssim \frac{|h|}{k} \left( |h| \vee [\mathcal{T}] \right) \mathcal{F}_{\mathcal{T}}(f, A), \quad (8.7)$$

where  $\tau_h \varphi(\cdot) := \varphi(\cdot - h)$  and  $k > 0$  is the lower bound in (lb).

*Proof.* For any  $h \in \mathbb{R}^d$  we have

$$\|\tau_h \varphi - \varphi\|_{L^2(A_{|h|})}^2 = \int_{A_{|h|}} (\varphi(x-h) - \varphi(x))^2 dx \leq \sum_{K, L \in \mathcal{T}|_A} |S_{KL}| (f(L) - f(K))^2, \quad (8.8)$$

where  $S_{KL} = \{x \in K : x - h \in L\}$ . For  $K, L \in \mathcal{T}|_A$  we use Lemma 8.3 and the Cauchy-Schwarz inequality to write

$$(f_N(K) - f_N(L))^2 \leq n_{KL} \sum_{i=1}^{n_{KL}} (f_N(K_{i-1}) - f_N(K_i))^2, \quad (8.9)$$

where  $K = K_0 \sim K_1 \sim \dots \sim K_{n_{KL}} = L$  and  $n_{KL} \lesssim \frac{d_{KL}}{[\mathcal{T}]}$ . Observe that  $d_{KL} \lesssim [\mathcal{T}] \vee |h|$ , whenever  $S_{KL} \neq \emptyset$ .

To estimate the measure of  $S_{KL}$ , we pick a hyperplane  $H$  that separates  $K$  and  $L$  (which exists by the Hahn-Banach theorem, in view of the convexity of the cells). By construction,  $S_{KL}$  is contained in the strip between  $H$  and  $H+h$ . Moreover, we have  $S_{KL} \subseteq K$ , which means that  $S_{KL}$  is contained in a ball of radius  $\lesssim [\mathcal{T}]$ . Combining these two facts, we infer that  $|S_{KL}| \lesssim [\mathcal{T}]^{d-1} |h|$ ; hence,  $|S_{KL}| \lesssim [\mathcal{T}]^{d-1} (|h| \wedge [\mathcal{T}])$  by  $\zeta$ -regularity.

Putting these estimates together, we obtain

$$|S_{KL}| (f(K) - f(L))^2 \lesssim [\mathcal{T}]^{d-1} |h| \sum_{i=1}^{n_{KL}} (f(K_{i-1}) - f(K_i))^2. \quad (8.10)$$

Let  $\alpha_{KL}$  denote the left-hand side in (8.2). Using (8.8) and (8.10) we find that

$$\|\tau_h \varphi - \varphi\|_{L^2(A_{|h|})}^2 \lesssim [\mathcal{T}]^{d-1} |h| \sum_{\substack{K, L \in \mathcal{T}|_A \\ L \sim K}} \alpha_{KL} (f(L) - f(K))^2.$$

On the other hand, since  $w_{KL} \gtrsim [\mathcal{T}]^{d-2}$  by  $\zeta$ -regularity and  $r_N \geq k$  by assumption (lb), we have

$$\mathcal{F}_{\mathcal{T}}(f, A) \gtrsim k [\mathcal{T}]^{d-2} \sum_{\substack{K, L \in \mathcal{T}|_A \\ L \sim K}} (f(K) - f(L))^2.$$

The desired result follows since  $\alpha_{KL} \leq 1 \vee \frac{|h|}{|\mathcal{T}|}$  by Lemma 8.3.  $\square$

The compactness result now follows easily.

**Proposition 8.5** (Compactness). *Fix  $A \in \mathcal{O}(\Omega)$  and assume that the lower bound (lb) holds. Let  $(\mathcal{T}_N)_N$  be a vanishing sequence of  $\zeta$ -regular meshes. Let  $f_N \in L^2(\mathcal{T}_N|_A)$  be such that*

$$\alpha := \sup_{N \in \mathbb{N}} \mathcal{F}_N(f_N, A) < +\infty$$

and define  $\varphi_N := \iota_N f_N \in L^2(A)$ . Then the sequence  $(\varphi_N)_N$  is relatively compact in  $L^2(A)$ . Moreover, any subsequential limit  $\varphi$  belongs to  $H^1(A)$  and satisfies

$$\|\nabla \varphi\|_{L^2(A)} \lesssim \sqrt{\frac{\alpha}{k}}.$$

*Proof.* The  $L^2(\Omega)$ -compactness follows from (8.7) in view of the Kolmogorov-Riesz-Fréchet theorem [Bre10, Theorem 4.26]. Let  $\varphi$  be any subsequential limit point of  $\varphi_N$  as  $[\mathcal{T}_N] \rightarrow 0$ . Another application of (8.7) yields for any  $h \in \mathbb{R}^d$  and  $\delta > 0$ ,

$$\|\tau_h \varphi - \varphi\|_{L^2(A_\delta)}^2 = \lim_{N \rightarrow \infty} \|\tau_h \varphi_N - \varphi_N\|_{L^2(A_\delta)}^2 \lesssim \frac{\alpha}{k} |h|^2,$$

which implies that  $\varphi \in H^1(A)$  by the characterization of  $H^1(A)$  as the space of functions which are Lipschitz continuous in  $L^2$ -norm (see, e.g. [Bre10, Proposition 9.3]).  $\square$

*Proof of Theorem 8.1.* Proposition 8.5 shows that  $\varphi \in H^1(\Omega)$  whenever  $\mathbf{F}_{0,\rho}(\varphi) < +\infty$ . It follows from Proposition 8.5 that every  $L^2$ -weakly convergent sequence  $\varphi_N = \iota_N f_N$  with bounded energy  $\sup_N \mathcal{F}_N(f_N, A) < +\infty$  converges strongly in  $L^2$ . Therefore, Mosco and  $\Gamma$ -convergence are equivalent in this situation.  $\square$

**8.2. Sobolev bound and inner regularity.** This second part focuses on the proof of the Sobolev upper bound (iii) in Theorem 9.3, which turns out to be useful for several results in the sequel.

**Proposition 8.6** (Sobolev upper bound). *Assume (ub). Then we have the Sobolev upper bound*

$$\mathbf{F}_{0,\rho}(\varphi, A) \lesssim \bar{k} \int_A |\nabla \varphi|^2 d\bar{\mathbf{m}} \quad (8.11)$$

for any  $\varphi \in H^1(\Omega)$  and  $A \in \mathcal{O}(\Omega)$ .

*Proof.* Let us first prove (8.11) for  $\varphi \in C_c^\infty(\mathbb{R}^d)$ . For  $N \in \mathbb{N}$ , define  $f_N : \mathcal{T}_N \rightarrow \mathbb{R}$  by

$$f_N(K) := \varphi(x_K) \quad \text{for } K \in \mathcal{T}_N.$$

Clearly,  $\varphi_N := \iota_N f_N$  converges uniformly to  $\varphi$  as  $N \rightarrow \infty$ . Moreover, by smoothness of  $\varphi$  and continuity of  $\sigma$  we also have

$$\varepsilon_N := \sup_{K, L \in \mathcal{T}_N} \left| \left( \frac{f_N(K) - f_N(L)}{d_{KL}} \right)^2 S_{KL} - (\nabla \varphi(x_K) \cdot \nu_{KL})^2 \sigma(x_K) \right| \rightarrow 0 \quad (8.12)$$

as  $N \rightarrow \infty$ . Similarly,

$$\left| \sum_{K \in \mathcal{T}_N|_A} |\nabla \varphi(x_K)|^2 \sigma(x_K) |K| - \int_A |\nabla \varphi|^2 d\bar{\mathbf{m}} \right| \leq \varepsilon_N. \quad (8.13)$$

Now we simply argue by  $\zeta$ -regularity of the meshes (in particular we use the fact that the number of neighbours is universally bounded) and (ub) to show that

$$\begin{aligned} \bar{k}^{-1} \tilde{\mathbf{F}}_N(\varphi_N, A) &= \sum_{K, L \in \mathcal{T}_N|_A} \left( \frac{f_N(K) - f_N(L)}{d_{KL}} \right)^2 \theta_{\log}(r_N(K), r_N(L)) d_{KL} |\Gamma_{KL}| S_{KL} \\ &\lesssim \sum_{K \in \mathcal{T}_N|_A} d_{KL} |\Gamma_{KL}| |\nabla \varphi(x_K)|^2 \sigma(x_K) + \varepsilon_N \sum_{K \in \mathcal{T}_N|_A} d_{KL} |\Gamma_{KL}| \\ &\lesssim \sum_{K \in \mathcal{T}_N|_A} |\nabla \varphi(x_K)|^2 \sigma(x_K) |K| + \varepsilon_N \mathcal{L}^d(A) \\ &\lesssim \int_A |\nabla \varphi|^2 d\bar{m} + \varepsilon_N (\mathcal{L}^d(A) + 1), \end{aligned}$$

where we used (8.12), the regularity of the mesh and (8.13). Passing to the limit  $N \rightarrow \infty$  we obtain

$$\mathbf{F}_{0,\rho}(\varphi, A) \leq \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N, A) \lesssim \bar{k} \int_A |\nabla \varphi|^2 d\bar{m},$$

which is the desired bound.

It remains to extend the result to  $H^1(\Omega)$  by a density argument. Indeed, for any  $\varphi \in H^1(\Omega)$  there exists a sequence  $(\varphi_i)_i \subseteq C_c^\infty(\mathbb{R}^d)$  such that  $\varphi_i \rightarrow \varphi$  in  $H^1(\Omega)$ . Using that  $\mathbf{F}_{0,\rho}$  is lower semicontinuous with respect to  $L^2(\Omega)$ , we apply (8.11) to  $\varphi_i$  to obtain

$$\mathbf{F}_{0,\rho}(\varphi, A) \leq \liminf_{i \rightarrow \infty} \mathbf{F}_{0,\rho}(\varphi_i, A) \lesssim \bar{k} \liminf_{i \rightarrow \infty} \int_A |\nabla \varphi_i|^2 d\bar{m} = \bar{k} \int_A |\nabla \varphi|^2 d\bar{m},$$

which shows (8.11) for  $\varphi \in H^1(\Omega)$ .  $\square$

*Remark 8.7.* In the case when  $m_N = \pi_N$  (or more generally, when  $m_N = P_N(\rho dx)$  for some continuous  $\rho$ ), it is even possible to prove (iii) with  $a = 0$  and  $c = 1$ . In other words, the way one can prove (iii) is to give a proof of the limsup inequality. Albeit simple, the proof of the existence of a recovery sequence reveals to be quite insufficient for our purposes, due to the fact there is no simple way to obtain the liminf inequality, which is the reason one has to pass through the compactness and representation scheme.

We now focus on the inner regularity as set-valued limit functional of  $(\tilde{\mathbf{F}}_N(\cdot, A))_N$  for every  $A \in \mathcal{O}(\Omega)$ . Note that we prove something slightly stronger than the classical inner regularity. More precisely, we are able to show an inner approximation with sets of Lebesgue measure 0, which will be particularly useful in the proof of the locality in Proposition 9.5 below.

**Proposition 8.8** (Inner regularity). *Assume (ub). For any  $\varphi \in H^1(\Omega)$  the function  $A \mapsto \mathbf{F}_{0,\rho}(\varphi, A)$  is inner regular on  $\mathcal{O}(\Omega)$ , in the sense that*

$$\sup_{\substack{A' \in \mathcal{A}, \\ \mathcal{L}^d(\partial A')=0}} \mathbf{F}_{0,\rho}(\varphi, A') = \sup_{A' \in \mathcal{A}} \mathbf{F}_{0,\rho}(\varphi, A') = \mathbf{F}_{0,\rho}(\varphi, A), \quad \forall A \in \mathcal{O}(\Omega). \quad (8.14)$$

*Proof.* We adapt the proof for the cartesian grid as given in [AC04, Proposition 3.9]. Fix  $\varphi \in H^1(\Omega)$  and  $\delta > 0$  and consider a non-empty set  $A'' \in \mathcal{O}(\Omega)$  such that

$A'' \Subset A$  (i.e.  $A''$  is relatively compact in  $A$ ) and

$$\int_{A \setminus \overline{A''}} |\nabla \varphi|^2 dx < \delta.$$

Let  $\varepsilon_N := \iota_N e_N$  be a recovery sequence for  $\mathbf{F}_{0,\rho}(\varphi, A \setminus \overline{A''})$ , i.e.

$$\varepsilon_N \rightarrow \varphi \text{ in } L^2(\Omega) \quad \text{and} \quad \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varepsilon_N, A \setminus \overline{A''}) \leq \mathbf{F}_{0,\rho}(\varphi, A \setminus \overline{A''}) \lesssim \bar{k}\delta, \quad (8.15)$$

where the last bound is a consequence of Proposition 8.6.

Take  $A' \in \mathcal{O}(\Omega)$  such that  $A'' \Subset A' \Subset A$  and  $\mathcal{L}^d(\partial A') = 0$ . Note that this can always be done since one can pick a compact set  $K$  satisfying  $A'' \subset K \Subset A$  and then choose  $A'$  as the union of any finite open cover of  $K$  by balls whose closures are contained in  $A$ . Let  $\varphi_N := \iota_N f_N$  be a recovery sequence for  $\mathbf{F}_{0,\rho}(\varphi, A')$  such that

$$\varphi_N \rightarrow \varphi \text{ in } L^2(\Omega) \quad \text{and} \quad \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N, A') \leq \mathbf{F}_{0,\rho}(\varphi, A').$$

Fix  $M \in \mathbb{N}$  and suppose that  $[\mathcal{T}_N] < \frac{1}{5(M+1)}$ . Define  $A'' \subset A_1 \subset A_2 \subset \dots \subset A_{5(M+1)} \subset A'$  by

$$A_j := \left\{ x \in A' : d(x, A'') < \frac{j}{5(M+1)} d((A')^c, A'') \right\}.$$

Moreover, for  $i \in \{1, \dots, M\}$  we consider a cutoff function  $\rho_i \in C^\infty(\mathbb{R}^d)$  satisfying

$$\rho_i|_{A_{5i+2}} = 1, \quad \rho_i|_{\Omega \setminus A_{5i+3}} = 0, \quad 0 \leq \rho_i \leq 1, \quad |\nabla \rho_i| \lesssim M. \quad (8.16)$$

Set  $r_N^i := P_N \rho_i$  and define

$$f_N^i := r_N^i f_N + (1 - r_N^i) e_N, \quad \text{so that } \varphi_N^i := \iota_N f_N^i \rightarrow \varphi$$

as  $N \rightarrow \infty$ . As  $[\mathcal{T}_N] < \frac{1}{5(M+1)}$ , we have by (8.16),

$$\varphi_N^i \equiv \varphi_N \text{ in } A_{5i+1}, \quad \varphi_N^i \equiv \varepsilon_N \text{ in } A \setminus \overline{A_{5i+4}}. \quad (8.17)$$

Using these identities and the inclusions  $A_{5i+1} \subset A'$  and  $A'' \subset A_{5i+4}$  we obtain

$$\begin{aligned} \tilde{\mathbf{F}}_N(\varphi_N^i, A) &\leq \tilde{\mathbf{F}}_N(\varphi_N^i, A_{5i+1}) + \tilde{\mathbf{F}}_N(\varphi_N^i, A_{5(i+1)} \setminus \overline{A_{5i}}) + \tilde{\mathbf{F}}_N(\varphi_N^i, A \setminus \overline{A_{5i+4}}) \\ &\leq \tilde{\mathbf{F}}_N(\varphi_N, A') + \tilde{\mathbf{F}}_N(\varphi_N^i, A_{5(i+1)} \setminus \overline{A_{5i}}) + \tilde{\mathbf{F}}_N(\varepsilon_N, A \setminus \overline{A''}) \end{aligned} \quad (8.18)$$

To estimate the middle term, let  $\nabla g(K, L) := g(L) - g(K)$  denote the discrete derivative and observe that

$$\begin{aligned} \nabla f_N^i(K, L) &= r_N^i(L) \nabla f_N(K, L) + (1 - r_N^i(L)) \nabla e_N(K, L) \\ &\quad + (f_N(K) - e_N(K)) \nabla r_N^i(K, L) \end{aligned}$$

for any  $K, L \in \mathcal{T}_N$ . Consequently,

$$|\nabla f_N^i(K, L)|^2 \lesssim |\nabla f_N(K, L)|^2 + |\nabla e_N(K, L)|^2 + M^2 d_{KL}^2 |f_N(K) - e_N(K)|^2.$$

Using this bound and the  $\zeta$ -regularity of the mesh we obtain

$$\begin{aligned}
& \frac{1}{M} \sum_{i=1}^M \tilde{\mathbf{F}}_N(\varphi_N^i, A_{5(i+1)} \setminus \overline{A_{5i}}) \\
& \lesssim \frac{1}{M} \sum_{i=1}^M \left( \tilde{\mathbf{F}}_N(\varphi_N, A_{5(i+1)} \setminus \overline{A_{5i}}) + \tilde{\mathbf{F}}_N(\varepsilon_N, A_{5(i+1)} \setminus \overline{A_{5i}}) + \bar{k}M^2 \|\varphi_N - \varepsilon_N\|_{L^2(\Omega)} \right) \\
& \leq \frac{2}{M} \left( \tilde{\mathbf{F}}_N(\varphi_N, A' \setminus \overline{A''}) + \tilde{\mathbf{F}}_N(\varepsilon_N, A' \setminus \overline{A''}) \right) + \bar{k}M^2 \|\varphi_N - \varepsilon_N\|_{L^2(\Omega)} \\
& \leq \frac{2E}{M} + \bar{k}M^2 \|\varphi_N - \varepsilon_N\|_{L^2(\Omega)},
\end{aligned}$$

where

$$E := E(\delta, A) := \sup_{N \in \mathbb{N}} \left( \tilde{\mathbf{F}}_N(\varphi_N, A') + \tilde{\mathbf{F}}_N(\varepsilon_N, A \setminus \overline{A''}) \right) < +\infty.$$

Inserting this error estimate into (8.18) we deduce that

$$\frac{1}{M} \sum_{i=1}^M \tilde{\mathbf{F}}_N(\varphi_N^i, A) - \tilde{\mathbf{F}}_N(\varphi_N, A') - \tilde{\mathbf{F}}_N(\varepsilon_N, A \setminus \overline{A''}) \lesssim \frac{E}{M} + \bar{k}M^2 \|\varphi_N - \varepsilon_N\|_{L^2(\Omega)}.$$

Next we pass to the limit  $N \rightarrow \infty$  for fixed  $M \in \mathbb{N}$ . Since  $\varphi_N, \varepsilon_N \rightarrow \varphi$  in  $L^2$ , it follows from (8.15) that

$$\limsup_{N \rightarrow \infty} \frac{1}{M} \sum_{i=1}^M \tilde{\mathbf{F}}_N(\varphi_N^i, A) - \mathbf{F}_{0,\rho}(\varphi, A') - \bar{k}\delta \lesssim \frac{E}{M}. \quad (8.19)$$

It remains to note that for any  $M \in \mathbb{N}$ , there exists a subsequence  $(\varphi_N^{i_N})_N$  such that  $\varphi_N^{i_N} \rightarrow \varphi$  in  $L^2(\Omega)$  as  $N \rightarrow \infty$  and

$$\tilde{\mathbf{F}}_N(\varphi_N^{i_N}, A) \leq \frac{1}{M} \sum_{i=1}^M \tilde{\mathbf{F}}_N(\varphi_N^i, A) \quad \forall N \in \mathbb{N}.$$

Together with (8.19) this bound yields

$$\mathbf{F}_{0,\rho}(\varphi, A) \leq \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N^{i_N}, A) \leq \mathbf{F}_{0,\rho}(\varphi, A') + C \left( \delta + \frac{E}{M} \right),$$

where  $C = C(d, \zeta)$  and  $E = E(\delta, A)$ . Taking the limit  $M \rightarrow \infty$  and then  $\delta \rightarrow 0$  we find

$$\mathbf{F}_{0,\rho}(\varphi, A) \leq \sup_{\substack{A' \in \mathcal{A}, \\ \mathcal{L}^d(\partial A')=0}} \mathbf{F}_{0,\rho}(\varphi, A').$$

As the reverse inequality trivially holds, this concludes the proof.  $\square$

*Proof of Theorem 8.2.* By Proposition 8.8 and [BD98, Theorem 10.3], the sequence  $(\tilde{\mathbf{F}}_N(\cdot, A))_N$  has a subsequence which is  $\Gamma$ -converging in  $L^2(\Omega)$ -topology to a limit functional  $\mathbf{F}_{0,\rho}(\cdot, A)$  for every  $A \in \mathcal{O}(\Omega)$ . The fact that  $\Gamma$ -convergence implies Mosco convergence, has already been observed in Theorem 8.1.  $\square$

## 9. REPRESENTATION AND CHARACTERISATION OF THE LIMIT

In this section we show the following representation formula for the  $\Gamma$ -limits from Section 8.

**Theorem 9.1** (Representation of the  $\Gamma$ -limit). *Let  $\mathbf{F}_{0,\rho}$  be as in Theorem 8.2, i.e. suppose that for every  $A \in \mathcal{O}(\Omega)$ , there exists a subsequence of  $(\tilde{\mathbf{F}}_N(\cdot, A))_N$  that is  $L^2(\Omega)$ -Mosco convergent to  $\mathbf{F}_{0,\rho}(\cdot, A)$ . Then the functional  $\mathbf{F}_{0,\rho}$  can be represented as*

$$\mathbf{F}_{0,\rho}(\varphi, A) = \begin{cases} \int_A f_\rho(x, \varphi, \nabla \varphi) \, dx & \text{if } \varphi \in H^1(\Omega), \\ +\infty, & \text{if } \varphi \in L^2(\Omega) \setminus H^1(\Omega), \end{cases} \quad (9.1)$$

for some measurable function  $f_\rho : \Omega \times \mathbb{R} \times \mathbb{R}^d \rightarrow [0, +\infty)$ .

Combined with the following result, this will complete the proof of Theorem 7.2.

**Theorem 9.2** (Characterization of  $f_\rho$ ). *Suppose that  $\sigma \in C_b(\bar{\Omega})$ . Then the function  $f_\rho : \Omega \times \mathbb{R}^d \rightarrow [0, +\infty)$  defined in Theorem 9.1 is given by*

$$f_\rho(x, u, \xi) = |\xi|^2 \rho(x) \sigma(x), \quad \forall x \in \Omega, u \in \mathbb{R}, \xi \in \mathbb{R}^d.$$

In particular, the sequence  $(\tilde{\mathbf{F}}_N(\cdot, A))_N$  is  $L^2(\Omega)$ -Mosco convergent to  $\mathbf{F}_{0,\rho}(\cdot, A)$ .

To prove Theorem 9.1, we use a representation result from [BFLM02] for functionals on Sobolev spaces, which can be applied here in view of Theorem 8.1. For our application, we have  $E(\cdot, A) := \mathbf{F}_{0,\rho}(\cdot, A)$  for any subsequential  $\Gamma$ -limit point  $\mathbf{F}_{0,\rho}(\cdot, A)$  of  $(\tilde{\mathbf{F}}_N(\cdot, A))_N$ .

**Theorem 9.3.** *Let  $E : H^1(\Omega) \times \mathcal{O}(\Omega) \rightarrow [0, +\infty]$  be a functional satisfying the following conditions:*

- (i) locality:  *$E$  is local, i.e. for all  $A \in \mathcal{O}(\Omega)$  we have  $E(\varphi, A) = E(\psi, A)$  if  $\varphi = \psi$  a.e. on  $A$ .*
- (ii) measure property: *For every  $\varphi \in H^1(\Omega)$  the set map  $E(\varphi, \cdot)$  is the restriction of a Borel measure to  $\mathcal{O}(\Omega)$ .*
- (iii) Sobolev bound: *There exists a constant  $c > 0$  and  $a \in L^1(\Omega)$  such that*

$$\frac{1}{c} \int_A |\nabla \varphi|^2 \, dx \leq E(\varphi, A) \leq c \int_A (a(x) + |\nabla \varphi|^2) \, dx$$

for all  $\varphi \in H^1(\Omega)$  and  $A \in \mathcal{O}(\Omega)$ .

- (iv) lower semicontinuity:  *$E(\cdot, A)$  is weakly sequentially lower semicontinuous in  $H^1(\Omega)$ .*

Then  $E$  can be represented in integral form

$$E(\varphi, A) = \int_A f(x, \varphi, \nabla \varphi) \, dx,$$

where the measurable function  $f : \Omega \times \mathbb{R} \times \mathbb{R}^d \rightarrow [0, +\infty)$  satisfies the self-consistent formula

$$f(x, u, \xi) := \limsup_{\varepsilon \rightarrow 0^+} \frac{M(u + \xi(\cdot - x), Q_\varepsilon(x))}{\varepsilon^d}, \quad (9.2)$$

where  $Q_\varepsilon(x)$  is the open cube of side-length  $\varepsilon > 0$  centred at  $x$  and

$$M(\psi, A) := \inf \{ E(\varphi, A) : \varphi \in H^1(\Omega), \varphi - \psi \in H_0^1(A) \} \quad (9.3)$$

for any  $\psi \in H^1(\Omega)$  and any open cube  $A \subseteq \Omega$ .

*Remark 9.4* (Equivalence of definitions). The paper [BFLM02] contains the statement of Theorem 9.3 with  $M(\psi, A)$  replaced by

$$\bar{M}(\psi, A) := \inf \{ E(\varphi, A) : \varphi \in H^1(\Omega), \varphi = \psi \text{ in a neighbourhood of } A \}.$$

We claim that  $M = \bar{M}$ . As any competitor  $\varphi$  for  $M$  is a competitor for  $\bar{M}$ , it is clear that  $M \geq \bar{M}$ . To show the opposite inequality, we fix  $\varepsilon > 0$  and take  $\varphi \in H^1(A)$  such that  $E(\varphi, A) \leq \bar{M}(\psi, A) + \varepsilon$ . It follows that  $\varphi - \psi \in H_0^1(A)$ , and there exists a sequence  $(\eta_n)_n \subseteq C_c^\infty(A)$  such that  $\eta_n \rightarrow \varphi - \psi$  in  $H^1(\Omega)$  as  $n \rightarrow \infty$ . Set  $\varphi_n := \psi + \eta_n$ , so that  $\varphi_n \rightarrow \varphi$  in  $H^1(\Omega)$ . Note that  $\varphi_n$  is a competitor for  $M(\psi, A)$  as it coincides with  $\psi$  on  $A \setminus \text{spt}(\eta_n)$ . Hence,  $M(\psi, A) \leq E(\varphi_n, A)$  for all  $n \in \mathbb{N}$ .

Using the continuity of  $E(\cdot, A)$  with respect to the strong  $H^1(\Omega)$  convergence (as follows from (iii)), we may pass to the limit to obtain

$$M(\psi, A) \leq \lim_{n \rightarrow \infty} E(\varphi_n, A) = E(\varphi, A) \leq \bar{M}(\psi, A) + \varepsilon.$$

As  $\varepsilon > 0$  is arbitrary, the claim follows.

In the remainder of this section we will verify that  $\mathbf{F}_{0,\rho}$  satisfies the conditions of Theorem 9.3.

First we observe that the Sobolev upper bound (iii) has already been proved in Proposition 8.6. Moreover, we claim that the corresponding lower bound follows from Lemma 8.4. To prove this, take a recovery sequence  $\varphi_N \rightarrow \varphi$  in  $L^2(\Omega)$  for  $\tilde{\mathbf{F}}_N(\cdot, A)$ . For any  $h \in \mathbb{R}^d$  and  $\delta > 0$  sufficiently small, it follows from Lemma 8.4 that

$$\begin{aligned} \|\tau_h \varphi - \varphi\|_{L^2(A_\delta)}^2 &= \lim_{N \rightarrow \infty} \|\tau_h \varphi_N - \varphi_N\|_{L^2(A_\delta)}^2 \\ &\lesssim \frac{|h|^2}{k} \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N, A) = \frac{|h|^2}{k} \mathbf{F}_\rho(\varphi, A). \end{aligned}$$

From the usual characterisation of Sobolev norms (see e.g. [Bre10, Proposition 9.3]) we infer that  $\|\nabla \varphi\|_{L^2(A_\delta)}^2 \lesssim k^{-1} \mathbf{F}_\rho(\varphi, A)$ , which yields the result.

We also observe that (iv) follows immediately since any  $\Gamma$ -limit is lower semicontinuous [Bra02, Proposition 1.28] with respect to the  $L^2(\Omega)$ -topology.

Thus, to verify that  $\mathbf{F}_{0,\rho}$  satisfies the conditions of Theorem 9.3, it remains to prove the locality (Section 9.1) and the subadditivity (Section 9.2). The proof of Theorem 9.2 is contained in Section 9.3.

**9.1. Locality.** A consequence of the inner regularity result from Proposition 8.8 is the following simple proof of the locality of  $\mathbf{F}_{0,\rho}$ .

**Proposition 9.5** (Locality). *Assume that (ub) holds. Then  $\mathbf{F}_{0,\rho}$  is local, i.e. for any  $A \in \mathcal{O}(\Omega)$  and  $\varphi, \psi \in L^2(\Omega)$  such that  $\varphi = \psi$  a.e. on  $A$ , we have  $\mathbf{F}_{0,\rho}(\varphi, A) = \mathbf{F}_{0,\rho}(\psi, A)$ .*

*Proof.* Let  $A \in \mathcal{O}(\Omega)$  and take  $\varphi, \psi \in L^2(\Omega)$  such that  $\varphi = \psi$  a.e. on  $A$ . In view of the inner regularity result from Proposition 8.8 we may assume that  $\mathcal{L}^d(\partial A) = 0$ . By symmetry, it suffices to prove that  $\mathbf{F}_{0,\rho}(\varphi, A) \geq \mathbf{F}_{0,\rho}(\psi, A)$ .

Define  $C_N := \bigcup\{K : K \in \mathcal{T}_N|_A\}$  and  $C := \bigcup_N C_N$ , so that  $C \supseteq A$ . We claim that

$$C \setminus A \subseteq B_N, \quad \text{where } B_N := \{x \in \Omega : d(x, \partial A) < 2[\mathcal{T}_N]\}. \quad (9.4)$$

Indeed, for every  $x \in C \setminus A$  there exists  $N \geq 1$  and  $K \in \mathcal{T}_N$  such that  $x \in K \setminus A$  and  $\bar{K} \cap A \neq \emptyset$ . Therefore,  $d(x, \partial A) = d(x, A) \leq \text{diam}(K) \leq [\mathcal{T}_N]$ , which implies (9.4).

Let  $(\varphi_N)_N$  be a recovery sequence for  $\mathbf{F}_{0,\rho}(\varphi, A)$ , i.e.  $\varphi_N \rightarrow \varphi$  in  $L^2(\Omega)$  and

$$\lim_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N, A) = \mathbf{F}_{0,\rho}(\varphi, A). \quad (9.5)$$

Fix  $\hat{\psi}_N \in PC_N$  such that  $\hat{\psi}_N \rightarrow \psi$  in  $L^2(\Omega)$  as  $N \rightarrow \infty$  and define  $\psi_N : \Omega \rightarrow \mathbb{R}$  by

$$\psi_N(x) := \begin{cases} \varphi_N(x) & \text{if } x \in C, \\ \hat{\psi}_N(x) & \text{if } x \in \Omega \setminus C. \end{cases}$$

We claim that  $\psi_N \rightarrow \psi$  in  $L^2(\Omega)$  as  $N \rightarrow \infty$ . Indeed, since  $\varphi = \psi$  a.e. on  $A$ , we have

$$\|\psi_N - \psi\|_{L^2(\Omega)}^2 = \|\hat{\psi}_N - \psi\|_{L^2(\Omega \setminus C)}^2 + \|\varphi_N - \psi\|_{L^2(C \setminus A)}^2 + \|\varphi_N - \varphi\|_{L^2(A)}^2. \quad (9.6)$$

The first and the last term on the right-hand side vanish as  $N \rightarrow \infty$  since  $\varphi_N \rightarrow \varphi$  and  $\hat{\psi}_N \rightarrow \psi$  in  $L^2(\Omega)$ . On the other hand, (9.4) yields

$$\begin{aligned} \limsup_{N \rightarrow \infty} \|\varphi_N - \psi\|_{L^2(C \setminus A)} &\leq \limsup_{N \rightarrow \infty} (\|\varphi\|_{L^2(B_N)} + \|\psi\|_{L^2(B_N)}) \\ &= \|\varphi\|_{L^2(\partial A)} + \|\psi\|_{L^2(\partial A)} = 0, \end{aligned}$$

since  $\mathcal{L}^d(\partial A) = 0$ . Together with (9.6) we infer that  $\psi_N \rightarrow \psi$  in  $L^2(\Omega)$  as  $N \rightarrow \infty$ . Using this fact, together with the  $\Gamma$ -convergence of  $\tilde{\mathbf{F}}_N$  in  $L^2$ , the equality  $\varphi_N = \psi_N$  a.e. on  $C$  and (9.5), we obtain

$$\mathbf{F}_{0,\rho}(\psi, A) \leq \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\psi_N, A) = \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N, A) = \mathbf{F}_{0,\rho}(\varphi, A),$$

which concludes the proof.  $\square$

**9.2. Subadditivity.** In this section we prove subadditivity of the functional  $A \mapsto \mathbf{F}_{0,\rho}(\varphi, A)$  for any  $\varphi \in H^1(\Omega)$ . This is the first step towards the verification of (ii) in Theorem 9.3.

**Proposition 9.6** (Subadditivity). *Assume (ub). Then the functional  $\mathbf{F}_{0,\rho}(\varphi, \cdot)$  is subadditive for any  $\varphi \in H^1(\Omega)$  in the sense that*

$$\mathbf{F}_{0,\rho}(\varphi, A \cup B) \leq \mathbf{F}_{0,\rho}(\varphi, A) + \mathbf{F}_{0,\rho}(\varphi, B), \quad \forall A, B \in \mathcal{O}(\Omega). \quad (9.7)$$

*Proof.* We prove that for all  $A' \Subset A$ ,  $B' \Subset B$ ,  $\varphi \in H^1(\Omega)$

$$\mathbf{F}_{0,\rho}(\varphi, A' \cup B') \leq \mathbf{F}_{0,\rho}(\varphi, A) + \mathbf{F}_{0,\rho}(\varphi, B)$$

and deduce (9.7) from the inner regularity Proposition (8.8). Once again, the proof is inspired by [AC04, Proposition 3.7] and follows similar ideas as in the proof of Proposition (8.8). Pick  $A' \Subset A$  and  $B' \Subset B$  and let  $(\psi_N)_N, (\phi_N)_N$  being recovery sequences respectively for  $\mathbf{F}_{0,\rho}(\varphi, A)$  and  $\mathbf{F}_{0,\rho}(\varphi, B)$ , which we can assume to be



finite. Set  $d := d(A', A^c)$  and pick any  $M \in \mathbb{N}$ . Suppose that  $[\mathcal{T}_N] < \frac{1}{5(M+1)}$ . We define the sets

$$A_j := \left\{ x \in A : d(x, A') < j \frac{d}{5(M+1)} \right\} \subset A$$

for  $j \in \{1, \dots, 5(M+1)\}$ . Moreover, for  $i \in \{1, \dots, M\}$  let  $\rho_i$  be a cutoff function  $\rho_i \in C^\infty(\mathbb{R}^d)$  satisfying

$$\rho_i|_{A_{5i+2}} = 1, \quad \rho_i|_{\Omega \setminus A_{5i+3}} = 0, \quad 0 \leq \rho_i \leq 1, \quad |\nabla \rho_i| \lesssim M.$$

Introduce sequences converging in  $L^2(\Omega)$  by

$$\varphi_N^i := \iota_N P_N \left( \rho_i \psi_N + (1 - \rho_i) \phi_N \right) \xrightarrow{N \rightarrow \infty} \varphi \quad \forall i \in \{1, \dots, M\}$$

and note that  $\varphi_N^i \equiv \psi_N$  in  $A_{5i+1}$  and  $\varphi_N^i \equiv \phi_N$  in  $\Omega \setminus \overline{A_{5i+4}}$ . Arguing as in the proof of Proposition (8.8), one deduces the bound

$$\tilde{\mathbf{F}}_N(\varphi_N^i, A' \cup B') \leq \tilde{\mathbf{F}}_N(\psi_N, A) + \tilde{\mathbf{F}}_N(\varphi_N^i, (A_{5(i+1)} \setminus \overline{A_{5i}}) \cap B') + \tilde{\mathbf{F}}_N(\phi_N, B) \quad (9.8)$$

for  $i \in \{1, \dots, M\}$ , as well as the bound

$$\frac{1}{M} \sum_{i=1}^M \tilde{\mathbf{F}}_N(\varphi_N^i, (A_{5(i+1)} \setminus \overline{A_{5i}}) \cap B') \lesssim \frac{E}{M} + \bar{k} M^2 \|\psi_N - \phi_N\|_{L^2(\Omega)},$$

where we used that  $(A_{5(i+1)} \setminus \overline{A_{5i}}) \cap B' \subset A \cap B$  and that the energy of the recovery sequences  $\psi_N$  and  $\phi_N$  is bounded from above. Thus,

$$\sup_{N \in \mathbb{N}} \tilde{\mathbf{F}}_N(\psi_N, A) \vee \sup_{N \in \mathbb{N}} \tilde{\mathbf{F}}_N(\phi_N, B) \leq E = E(A, B) < +\infty.$$

We may combine the error estimates above with (9.8) to deduce

$$\frac{1}{M} \sum_{i=1}^M \tilde{\mathbf{F}}_N(\varphi_N^i, A' \cup B') - \tilde{\mathbf{F}}_N(\psi_N, A) - \tilde{\mathbf{F}}_N(\phi_N, B) \lesssim \frac{E}{M} + \bar{k} M^2 \|\psi_N - \phi_N\|_{L^2(\Omega)}.$$

Passing to the limit as  $N \rightarrow \infty$  for a fixed  $M \in \mathbb{N}$ , from the previous bound and the fact that both  $\psi_N, \phi_N \rightarrow \varphi$ , we obtain

$$\limsup_{N \rightarrow \infty} \frac{1}{M} \sum_{i=1}^M \tilde{\mathbf{F}}_N(\varphi_N^i, A' \cup B') - \mathbf{F}_{0,\rho}(\varphi, A) - \mathbf{F}_{0,\rho}(\varphi, B) \lesssim \frac{E}{M}. \quad (9.9)$$

Once again, in order to conclude the proof we note that for any fixed  $M \in \mathbb{N}$ , one can find a sequence of  $\varphi_N^{i_N}$  such that  $\varphi_N^{i_N} \rightarrow \varphi$  in  $L^2(\Omega)$  as  $N \rightarrow \infty$  and

$$\tilde{\mathbf{F}}_N(\varphi_N^{i_N}, A' \cup B') \leq \frac{1}{M} \sum_{i=1}^M \tilde{\mathbf{F}}_N(\varphi_N^i, A' \cup B').$$

Together with (9.9), this yields

$$\mathbf{F}_{0,\rho}(\varphi, A' \cup B') \leq \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N^{i_N}, A' \cup B') \leq \mathbf{F}_{0,\rho}(\varphi, A) + \mathbf{F}_{0,\rho}(\varphi, B) + C \frac{E}{M}$$

for every  $M \in \mathbb{N}$  and some constants  $C = C(d, \zeta) > 0$  and  $E = E(A, B) > 0$ . Taking the limit  $M \rightarrow \infty$ , we infer that

$$\mathbf{F}_{0,\rho}(\varphi, A' \cup B') \leq \mathbf{F}_{0,\rho}(\varphi, A) + \mathbf{F}_{0,\rho}(\varphi, B),$$

which completes the proof.  $\square$

The following additivity property turns out to be much easier to prove than the correspondent result on the grid in [AC04], due to inner regularity in combination with the very short range of interaction (nearest neighbours on a scale of order  $[\mathcal{T}_N]$ ).

**Proposition 9.7** (Additivity on disjoint sets). *Assume (ub). For any  $\varphi \in H^1(\Omega)$  the function  $\mathbf{F}_{0,\rho}(\varphi, \cdot)$  is additive on disjoint sets, i.e.*

$$\mathbf{F}_{0,\rho}(\varphi, A \cup B) = \mathbf{F}_{0,\rho}(\varphi, A) + \mathbf{F}_{0,\rho}(\varphi, B) \quad (9.10)$$

for all  $A, B \in \mathcal{O}(\Omega)$  such that  $A \cap B = \emptyset$ .

*Proof.* In view of the subadditivity result from Proposition 9.6, it remains to show the superadditivity. Furthermore, by inner regularity (Proposition 8.8) we may assume that  $d(A, B) > 0$ . Consequently, for  $N$  sufficiently large we have

$$\tilde{\mathbf{F}}_N(\varphi, A \cup B) = \tilde{\mathbf{F}}_N(\varphi, A) + \tilde{\mathbf{F}}_N(\varphi, B) \quad \forall \varphi \in H^1(\Omega).$$

Fix  $\varphi \in H^1(\Omega)$  and let  $(\varphi_N)_N$  be a recovery sequence for  $\mathbf{F}_{0,\rho}(\varphi, A \cup B)$ . Using the previous identity we obtain

$$\begin{aligned} \mathbf{F}_{0,\rho}(\varphi, A) + \mathbf{F}_{0,\rho}(\varphi, B) &\leq \liminf_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N, A) + \liminf_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N, B) \\ &\leq \liminf_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N, A) + \tilde{\mathbf{F}}_N(\varphi_N, B) \\ &= \liminf_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\varphi_N, A \cup B) \\ &= \mathbf{F}_{0,\rho}(\varphi, A \cup B), \end{aligned}$$

which is the desired superadditivity inequality.  $\square$

We are now in a position to collect all the pieces for the proof of Theorem 9.1.

*Proof of Theorem 9.1.* In view of Proposition 8.6, it suffices to check that  $\mathbf{F}_{0,\rho}(\cdot, A)$  satisfies the conditions of Theorem 9.3.

The locality (i) has been shown in Proposition 9.5.

To prove (ii), we apply the De Giorgi-Letta criterion; cf. [DGL77], [BD98]. For any  $\varphi \in H^1(\Omega)$ , it follows from Proposition 8.8, Proposition 9.6 and Proposition 9.7 that  $\mathbf{F}_{0,\rho}(\varphi, \cdot)$  is the restriction of a Borel measure to  $\mathcal{O}(\Omega)$ .

The Sobolev bound (iii) has been proved in Proposition 8.6.

Finally, to prove the lower semicontinuity (iv) we note that the lower semicontinuity with respect to strong  $L^2(\Omega)$ -convergence follows from the fact that any  $\Gamma$ -limit is lower semicontinuous; see [Bra02, Proposition 1.28]. Since  $H^1(\Omega)$  is compactly embedded in  $L^2(\Omega)$ , the result follows.  $\square$

**9.3. The characterization of the  $\Gamma$ -limit.** To prove Theorem 7.2 it remains to characterize the  $\Gamma$ -limit  $\mathbf{F}_{0,\rho}$  obtained in Theorem 9.1. Thus, we have to compute the function  $f_\rho$  appearing in Theorem 9.1. From (9.2) it follows that for  $x \in \Omega$ ,  $u \in \mathbb{R}$  and  $\xi \in \mathbb{R}^d$ ,

$$f_\rho(x, u, \xi) = \limsup_{\varepsilon \rightarrow 0^+} \frac{\mathbf{M}(u + \xi(\cdot - x); Q_\varepsilon(x))}{\varepsilon^d}, \quad (9.11)$$

where  $Q_\varepsilon(x)$  denotes the open cube of side-length  $\varepsilon$  centred at  $x$  and

$$\mathbf{M}(\phi, A) := \inf_{\psi} \{ \mathbf{F}_{0,\rho}(\psi, A) : \psi \in H^1(\Omega) \text{ s.t. } \psi - \phi \in H_0^1(A) \}$$

for any Lipschitz function  $\phi : \Omega \rightarrow \mathbb{R}$  and any open set  $A \subseteq \Omega$  with Lipschitz boundary.

In order to compute  $\mathbf{M}$  by discrete approximation, we consider its discrete counterpart  $\mathcal{M}_{\mathcal{T}}$  defined by

$$\mathcal{M}_{\mathcal{T}}(f, A) := \inf_g \{ \mathcal{F}_{\mathcal{T}}(g, A) : g \in \mathbb{R}^{\mathcal{T}} \text{ s.t. } f = g \text{ on } \mathcal{T}|_{A^c} \} \quad \text{for } f : \mathcal{T} \rightarrow \mathbb{R}.$$

The following result is crucial for the proof of Theorem 9.2 below.

**Lemma 9.8.** *Let  $A \subseteq \Omega$  be an open set with Lipschitz boundary. For any Lipschitz function  $\phi : \Omega \rightarrow \mathbb{R}$  we define  $f_N : \mathcal{T}_N \rightarrow \mathbb{R}$  by  $f_N(K) := \phi(x_K)$  for  $K \in \mathcal{T}_N$ . Suppose that  $\tilde{\mathbf{F}}_N(\cdot, A) \xrightarrow{\Gamma} \mathbf{F}_{0,\rho}(\cdot, A)$  in  $L^2(\Omega)$  as  $N \rightarrow \infty$  for any  $A \in \mathcal{O}(\Omega)$ . Then we have*

$$\mathcal{M}_N(f_N, A) \rightarrow \mathbf{M}(\phi, A) \tag{9.12}$$

as  $N \rightarrow \infty$ .

*Proof.* First we embed the discrete functionals in the continuous setting. For any Lipschitz function  $\phi : \bar{\Omega} \rightarrow \mathbb{R}$  and any open set  $A \subseteq \Omega$  we set

$$PC_N(\phi, A) := \{ \psi \in PC_N : \psi(x_K) = \phi(x_K) \ \forall K \in \mathcal{T}_N|_{A^c} \}. \tag{9.13}$$

We consider the embedded discrete energies  $\tilde{\mathbf{F}}_N^\phi : L^2(\Omega) \rightarrow [0, +\infty]$  defined by

$$\tilde{\mathbf{F}}_N^\phi(\psi, A) := \begin{cases} \mathcal{F}_N(P_N\psi, A), & \text{if } \psi \in PC_N(\phi, A) \\ +\infty & \text{otherwise,} \end{cases}$$

and their continuous counterpart  $\mathbf{F}_{0,\rho}^\phi : L^2(\Omega) \rightarrow [0, +\infty]$  defined by

$$\mathbf{F}_{0,\rho}^\phi(\psi, A) := \begin{cases} \mathbf{F}_{0,\rho}(\psi, A), & \text{if } \psi - \phi \in H_0^1(A), \\ +\infty & \text{otherwise.} \end{cases}$$

We claim that

$$\tilde{\mathbf{F}}_N^\phi(\cdot, A) \xrightarrow{\Gamma} \mathbf{F}_{0,\rho}^\phi(\cdot, A), \quad \forall A \subseteq \Omega \text{ with Lipschitz boundary, } \phi \in \text{Lip}(\mathbb{R}^d),$$

which implies, together with Proposition 8.5 and basic results from the theory of  $\Gamma$ -convergence, the desired convergence of the minima in (9.12).

To prove the claim, we argue as in [AC04, Theorem 3.10].

To prove the liminf inequality, we consider a sequence  $\psi_N \rightharpoonup \psi$  in  $L^2(\Omega)$  satisfying  $\sup_N \tilde{\mathbf{F}}_N^\phi(\psi_N, A) < +\infty$ . In particular, this implies that  $\psi_N \in PC_N(P_N\phi, A)$  and  $\tilde{\mathbf{F}}_N^\phi(\psi_N, A) = \tilde{\mathbf{F}}_N(\psi_N, A)$ . Since  $\tilde{\mathbf{F}}_N(\cdot, A) \xrightarrow{\Gamma} \mathbf{F}_{0,\rho}(\cdot, A)$ , it remains to prove that  $\psi - \phi \in H_0^1(A)$ . In view of the boundary condition and the fact that  $\phi \in \text{Lip}(\mathbb{R}^d)$ , we have

$$\tilde{\mathbf{F}}_N(\psi_N, \Omega) \leq \tilde{\mathbf{F}}_N(\psi_N, A) + \tilde{\mathbf{F}}_N(P_N\phi, \Omega) \lesssim \tilde{\mathbf{F}}_N(\psi_N, A) + \text{Lip}(\phi).$$

It follows from Proposition 8.5 that  $\psi_N \rightarrow \psi$  strongly in  $L^2(\Omega)$  with  $\psi \in H^1(\Omega)$ . Moreover, by construction we have  $\psi_N \rightarrow \phi$  in  $L^2(\Omega \setminus A)$ . Since  $A$  has a Lipschitz boundary, we conclude that  $\psi - \phi \in H_0^1(A)$ .

Let us now prove the limsup inequality. Pick  $\psi \in L^2(\Omega)$  such that  $\mathbf{F}_{0,\rho}^\phi(\psi, A) < +\infty$ . In particular,  $\psi - \phi \in H_0^1(A)$ . Without loss of generality, we may assume that  $\text{supp}(\psi - \phi) \Subset A$ , as the general case follows then by a density argument using the continuity of  $\mathbf{F}_{0,\rho}$  in the strong  $H^1(\Omega)$ -topology. Consider a recovery sequence

$\psi_N \rightarrow \psi$  in  $L^2(\Omega)$  such that  $\tilde{\mathbf{F}}_N(\psi_N, A) \rightarrow \mathbf{F}_{0,\rho}(\psi, A) = \mathbf{F}_{0,\rho}^\phi(\psi, A)$  as  $N \rightarrow +\infty$ . As in the proof of Proposition 8.8, one can find for any  $\delta > 0$  a cutoff function  $\phi_\delta$  with the following properties:

- (i)  $\text{supp}(\psi - \phi) \Subset \text{supp} \phi_\delta \Subset A$ ;
- (ii) the functions  $\psi_N^\delta := i_N \circ P_N(\phi_\delta \psi_N + (1 - \phi_\delta)\phi)$  satisfy

$$\begin{aligned} \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N^\phi(\psi_N^\delta, A) &= \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\psi_N^\delta, A) \\ &\leq \limsup_{N \rightarrow \infty} \tilde{\mathbf{F}}_N(\psi_N, A) + \delta = \mathbf{F}_{0,\rho}^\phi(\psi, A) + \delta. \end{aligned}$$

Passing to the limit along a diagonal subsequence  $\psi_N^{\delta(N)} \rightarrow \psi$  in  $L^2(\Omega)$  as  $\delta \rightarrow 0$ , the result follows.  $\square$

*Proof of Theorem 9.2.* We split the proof into two parts.

*Step 1.* We first suppose that  $\sigma, \rho \equiv 1$  and  $m_N = \pi_N$  and we fix  $\varepsilon > 0$ . For fixed  $u \in \mathbb{R}$ ,  $z \in \Omega$ , and  $\xi \in \mathbb{R}^d$  we will compute

$$\mathcal{M}_N(f_{u,z}^\xi, Q_\varepsilon(z)), \quad \text{where } f_{u,z}^\xi(K) := \phi_{u,z}^\xi(x_K) \text{ and } \phi_{u,z}^\xi(\cdot) := u + \xi(\cdot - z).$$

As a shorthand we write  $f := f_{u,z}^\xi$  and  $Q_\varepsilon := Q_\varepsilon(z)$ , suppressing the  $N$ -dependence of  $f$ . Recall that

$$\mathcal{M}_N(f, Q_\varepsilon) = \inf_g \{ \mathcal{F}_N(g, Q_\varepsilon) : g \in \mathbb{R}^{\mathcal{T}_N} \text{ and } g(K) = f(K) \text{ for } K \in \mathcal{T}_N|_{Q_\varepsilon} \}.$$

In other words, we minimize the discrete Dirichlet energy localized on  $Q_\varepsilon$  with Dirichlet boundary conditions given by the discretised affine function  $f$ .

By computing the first variation of the action, the unique minimizer is given by the solution  $h : \mathcal{T}_N \rightarrow \mathbb{R}$  of the corresponding discrete Laplace equation

$$\begin{cases} \mathcal{L}_N h(K) = 0 & \text{for } K \in \mathcal{T}_N \setminus \mathcal{T}_N|_{Q_\varepsilon}, \\ h(K) = f(K) & \text{for } K \in \mathcal{T}_N|_{Q_\varepsilon}. \end{cases} \quad (9.14)$$

We claim that the function  $f$  solves (9.14). Indeed, the boundary conditions hold trivially. Moreover, writing  $\tau_{KL} := \frac{x_K - x_L}{|x_K - x_L|}$  we obtain for any  $K \in \mathcal{T}_N \setminus \mathcal{T}_N|_{Q_\varepsilon}$ ,

$$\begin{aligned} \pi_K \mathcal{L}_N f(K) &= \sum_{L \sim K} w_{KL} (f(L) - f(K)) = \sum_{L \sim K} |\Gamma_{KL}| \langle \xi, \tau_{KL} \rangle \\ &= \int_{\partial K} \langle \xi, \nu_{\text{ext}} \rangle d\mathcal{H}^{d-1} = 0, \end{aligned}$$

where  $\nu_{\text{ext}}$  denotes the outward normal unit normal and in the last step we used Stokes' theorem. This computation shows the optimality of  $f$  and, hence,

$$\mathcal{M}_N(f, Q_\varepsilon) = \mathcal{F}_N(f, Q_\varepsilon).$$

For the asymptotic computation of  $\mathcal{F}_N(f, Q_\varepsilon)$  we use the average isotropy property of any regular mesh (see [GKM18, Lemma 5.4]) to obtain

$$\begin{aligned} |\mathcal{F}_N(f, Q_\varepsilon) - \varepsilon^d |\xi|^2| &= \left| \left( \frac{1}{2} \sum_{\substack{K, L \in \mathcal{T}_N \\ \bar{K}, \bar{L} \cap Q_\varepsilon \neq \emptyset}} d_{KL} |\Gamma_{KL}| \langle \xi, \tau_{KL} \rangle^2 \right) - |\xi|^2 |Q_\varepsilon| \right| \\ &\leq |B(\partial Q_\varepsilon, 5[\mathcal{T}_N])| \rightarrow 0 \text{ as } N \rightarrow \infty. \end{aligned}$$

Note that we get  $|B(\partial Q_\varepsilon, 5[\mathcal{T}_N])|$  instead of  $|B(\partial Q_\varepsilon, 4[\mathcal{T}_N])|$  as in [GKM18, Lemma 5.4] because we take into account all the cells whose closure intersects the cube  $Q_\varepsilon$  and not only the ones contained in it. Together with Lemma 9.8, we obtain for all  $\xi \in \mathbb{R}^d$  and  $\varepsilon > 0$ ,

$$\mathbf{M}(\phi_{u,z}^\xi, Q_\varepsilon) = \lim_{N \rightarrow \infty} \mathcal{M}_N(f, Q_\varepsilon) = \lim_{N \rightarrow \infty} \mathcal{F}_N(f, Q_\varepsilon) = \varepsilon^d |\xi|^2. \quad (9.15)$$

Hence,

$$f_\rho(z, u, \xi) = \limsup_{\varepsilon \rightarrow 0^+} \frac{\mathbf{M}(\phi_{u,z}^\xi, Q_\varepsilon)}{\varepsilon^d} = |\xi|^2,$$

which concludes the proof in the special case  $\sigma, \rho \equiv 1, m_N = \pi_N$ .

*Step 2.* Let us now consider the general case when  $\sigma \in C_b(\Omega)$  and  $m_N, \rho$  satisfy (lb), (ub) and (pc). We write  $\bar{\mathcal{F}}_N, \bar{\mathcal{M}}_N$  for the respective analogues of  $\mathcal{F}_N, \mathcal{M}_N$  from the special case  $\sigma, \rho \equiv 1$  and  $m_N = \pi_N$ , which we considered in Step 1.

Fix  $u \in \mathbb{R}, z \in \Omega, \xi \in \mathbb{R}^d$  and let  $Q_\varepsilon, \phi_{u,z}^\xi, f$  be as above.

For all  $g : \mathcal{T}_N \rightarrow \mathbb{R}$  we have by construction,

$$\left( \inf_{Q_{2\varepsilon}} \rho_N \sigma \right) \bar{\mathcal{F}}_N(g, Q_\varepsilon) \leq \mathcal{F}_N(g, Q_\varepsilon) \leq \left( \sup_{Q_{2\varepsilon}} \rho_N \sigma \right) \bar{\mathcal{F}}_N(g, Q_\varepsilon).$$

Hence, in particular,

$$\left( \inf_{Q_{2\varepsilon}} \rho_N \sigma \right) \bar{\mathcal{M}}_N(f, Q_\varepsilon) \leq \mathcal{M}_N(f, Q_\varepsilon) \leq \left( \sup_{Q_{2\varepsilon}} \rho_N \sigma \right) \bar{\mathcal{M}}_N(f, Q_\varepsilon).$$

As a consequence of the first part of the proof and (9.15), passing to the limit as  $N \rightarrow \infty$  and applying (9.12), we deduce

$$\begin{aligned} \left( \limsup_{N \rightarrow \infty} \inf_{Q_{2\varepsilon}} \rho_N \right) \left( \inf_{Q_{2\varepsilon}} \sigma \right) |\xi|^2 \varepsilon^d &\leq \mathbf{M}(\phi_{u,z}^\xi, Q_\varepsilon) \\ &\leq \left( \liminf_{N \rightarrow \infty} \sup_{Q_{2\varepsilon}} \rho_N \right) \left( \sup_{Q_{2\varepsilon}} \sigma \right) |\xi|^2 \varepsilon^d. \end{aligned}$$

Passing to the limsup as  $\varepsilon \rightarrow 0$ , we deduce from (9.11), both the continuity of  $\sigma$  and the (pc) condition

$$f_\rho(z, u, \xi) = \limsup_{\varepsilon \rightarrow 0} \frac{\mathbf{M}(\phi_{u,z}^\xi, Q_\varepsilon)}{\varepsilon^d} = |\xi|^2 \rho(z) \sigma(z) \quad \text{for a.e. } z \in \Omega,$$

which concludes the proof.  $\square$

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# PARABOLIC HARNACK INEQUALITIES FOR LINEAR DIFFUSIONS WITH AN APPLICATION TO MARKOV CHAINS ON LOCALLY FINITE GRAPHS

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## 1. INTRODUCTION

This short note is devoted to the analysis of quadratic diffusion processes on metric measure spaces, with particular attention to the case of locally finite graphs. The main result shows that under a two-sided bounded horizon condition on the associated jump process, a Poincaré inequality and a volume growth condition, one can prove a parabolic Harnack inequality for the correspondent diffusion process. The importance of such an inequality is well-established in the literature and its origins go back to Carl Gustav Axel von Harnack in the 19th century, in the context of harmonic functions in Euclidean domains. One particularly significant application of Harnack inequalities is the Hölder continuity of the correspondent solution – a parabolic version of the Harnack inequality even implies Hölder regularity of the associated flow. We refer the reader to [Kas07] for a general introduction to the topic.

Given their fundamental impact, Harnack inequalities have been widely studied. Let us recall the works of Grigor'yan [Gri09] and Saloff-Coste [SC02] for Laplace-Beltrami operators on Riemannian manifolds, where equivalent characterizations for parabolic Harnack inequalities have been investigated. In particular, they showed that a parabolic Harnack inequality is equivalent to a Poincaré inequality together with a doubling condition for the volume measure; thus, highlighting a deep connection between properties of solutions to the heat flow on a manifold and more geometric and analytic aspects of the space itself. Similar results have been extended to the case of symmetric diffusions on metric measure spaces by Sturm [Stu96] and to random walks on graphs by Delmotte [Del99]. All these results concern a classical linear diffusion regime. Other regimes have been considered in [BBK09].

More recently, a more unifying picture for different diffusions on general metric measure spaces has been proposed in a series of works by Chen, Kumagai and Wand [CKW17],[CKW18],[CKW19a], [CKW19b], where the authors proposed several equivalent conditions for parabolic Harnack inequalities, amongst them elliptic Harnack inequalities, elliptic and parabolic Hölder regularity as well as upper and lower bounds on the heat kernel.

Albeit the existence of such an involved history of works, the particular case of linear diffusions on locally finite graphs appeared, to our knowledge, slightly incomplete. In particular, the main reference work in this setting, given by [Del99], deals with parabolic Harnack inequalities for diffusions where the reference measure  $\mu$  and the jump kernel  $j$  are related by the condition

$$\mu(x) = \sum_y j(x, y). \tag{1}$$

In [BBK09], the authors discuss similar problems with more flexibility, thus, not assuming the previous condition; even though they assume two-sided bounds on  $\mu$  and  $j$ , which is a stricter condition not assumed in [Del99]. In [BBK09, Theorem 1.5] the authors describe the connections between upper bounds on the jump kernel, the doubling conditions and the Poincaré inequalities with parabolic Harnack inequalities. Nonetheless, those results only apply to certain nonlinear diffusion regimes. Indeed, the reason why the linear case is left out, is the presence of long-range interactions, with consequent issues of integrability in a linear regime.

The same authors in [CKW17, Remark 1.7] discuss the possible application of their general equivalence result to different diffusion regimes but they exclude the linear case.

Another generalization of the results in [Del99] is also pursued in [ADS16]. In this work elliptic and parabolic Harnack inequalities are established for locally finite graphs satisfying volume regularity as well as a relative isoperimetric inequality which is, for instance, satisfied on the Euclidean lattice. Despite working under the assumption (1), the approach of the authors allows for more general reference measures (cf. [ADS16, Remark 1.5]).

The goal of this short work is to fill this gap and prove, in the same spirit of [CKW17, Remark 1.7], a parabolic Harnack inequality (and a Hölder regularity result as a consequence) in the linear case for bounded-horizon jump processes, where integrability issues as appearing in a long-range regime do not pose a problem.

Finally, we discuss an application of this result to a finite volume framework and prove a Hölder regularity result for approximating solutions to a Fokker-Planck equation in  $\mathbb{R}^d$ . This turns out to be the key point in [FMP20], in order to obtain evolutionary  $\Gamma$ -convergence of discrete gradient structures for the Fokker-Planck equation in  $\mathbb{R}^d$  with respect to the discrete optimal transport metric, introduced independently by Maas in [Maa11] and Mielke in [Mie11].

## 2. PARABOLIC HARNACK INEQUALITIES FOR LINEAR DIFFUSIONS ON METRIC MEASURE SPACES

Let  $(X, d, \mu)$  be a metric measure space. Throughout these notes we assume that  $(X, d)$  is a locally compact Polish space and  $\mu$  is a positive Radon measure on  $X$  with full support. In this section we present a result showing a Harnack inequality for linear diffusions on a metric measure space, where the associated jump process has a bounded horizon (both from below and above, see (9)).

We start with some definitions.

**Definition 2.1.**  *$(X, d, \mu)$  is said to satisfy (VG) (volume growth condition) with parameter  $\alpha > 0$  if*

$$C_V^{-1}r^\alpha \leq \mu(B(x, r)) \leq C_V r^\alpha, \quad \forall x \in X, r \geq 0.$$

We are interested in a regular Dirichlet form  $\mathcal{E}$  with dense domain  $\mathcal{F}$  in  $L^2(X, \mu)$ , with only pure-jump part as follows: For a symmetric Radon measure  $J$  on  $X \times X \setminus \text{diag}$  (here  $\text{diag}$  denotes the diagonal set  $\{(x, x) : x \in X\}$ ), we consider

$$\mathcal{E}(f, g) := \int_{X \times X \setminus \text{diag}} (f(x) - f(y))(g(x) - g(y)) \, dJ(x, y) \quad \forall f, g \in \mathcal{F}. \quad (2)$$

Associated to  $\mathcal{E}$ , one can consider the corresponding *carré du champ*  $\mathbf{\Gamma}$ , given for each pair of functions  $f, g \in \mathcal{F}$ , by the measure

$$\mathbf{\Gamma}(f, g)(A) := \int_{A \times X \setminus \text{diag}} (f(x) - f(y))(g(x) - g(y)) \, dJ(x, y) \quad (3)$$

for all Borel sets  $A \subseteq X$ . By definition, we have  $\mathcal{E}(f, g) = \mathbf{\Gamma}(f, g)(X)$ .

We want to describe some of the properties of the semigroup generated by  $\mathcal{E}$ , in particular, the validity of Harnack type inequalities and the Hölder regularity of the solutions, in the specific case of a classical linear diffusion regime. Let  $\phi : \mathbb{R}^+ \rightarrow \mathbb{R}^+$  be a strictly increasing continuous function with  $\phi(0) = 0$  and  $\phi(1) = 1$ , satisfying

$$c_1 \left(\frac{R}{r}\right)^{\beta_1} \leq \frac{\phi(R)}{\phi(r)} \leq c_2 \left(\frac{R}{r}\right)^{\beta_2} \quad \forall 0 < r \leq R \quad (4)$$

for certain constants  $c_1, c_2 > 0$  and  $\beta_2 \geq \beta_1 > 0$ .

We make use of several abbreviations throughout the article, consistent with respect to the works [CKW17],[CKW18],[CKW19a], [CKW19b] of Chen, Kumagai and Wang.

**Definition 2.2.** We say  $J_{\phi, \leq}$  (upper bound on the jump kernel) is satisfied if  $J$  is absolutely continuous with respect to  $\mu \times \mu$  with density  $j$ , satisfying

$$j(x, y) \leq \frac{c}{V(x, d(x, y))\phi(d(x, y))} \quad \mu \times \mu\text{-a.e. } x, y \in X \quad (5)$$

for a constant  $c > 0$ , where  $V(x, r)$  denotes the  $\mu$ -volume of the closed ball centred in  $x$  of radius  $r$ .

One of the key properties that is often used to obtain regularity estimates for the solution of the correspondent heat flow, as introduced in [CKW17], reads as follows.

**Definition 2.3.** For Borel sets  $A, B \subseteq X$  such that  $\bar{A} \subset B$ , we say that  $\varphi$  is a cut-off function for  $A \subset B$  if  $0 \leq \varphi \leq 1$  on  $X$  such that  $\varphi = 1$  on  $A$  and  $\varphi = 0$  on  $B^c$ .

**Definition 2.4.** We say that CSJ( $\phi$ ) (cut-off Sobolev inequality for the jump kernel) is satisfied if there exist  $C_0 \in (0, 1]$  and  $C_1, C_2 > 0$  such that for every  $0 < r \leq R$ , almost every  $x_0 \in X$  and any  $f \in \mathcal{F}$ , there exists a cut-off function  $\varphi \in \mathcal{F}_b := \mathcal{F} \cap L^\infty(X, \mu)$  for  $B(x_0, R) \subset B(x_0, R + r)$ , satisfying

$$\int_{B_{x_0}(R+(1+C_0)r)} f^2 \, d\mathbf{\Gamma}(\varphi, \varphi) \leq C_1 \int_{U \times U^*} (f(x) - f(y))^2 \, dJ(x, y) \quad (6)$$

$$+ \frac{C_2}{\phi(r)} \int_{B_{x_0}(R+(1+C_0)r)} f^2 \, d\mu, \quad (7)$$

where  $U = B(x_0, R + r) \setminus B(x_0, R)$  and  $U^* = B(x_0, R + (1 + C_0)r) \setminus B(x_0, R - C_0r)$ .

A substantially stronger version of the condition above is the following upper bound on the carré du champ of  $\mathcal{E}$ .

**Definition 2.5.** We say that  $U\mathbf{\Gamma}(\phi)$  (upper bound on the carré du champ) holds if for every  $0 < r \leq R$  and every  $x_0 \in X$ , there exist  $C_2 > 0$  and a cut-off function  $\varphi \in \mathcal{F}_b$  for  $B(x_0, R) \subset B(x_0, r + R)$  such that

$$\frac{d\mathbf{\Gamma}(\varphi, \varphi)}{d\mu}(x) \leq \frac{C_2}{\phi(r)} \quad \mu\text{-a.e. } x \in X. \quad (8)$$

Note that  $\mathbf{U}\Gamma(\phi)$  implies  $\text{CSJ}(\phi)$  for any  $C_0$  and  $C_1 = 0$  (even stronger, the choice of  $\varphi$  is uniform in  $f \in \mathcal{F}$ ).

In the following result we describe a particular setting where the  $\mathbf{U}\Gamma(\phi)$  condition is indeed satisfied. For a general picture of the relations between various conditions, amongst them the ones introduced above, we refer to the works [CKW17], [CKW18].

**Theorem 2.6** ( $\mathbf{U}\Gamma(\phi)$  for linear diffusion with two-sided bounded horizon). *Assume  $\phi(r) = r^2$  and suppose there exist  $\alpha_*, \alpha^* \in R^+$  such that*

$$j(x, y) = 0 \quad \text{whenever} \quad d(x, y) \leq \alpha_* \quad \text{or} \quad d(x, y) \geq \alpha^*. \quad (9)$$

*Then (VG) and  $J_{\phi, \leq}$  imply  $\mathbf{U}\Gamma(\phi)$  with a constant  $C_2$  in (8) only depending on the constants in (VG),  $J_{\phi, \leq}$ ,  $\alpha^*$  and  $\alpha_*$ .*

*Remark 2.7.* A simple example of a metric measure space that satisfies (9) is given by an unweighted directed graph where a jump occurs, i.e.  $j(x, y) > 0$ , if and only if  $(x, y)$  is an edge. More generally, a graph setting with a more involved jump function  $j$  has been extensively studied in [CKW17], [CKW18]. Nonetheless, in those works only the case  $\phi(r) = r^\beta$  with  $\beta < 2$  has been investigated. In that case, no bounded horizon condition like (9) is needed.

In [Del99], [BBK09] the case  $\beta = 2$  is considered. Nevertheless, in the first work the extra assumption (1) between  $\mu$  and  $j$  is present, whereas in the second one, no result concerning the direct connection between  $J_{\phi, \leq}$  and  $\text{PHI}(\phi)$  is present for such a regime.

*Proof of Theorem 2.6.* The proof follows along the lines of [BBK09] and [CKW17, Remark 1.7]. For given  $0 < r \leq R$  and  $x_0 \in X$ , define  $\varphi(x) := h(d(x, x_0))$  for a function  $h \in C^1(\mathbb{R}_0^+; [0, 1])$  satisfying

$$h(s) = \begin{cases} 1 & s \leq R \\ 0 & s \geq r + R \end{cases} \quad \text{and} \quad |h'(s)| \leq \frac{2}{r} \quad \forall s \geq 0.$$

Then, by construction, we have

$$\begin{aligned} \frac{d\Gamma(\varphi, \varphi)}{d\mu}(x) &= \int (\varphi(x) - \varphi(y))^2 j(x, y) d\mu(y) \\ &\leq \int_{\{d(x, y) \geq r\}} j(x, y) d\mu(y) + \frac{4}{r^2} \int_{\{d(x, y) \leq r\}} d(x, y)^2 j(x, y) d\mu(y). \end{aligned} \quad (10)$$

*Step 1.* We show that for any given  $r > 0$ , there exists  $C_2 \in R^+$ , only depending on the constants in (VG),  $J_{\phi, \leq}$ , and (9), such that

$$\int_{\{d(x, y) \geq r\}} j(x, y) d\mu(y) \leq \frac{C_2}{\phi(r)}. \quad (11)$$

Indeed, as a consequence of  $J_{\phi, \leq}$ , (4) and (VG), one gets

$$\begin{aligned}
 \int_{\{d(x,y) \geq r\}} j(x,y) \, d\mu(y) &\leq c \int_{\{d(x,y) \geq r\}} \frac{1}{V(x, d(x,y))\phi(d(x,y))} \, d\mu(y) \\
 &= c \sum_{i=0}^{\infty} \int_{\{2^i r \leq d(x,y) < 2^{i+1} r\}} \frac{1}{V(x, d(x,y))\phi(d(x,y))} \, d\mu(y) \\
 &\leq c \sum_{i=0}^{\infty} \frac{1}{V(x, 2^i r)\phi(2^i r)} V(x, 2^{i+1} r) \\
 &\leq \frac{C_2}{\phi(r)} \sum_{i=0}^{\infty} 2^{-i\beta_2} \leq \frac{C_2}{\phi(r)}
 \end{aligned}$$

for some constant  $C_2$ , which shows (11).

*Step 2.* We show that for every  $r > 0$ , there exists  $C_2 \in R^+$ , only depending on the constants in (VG),  $J_{\phi, \leq}$  and (9), such that

$$\int_{\{d(x,y) \leq r\}} d(x,y)^2 j(x,y) \, d\mu(y) \leq C_2. \quad (12)$$

Indeed, if  $r \leq \alpha_*$ , then the left-hand side of (12) simply vanishes. Hence, we may assume without restriction that  $r \geq \alpha_*$ . As a consequence of  $J_{\phi, \leq}$  and (VG), together with  $\phi(r) = r^2$  and (9), we may deduce in a similar spirit as above

$$\begin{aligned}
 \int_{\{d(x,y) \leq r\}} d^2(x,y) j(x,y) \, d\mu(y) &\leq \int_{\{d(x,y) \leq r\}} d^2(x,y) j(x,y) \, d\mu(y) \\
 &= \sum_{i=0}^{\infty} \int_{\{2^{-i-1} r < d(x,y) \leq 2^{-i} r\}} d^2(x,y) j(x,y) \, d\mu(y) \\
 &= \sum_{i=i_*(r)}^{i^*(r)} \int_{\{2^{-i-1} r < d(x,y) \leq 2^{-i} r\}} d^2(x,y) j(x,y) \, d\mu(y) \\
 &\leq c \sum_{i=i_*(r)}^{i^*(r)} \int_{\{2^{-i-1} r < d(x,y) \leq 2^{-i} r\}} \frac{1}{V(x, d(x,y))} \, d\mu(y) \\
 &\leq c \sum_{i=i_*(r) \vee 0}^{i^*(r)} \frac{1}{V(x, 2^{-i-1} r)} V(x, 2^{-i} r) \\
 &\leq C_2(i^*(r) - i_*(r)),
 \end{aligned}$$

where to pass from the second to the third line we used (9) for functions  $i_*(r)$  and  $i^*(r)$  given by

$$i_*(r) := \left\lceil \log_2 \left( \frac{r}{\alpha_*} \right) \right\rceil \quad \text{and} \quad i^*(r) := \left\lfloor \log_2 \left( \frac{r}{\alpha_*} \right) \right\rfloor \geq 0,$$

respectively.

We end the proof of (12) by noticing that in fact  $i^*(r) - i_*(r) \leq \log_2 \left( \frac{\alpha_*}{\alpha_*} \right) + 1$  for any  $r > 0$ . Finally plugging (11) and (12) into (10), we obtain  $\mathbf{U}\Gamma(\phi)$ .  $\square$

*Remark 2.8.* Note that (11) neither relies on  $\phi$  being quadratic nor on (9). However, those two conditions are of fundamental importance in order to get (12).

*Remark 2.9.* The  $\mathbf{UF}(\phi)$  condition is crucial for the choice of  $\phi$ . Indeed, in a classical diffusion setting, say on a Riemannian manifold  $(M, g)$ , the quadratic choice is natural for the specific choice of  $\varphi$  as in the proof of Theorem 2.6.

The  $\mathbf{UF}(\phi)$  condition is known to be related to a parabolic Harnack inequality and Hölder regularity of the solution of the correspondent flow, as proved in [CKW17, Theorem 1.20].

**Definition 2.10** (Harnack Inequality). *Let  $(X, d, \mu)$  be a metric measure space,  $\mathcal{E}$  a pure-jump regular Dirichlet form with dense domain  $\mathcal{F}$  in  $L^2(X, \mu)$  as defined in (2), with a jump kernel given by a Radon measure  $J$  on  $X \times X \setminus \text{diag}$ , absolutely continuous with respect to  $\mu \times \mu$  with symmetric density  $j(x, y) = j(y, x)$ . Let  $\mathcal{L}$  be the associated generator, given by*

$$\mathcal{L}f(x) := \int_X j(x, y)(f(y) - f(x)) \, d\mu(y) \quad f \in \mathcal{F}. \quad (13)$$

We say that  $(X, d, \mu, J)$  satisfies a continuous-time parabolic Harnack inequality (in short  $\mathbf{PHI}(\phi)$ ) if there exist parameters  $\eta \in (0, 1)$ ,  $0 < \theta_1 < \theta_2 < \theta_3 < \theta_4$  and a constant  $c_H > 0$  such that for all  $x_0 \in X$ ,  $s \in \mathbb{R}$ ,  $r > 0$  and every non-negative solution of

$$\partial_t u = \mathcal{L}u, \quad \text{on } Q = [s, s + \theta_4\phi(r)] \times B(x_0, r),$$

one has

$$\sup_{Q_-} u \leq c_H \inf_{Q_+} u \quad (\mathbf{PHI}(\phi))$$

where  $Q_-$  and  $Q_+$  are defined by

$$Q_- := [s + \theta_1\phi(r), s + \theta_2\phi(r)] \times B(x_0, \eta r)$$

and

$$Q_+ := [s + \theta_3\phi(r), s + \theta_4\phi(r)] \times B(x_0, \eta r),$$

respectively.

*Remark 2.11.* Fix  $\eta' \in (0, 1)$  and  $0 < \theta'_1 < \theta'_2 < \theta'_3 < \theta'_4$  as above. One can show that a Harnack inequality with respect to  $(\eta, \theta_1, \theta_2, \theta_3, \theta_4, c_H)$  implies the existence of a constant  $c'_H > 1$ , only dependent on the aforementioned constants, such that a Harnack inequality with respect to  $(\eta', \theta'_1, \theta'_2, \theta'_3, \theta'_4, c'_H)$  holds as well; see [Del99, Definition 1.6].

There are two more ingredients required to obtain a parabolic Harnack inequality: a regularity property on the jump kernel and a (weak) Poincaré inequality.

**Definition 2.12.** *We say that (UJS) (upper bound for jump kernel smoothness) holds if  $J$  is absolutely continuous with respect to  $\mu \times \mu$  with symmetric density  $j(x, y) = j(y, x)$  and there exists a constant  $c > 0$  such that for  $\mu$ -a.e.  $x_0 \neq y$  in  $X$ , we have*

$$j(x_0, y) \leq \frac{c}{V(x_0, r)} \int_{B(x_0, r)} j(x, y) \, d\mu(x) \quad \forall r \leq \frac{d(x_0, y)}{2}.$$

**Definition 2.13.** We say that a weak-Poincaré inequality (in short  $\text{PI}(\phi)$ ) holds, whenever there exist  $C_P > 0$  and  $c \geq 1$  such that for every  $x_0 \in X$  and  $r > 0$ , the inequality

$$\int_{B(x_0, r)} |f(x)|^2 d\mu(x) \leq C_P \phi(r) \int_{B(x_0, cr) \times B(x_0, cr)} |f(x) - f(y)|^2 dJ(x, y) \quad (14)$$

holds for any given function  $f : B(x_0, r) \rightarrow \mathbb{R}$  satisfying  $\int_{B(x_0, r)} f(x) d\mu(x) = 0$ .

We are finally ready to state the main consequence of Theorem 2.6.

**Corollary 2.14.** Let  $(X, d, \mu)$  be a metric measure space that satisfies (VG) and let  $\mathcal{E}$  be a regular Dirichlet form with dense domain  $\mathcal{F}$  in  $L^2(X, \mu)$  as defined in (2). Set  $\phi(r) = r^2$  and suppose that

- (i)  $J_{\phi, \leq}$ , (UJS) and  $\text{PI}(\phi)$  are satisfied,
- (ii) the density  $j$  satisfies the bounded horizon assumption (9).

Then a parabolic Harnack inequality  $\text{PHI}(\phi)$  holds true. Moreover, one has Hölder regularity for the associated heat flow, i.e. there exist  $\lambda, \eta \in (0, 1)$ , and  $C_H > 0$  depending only on the constants in (VG),  $J_{\phi, \leq}$ , (UJS),  $\text{PI}(\phi)$ , and (9) such that for all  $x_0 \in X$ ,  $s \in \mathbb{R}$ ,  $R > 0$  and every continuous solution<sup>1</sup> of  $\partial_t v_t = \mathcal{L}v_t$  on  $Q = [s - R^2, s] \times B(x_0, R)$ , it holds

$$|v_t(x) - v_t(y)| \leq C_H \left( \frac{d(x, y)}{R} \right)^\lambda \sup_Q |v| \quad \forall (t, x), (t, y) \in Q^+,$$

where  $Q^+ = [s - \eta R^2, s] \times B(x_0, \eta R)$ .

*Proof.* Apply Theorem 2.6 and [CKW18, Theorem 1.20].  $\square$

#### APPLICATION TO MARKOV CHAINS ON INFINITE GRAPHS

A particular setting where the results of the previous section apply, is given by a locally finite graph  $\Gamma = (V, E)$  where  $V$  denotes the set of vertices and  $E$  the set of edges.

Write  $x \sim y$ , whenever  $x$  and  $y$  are neighbouring vertices in  $\Gamma$ . Let  $d_{\text{gra}}$  be the graph distance induced by  $\Gamma$  and let  $B_{\text{gra}}(x, r)$  be the corresponding closed ball centered in  $x$  of radius  $r > 0$ . Denote the corresponding volume with respect to  $\mu$  by  $V(x, r) := \mu(B_{\text{gra}}(x, r))$ .

For notational simplicity, we use subscripts in form of  $\mu_x$  and  $J_{xy}$  to denote the respective expressions  $\mu(x)$  and  $J(\{(x, y)\})$  in this section.

**Proposition 2.15** (Quadratic Harnack inequality on infinite graphs). *Let  $\Gamma = (V, E)$  be a locally finite (unweighted) graph. Let  $\mu \in \mathcal{M}(V)$  be a bounded measure on  $V$ , together with a measure  $J$  on  $V \times V$  such that  $J_{xy} = J_{yx}$  for all  $x, y \in V$  and  $J_{xy} > 0$ , precisely, when  $x \sim y$ . Assume that*

$$J_{xy} \leq C_J \mu_x \mu_y \quad \forall x, y \in V \quad (15)$$

for some constant  $C_J > 0$ . Consider the corresponding generator  $\mathcal{L}_{\mathcal{T}}$ , given by

$$\mathcal{L}_{\mathcal{T}} f(x) := \frac{1}{\mu_x} \sum_{y \sim x} J_{xy} (f(y) - f(x)). \quad (16)$$

Suppose the following geometric assumptions hold:

<sup>1</sup>For general bounded measurable solutions see [CKW18, Definition 1.15].

(i) Volume growth: *There exists a constant  $C_V > 0$  such that*

$$C_V^{-1}r^d \leq V(x, r) \leq C_V r^d \quad \forall x \in V, r > 0.$$

(ii) Weak Poincaré inequality: *There exist  $C_P > 0$  and  $c \geq 1$  such that for all  $x_0 \in \Gamma$  and  $r > 0$ , the inequality*

$$\sum_{x \in B_{\text{gra}}(x_0, r)} \mu_x |f(x)|^2 \leq C_P r^2 \sum_{x, y \in B_{\text{gra}}(x_0, cr)} J_{xy} |f(x) - f(y)|^2 \quad (17)$$

*holds for any function  $f : B_{\text{gra}}(x_0, r) \rightarrow \mathbb{R}$  satisfying  $\sum_{x \in B_{\text{gra}}(x_0, r)} \mu_x f(x) = 0$ .*

(iii) 2-sided bounded horizon: *There exist  $\alpha_*, \alpha^* > 0$  such that the density  $j(x, y) := J_{xy}$  satisfies (9).*

*Then  $(\Gamma, d_{\text{gra}}, \mu, J)$  satisfies a parabolic Harnack inequality  $\text{PHI}(\phi)$  for  $\phi(r) = r^2$  with a constant  $c_H$  only depending on  $C_J, C_V$  and  $C_P$ .*

*Remark 2.16.* Note that, under the additional assumption of a bounded, nowhere vanishing measure  $\mu$  on  $V$  and the 2-sided bounded horizon condition (9), the setting of [Del99] fits into the framework presented above with a constant in (15) given by  $C_J^{-1} = \inf_x \{\mu_x\}$ .

*Proof of Proposition 2.15.* We apply Theorem 2.6 to  $(X, d, \mu) = (\Gamma, d_{\text{gra}}, \mu)$  and  $J$  as given in this section.  $\square$

### 3. THE FINITE VOLUME FRAMEWORK

The aim of this section is to apply Proposition 2.15 to a finite volume framework; see [EGH00], [FMP20] for a detailed description of the setup and related analysis.

Let  $\mathcal{T}$  be a  $\zeta$ -regular, finite partition (called mesh) of a domain with compact closure  $\bar{\Omega} \subset \mathbb{R}^d$  into sets (called cells) with nonempty and convex interior. Denote by  $\varepsilon := [\mathcal{T}] := \max\{\text{diam}(K) : K \in \mathcal{T}\}$  the size of the mesh.

Assume a probability measure  $\bar{\mathfrak{m}}$  on  $\bar{\Omega}$ , absolutely continuous with respect to the  $d$ -dimensional Lebesgue measure, with a density  $\sigma := Z_V e^{-V}$  for some potential  $V \in C(\bar{\Omega}) \cap C^1(\Omega)$  and a normalising constant  $Z_V > 0$ .

We assume that  $\mathcal{T}$  is admissible in the sense that each cell  $K \in \mathcal{T}$  contains a point  $x_K \in \bar{K}$  such that  $x_K - x_L$  is orthogonal to the common interface  $\Gamma_{KL} := \partial K \cap \partial L$  for any neighbouring cell  $L$  of  $K$ , denoted by  $L \sim K$ . Let  $d_{KL} := |x_K - x_L|$  be the Euclidean distance between reference points of any two cells  $K, L \in \mathcal{T}$ .

We endow  $\mathcal{T}$  with a graph structure with cells corresponding to vertices and pair of adjacent cells in  $\mathcal{T}$  corresponding to edges. As before, we denote by  $d_{\text{gra}}(K, L)$  the graph distance induced by the (unweighted) graph corresponding to  $\mathcal{T}$  (not to be confused with the Euclidean distance  $d_{KL}$ ). Denote by  $B_{\text{gra}}(K, r)$  a closed ball centred in  $K \in \mathcal{T}$  of radius  $r > 0$  with respect to the graph metric  $d_{\text{gra}}$ .

We consider a nearest-neighbour jump process, given by

$$J_{KL} := \begin{cases} \varepsilon^{-d} (\varepsilon^2 w_{KL}) & \text{if } K \sim L \\ 0 & \text{otherwise} \end{cases}, \quad (18)$$

where

$$w_{KL} := \frac{\mathcal{H}^{d-1}(\Gamma_{KL})}{d_{KL}} S_{KL} \quad \text{and} \quad S_{KL} := \theta(\sigma(x_K), \sigma(x_L))$$



for some mean  $\theta : \mathbb{R}_0^+ \times \mathbb{R}_0^+ \rightarrow \mathbb{R}_0^+$  satisfying  $\min\{a, b\} \leq \theta(a, b) \leq \max\{a, b\}$ . The corresponding reference measure  $\mu \in \mathcal{P}(\mathcal{T})$  is given by

$$\mu_K := \mu(\{K\}) := \varepsilon^{-d} \pi(K) \quad \text{with} \quad \pi(K) = \bar{\mathfrak{m}}(K). \quad (19)$$

Then  $(\mathcal{T}, d_{\text{gra}}, \pi)$  defines a metric measure space, where  $\pi$  and  $J$  induce a correspondent regular Dirichlet form  $\mathcal{E}$  on  $L^2(\mathcal{T}, \pi)$ , given by

$$\mathcal{E}_{\mathcal{T}}(f, g) = \sum_{K \sim L} J_{KL} (f(L) - f(K))(g(L) - g(K)). \quad (20)$$

Moreover, define

$$V(K, r) := \mu(B_{\text{gra}}(K, r)) \quad \forall K \in \mathcal{T}.$$

*Remark 3.1.* The graph metric  $d_{\text{gra}}$  satisfies a *volume doubling condition* which is inherited from a comparison of metrics in form of

$$\frac{[\mathcal{T}]}{C} d_{\text{gra}}(K, L) \leq d_{KL} \leq C[\mathcal{T}] d_{\text{gra}}(K, L) \quad \forall K, L \in \mathcal{T} \quad (21)$$

for some constant  $C > 0$  only depending on  $\Omega$  and  $\zeta$ . Indeed, the first inequality in (21) follows from [GKM18, Lemma 1.12], whereas the second inequality is due to the fact that  $\sum_i d_{L_{i-1}, L_i} \leq d_{\text{gra}}(K, L)$  for any path  $K = L_0, L_1, \dots, L_N = L$  along neighbouring cells  $L_{i-1} \sim L_i$ .

A direct consequence of (21) are the following volume comparison bounds

$$B_{\text{gra}}(K, r[\mathcal{T}]/C) \subseteq \bigcup B(K, r) \subseteq B_{\text{gra}}(x_K, r[\mathcal{T}]C) \quad \forall K \in \mathcal{T}, r > 0. \quad (22)$$

Consider the correspondent diffusion, given by

$$\partial_t v_t(K) = \frac{1}{\mu_K} \sum_{L \in \mathcal{T}} (v_t(L) - v_t(K)) J_{KL} \quad \forall K \in \mathcal{T}. \quad (23)$$

Our goal is to prove a Harnack-type inequality for solutions of (23). We remark that it is not possible to directly apply [Del99, Theorem 1.7] to deduce such a result, due to the fact that not all assumptions are satisfied, namely,

$$\mu_K \neq \sum_{L \sim K} J_{KL}.$$

Nonetheless, equality holds above up to a small correction term.

Given all considerations above, we aim to apply the results from the previous section to  $\mathcal{T}$  with measures  $J$   $\mu$  as defined in (18) and (19), respectively.

First we need to prove a weak Poincaré inequality relative to the finite volume partition.

**Proposition 3.2** (Weak discrete weighted Poincaré inequality). *There exist constants  $c_0, c_1 > 0$ , depending only on  $\Omega$  and  $\zeta$  such that all functions  $u : \mathcal{T} \rightarrow \mathbb{R}$  satisfy*

$$\begin{aligned} & \sum_{K, L \in B_{\text{gra}}(K_0, r)} |u(K) - u(L)|^2 \pi(K) \pi(L) \\ & \leq c_1 d(K_0, c_0 r)^2 \pi(B_{\text{gra}}(K_0, r)) \sum_{K, L \in B_{\text{gra}}(K_0, c_0 r)} w_{KL} |u(K) - u(L)|^2 \end{aligned} \quad (24)$$

for any  $K_0 \in \mathcal{T}$  and  $r > 0$ , where  $d(K_0, c_0 r) := \text{diam}(B_{\text{gra}}(K_0, c_0 r))$ .

In particular, whenever  $\sum_{K \in B_{\text{gra}}(K_0, r)} u(K)\pi(K) = 0$ , we have

$$\sum_{K \in B_{\text{gra}}(K_0, r)} |u(K)|^2 \pi(K) \leq c_1 d(K_0, c_0 r)^2 \sum_{K, L \in B_{\text{gra}}(K_0, c_0 r)} w_{KL} |u(K) - u(L)|^2.$$

The proof is based on arguments taken from [GKM18, Proposition 4.5] and [EGH00, Lemma 3.7], adapted to account for a weight function as well as metric balls  $B_{\text{gra}}$  which need not be convex.

*Proof.* Write  $\rho := \nu_{\mathcal{T}} u$  and  $B_r := \bigcup B_{\text{gra}}(K_0, r)$  for fixed  $K_0 \in \mathcal{T}$  and  $r > 0$ .

Given two cells  $K, L \in \mathcal{T}$ , we define a function  $\mathbf{1}_{KL} : \Omega \times \Omega \rightarrow \{0, 1\}$  as follows: For any two points  $x, y \in B_r$ , we set  $\mathbf{1}_{KL}(x, y) = 1$ , whenever  $K \sim L$  such that the common interface  $\Gamma_{KL}$  intersects the straight line segment from  $x$  to  $y$  and  $(y - x) \cdot (x_L - x_K) > 0$ . In all other cases, we set  $\mathbf{1}_{KL}(x, y) = 0$ .

Note that the volume comparison bounds in (22) imply that the straight line segment from  $x$  to  $y$  is included in a slightly larger ball  $B_{\text{gra}}(K_0, c_0 r)$  for some constant  $c_0 \geq 1$  depending only on  $\Omega$  and  $\zeta$ . Therefore, we may use a telescopic sum to infer the estimate

$$|\rho(x) - \rho(y)| \leq \sum_{K, L \in B_{\text{gra}}(K_0, c_0 r)} |u(L) - u(K)| \mathbf{1}_{KL}(x, y) \quad \text{a.e. } x, y \in B_r. \quad (25)$$

Introduce

$$\alpha_{KL}(z) := \frac{z}{|z|} \cdot \frac{x_L - x_K}{d_{KL}} \quad \forall K, L \in \mathcal{T}, z \in \mathbb{R}^d$$

and notice that  $\alpha_{KL}(y - x) > 0$  whenever  $\mathbf{1}_{KL}(x, y) = 1$ . Hence, we may use the Cauchy-Schwarz inequality to estimate (25) as

$$\begin{aligned} & |\rho(x) - \rho(y)|^2 \\ & \leq \left( \sum_{K, L} \frac{|u(L) - u(K)|^2 S_{KL}}{\alpha_{KL}(y - x) d_{KL}} \mathbf{1}_{KL}(x, y) \right) \left( \sum_{K, L} \alpha_{KL}(y - x) \frac{d_{KL}}{S_{KL}} \mathbf{1}_{KL}(x, y) \right). \end{aligned} \quad (26)$$

Notice that  $\alpha_{KL}(x, y)$  vanishes, unless  $K$  and  $L$  are neighbouring cells intersecting the line segment from  $x$  to  $y$ . In particular, we may index subsequent intersecting cells, say  $L_0, L_1, \dots, L_N$ , such that  $\alpha_{KL}(x, y) = 1$  for any  $K, L \in \mathcal{T}$ , precisely, when  $(K, L) = (L_{i-1}, L_i)$ . Thus, using that the regularity of the mesh implies the bound  $1/C_1 \leq S_{KL} \leq C_1$  for some constant  $C_1 > 0$ , we infer

$$\begin{aligned} & \sum_{K, L} \alpha_{KL}(y - x) \frac{d_{KL}}{S_{KL}} \mathbf{1}_{KL}(x, y) \leq C_1 \sum_{i=1}^N \alpha_{L_{i-1}K_i}(y - x) d_{L_{i-1}L_i} \\ & \leq C_1 \sum_{i=1}^N \frac{y - x}{|y - x|} \cdot (x_{L_i} - x_{L_{i-1}}) = C_1 \frac{y - x}{|y - x|} \cdot (x_{L_N} - x_{L_0}) \leq C_1 d(K_0, c_0 r). \end{aligned} \quad (27)$$

Using that the density of  $\bar{\mathbf{m}}$  is bounded from above, we invoke a change of variables in form of  $z = y - x$  to estimate

$$\begin{aligned} & \int_{B_{c_0r}} \int_{B_{c_0r}} \frac{1}{\alpha_{KL}(y-x)} \mathbf{1}_{KL}(x, y) \, d\bar{\mathbf{m}}(x) \, d\bar{\mathbf{m}}(y) \\ & \leq C_1 \int_{\{-x\}+B_{c_0r}} \frac{1}{\alpha_{KL}(z)} \int_{B_{c_0r}} \mathbf{1}_{KL}(x, x+z) \, dx \, d\bar{\mathbf{m}}(z) \\ & \leq C_1 \int_{\{-x\}+B_{c_0r}} \mathcal{H}^{d-1}(\Gamma_{KL}) \cdot |z| \, d\bar{\mathbf{m}}(z) \leq C_2 d(K_0, c_0r) \bar{\mathbf{m}}(B_{c_0r}) \mathcal{H}^{d-1}(\Gamma_{KL}), \end{aligned} \quad (28)$$

for some constant  $C_2 > 0$ , where we used the volume formula

$$\int_{\mathbb{R}^d} \mathbf{1}_{KL}(x, x+z) \, dx = z \cdot (x_L - x_K) \frac{\mathcal{H}^{d-1}(\Gamma_{KL})}{d_{KL}},$$

to pass from the second to the last line.

Collecting both estimates (27) and (28) above, we may further estimate (26) as

$$\begin{aligned} & \int_{B_{c_0r}} \int_{B_{c_0r}} |\rho(x) - \rho(y)|^2 \, d\bar{\mathbf{m}}(x) \, d\bar{\mathbf{m}}(y) \\ & \leq C_3 d(K_0, c_0r)^2 \bar{\mathbf{m}}(B_{c_0r}) \sum_{\substack{K, L \in B_{\text{gra}}(K_0, c_0r): \\ \bar{K} \sim L}} |u(L) - u(K)|^2 w_{KL} \end{aligned} \quad (29)$$

for a constant  $C_3 > 0$ .

Using the Euclidean doubling volume property in tandem with (22), as well as the bounds on the density of  $\bar{\mathbf{m}}$ , we also have  $\bar{\mathbf{m}}(B_{c_0r}) \leq C_4 \bar{\mathbf{m}}(B_r)$  for some  $C_4 \geq 1$ . Consequently, (29) allows us to establish (24).

Finally, the second claim follows by an application of Jensen's inequality to the left-hand side of (24).  $\square$

*Remark 3.3 (Ultracontractivity).* Consider the generator  $\mathcal{L}_{\mathcal{T}}$  as defined in (16) with measures  $J$  and  $\mu$  given by (19) and (18), respectively. A consequence of the Poincaré inequality proved in Proposition 3.2 is the  $L^1 \rightarrow L^\infty$  ultracontractivity property of the flow associated to  $\mathcal{L}_{\mathcal{T}}$  viz

$$|v_t|_{L^\infty(\mathcal{T}, \mu)} \leq C t^{-\frac{d}{2}} |v_t|_{L^1(\mathcal{T}, \mu)}. \quad (30)$$

Indeed it is well-known (see e.g. [SC92]) that a Poincaré inequality as in (24) implies the Nash inequality

$$\|f\|_2^{2+\frac{4}{d}} \leq C \mathcal{E}_{\mathcal{T}}(f, f) \|f\|_2^{\frac{4}{d}},$$

which, in particular, yields the ultracontractivity property (30); see [CKS87, Theorem 2.1] for a proof.

Note that the scaling property of (30) implies

$$|u_t|_{L^\infty(\mathcal{T}, \pi)} \leq C t^{-\frac{d}{2}} |u_t|_{L^1(\mathcal{T}, \pi)},$$

where  $u_t$  is the flow associated with the rescaled generator  $\Delta_{\mathcal{T}} := \varepsilon^{-2} \mathcal{L}_{\mathcal{T}}$ .

Now we are ready to prove the main result of this section.

**Proposition 3.4.** *Let  $\mathcal{T}$  be an admissible and  $\zeta$ -regular mesh of  $\Omega \subset \mathbb{R}^d$ . Then  $(\mathcal{T}, d_{\text{gra}}, \mu, J)$  with  $\mu$  and  $J$  defined as in (19) and (18), respectively, satisfies a continuous-time parabolic Harnack inequality with a constant  $c_H$  depending only on  $\Omega$ ,  $\bar{\mathbf{m}}$  and  $\zeta$ .*

*Proof.* We show that  $(\mathcal{T}, d_{\text{gra}}, \mu, J)$  satisfies the assumptions of Proposition 2.15.

First of all, note that (15) is a straightforward consequence of the  $\zeta$ -regularity of the mesh. Thus, we have to check the three remaining geometric assumptions:

- (i) *Volume growth condition.* The volume comparison bounds in (22) immediately imply this condition.
- (ii) *Poincaré inequality.* For every choice of  $K_0 \in \mathcal{T}$  and  $r > 0$ , we apply Proposition 3.2 to the sub-problem

$$\Omega_r := \bigcup B_{\text{gra}}(K_0, r) \quad \text{and} \quad \mathcal{T}_r := B_{\text{gra}}(K_0, r),$$

in order to obtain

$$\sum_{K \in \mathcal{T}_r} |f(K)|^2 \pi(K) \leq C_P \text{diam}(\Omega_{c_0 r})^2 \sum_{K, L \in \mathcal{T}_{c_0 r}} w_{KL} |f(K) - f(L)|^2.$$

Recall that by  $\zeta$ -regularity of the mesh, we know that (22) holds. In particular, there exists a constant  $C_1 > 0$  such that  $\text{diam}(\Omega_{c_0 r}) \leq C_1 \varepsilon r$ , which shows that a weak local Poincaré inequality as in (17) holds.

- (iii) *2-sided bounded horizon.* This condition is a direct consequence of  $J$  being a nearest-neighbour jump process.

□

As a corollary, we infer from the continuous-time parabolic Harnack inequality above the Hölder regularity of solutions to the flow equation

$$\partial_t v_t = \mathcal{L}_{\mathcal{T}} v_t,$$

where  $\mathcal{L}_{\mathcal{T}}$  is a generator as defined in (16) with measures  $J$  and  $\mu$  given by (18) and (19), respectively.

**Proposition 3.5** (Hölderianity of the rescaled discrete flow). *There exists  $\lambda \in (0, 1)$  such that for every  $\eta \in (0, 1)$ , one can find  $C_H = C_H(\eta) > 0$ , depending only on  $\Omega$ ,  $\bar{\mathbf{m}}$  and  $\zeta$  by means of the constants in Proposition 2.15, such that for all  $K_0 \in \mathcal{T}$ ,  $s \in \mathbb{R}$ ,  $R > 0$  and every non-negative solution of  $\partial_t v_t = \mathcal{L}_{\mathcal{T}} v_t$  on  $Q = [s - R^2, s] \times B_{\text{gra}}(K_0, R)$ , there holds*

$$|v_t(K) - v_t(L)| \leq C_H \left( \frac{d_{\text{gra}}(K, L)}{R} \right)^\lambda \sup_Q |u| \quad \forall (t, K), (t, L) \in Q^+, \quad (31)$$

where  $Q^+ = [s - \eta R^2, s] \times B(K_0, \eta R)$ .

Moreover,  $C_H(\eta)$  satisfies the bound  $\sup_{\eta_0 \leq \eta \leq \eta_1} C_H(\eta) < +\infty$  for any  $\eta_0, \eta_1 \in (0, 1)$ .

*Proof.* Apply Corollary 2.14 (see also [CKW18, Remark 1.16]). □

Finally, we rescale (31) to obtain Hölder regularity for the solutions to the discrete Fokker-Planck equation  $\partial_t u_t = \Delta_{\mathcal{T}} u_t$  with a rescaled generator  $\Delta_{\mathcal{T}} := \varepsilon^{-2} \mathcal{L}_{\mathcal{T}}$ .

**Proposition 3.6** (Hölderianity of the discrete flow). *Let  $\mathcal{T}$  be an admissible and  $\zeta$ -regular mesh of  $\Omega \subset \mathbb{R}^d$ . Let  $(u_t)_{t \geq 0}$  be the solution of the discrete Fokker-Planck equation  $\partial_t u_t = \Delta_{\mathcal{T}} u_t$ . Then for every time  $t > 0$ , the Hölder estimate*

$$|u_t(K) - u_t(L)| \lesssim c(t) |x_K - x_L|^\lambda \sup_{\substack{L_0 \in \mathcal{T} \\ \frac{t}{2} \leq s < +\infty}} |u_s(L_0)| \quad \forall K, L \in \mathcal{T} \quad (32)$$

holds for some monotonically decreasing function  $c : \mathbb{R}^+ \rightarrow \mathbb{R}^+$  and some constant  $\lambda > 0$ , only depending on  $\Omega$ ,  $\bar{\mathbf{m}}$  and  $\zeta$ .

*Proof.* Note that, by unfolding the definitions, we have  $\mathcal{L}_{\mathcal{T}} = \varepsilon^2 \Delta_{\mathcal{T}}$  for  $\varepsilon = [\mathcal{T}]$  and  $\mathcal{L}_{\mathcal{T}}$  as in Proposition 3.5. This means for a given common initial datum, one has a scaling correspondence between the solutions  $(u_t)_{t \geq 0}$  and  $(v_t)_{t \geq 0}$  of the two respective flows, given by

$$u_t(K) = v_{t/\varepsilon^2}(K) \quad \forall t > 0, K \in \mathcal{T}. \quad (33)$$

Pick  $\eta = \eta(t) \in (1/2, 1)$  such that

$$\frac{t\eta^2}{2(1-\eta)} \geq C^2 \text{diam}(\Omega)^2,$$

where  $C$  denotes the constant appearing in (21). Moreover, define

$$R^2 := \frac{t}{2(1-\eta)\varepsilon^2} \quad \text{and} \quad s := \eta R^2 + \frac{t}{2\varepsilon^2}$$

in such a way that  $d_{\text{gra}}(K, L) \leq \eta R$  for all  $K, L \in \mathcal{T}$ .

Now we may apply Proposition 3.5 to every couple of cells  $K, L \in \mathcal{T}$ , together with

$$Q = \left[ \frac{t}{2\varepsilon^2}, C_{\eta} \frac{t}{\varepsilon^2} \right] \times B_{\text{gra}}(K, R), \quad Q^+ := \left[ \frac{t}{\varepsilon^2}, C_{\eta} \frac{t}{\varepsilon^2} \right] \times B_{\text{gra}}(K, \eta R) \ni \left( \frac{t}{\varepsilon^2}, L \right)$$

for a constant  $C_{\eta} \geq 1$ , only depending on  $\eta$ . As a result,

$$|v_{t/\varepsilon^2}(K) - v_{t/\varepsilon^2}(L)| \leq c |x_K - x_L|^\lambda \sup_Q |v| \leq c |x_K - x_L|^\lambda \sup_{\substack{L_0 \in \mathcal{T} \\ \frac{t}{2} \leq s < +\infty}} |u_s(L_0)|,$$

with  $c$  only depending on  $\eta = \eta(t)$  and  $C_H = C_H(\eta)$ . This bound, together with (33), allows us to conclude the proof.  $\square$

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# GRADIENT FLOWS FOR METRIC GRAPHS

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## 1. INTRODUCTION

This article investigates the geometry of Wasserstein spaces over metric graphs and the relation of corresponding energy functionals to Fokker-Planck equations.

A metric graph  $\mathfrak{G}$  may be understood as a (discrete) graph  $(V, E)$  with a weight function  $m : E \rightarrow \mathbb{R}^+$ , where each edge  $e \in E$  is identified with with an interval  $(0, m_e)$  of length corresponding to the edge weight  $m_e := m(e)$ .

We say that a point  $x$  belongs to  $\mathfrak{G}$  if either  $x$  corresponds to a node in  $V$  or there exists an edge  $e \in E$  such that  $x \in \{e\} \times (0, m_e)$ .

Endowed with its natural metric  $\mathbf{d}$  which measures the total length of the shortest paths between any two points,  $\mathfrak{G}$  becomes a metric space. Hence, assuming that the underlying graph  $(V, E)$  is finite and connected, we may define the  $L^p$ -Wasserstein distance between two Borel probability measures  $\mu$  and  $\nu$  on  $\mathfrak{G}$  by means of the Kantorovich transport problem

$$W_p^p(\mu, \nu) := \min_{\sigma} \left\{ \int_{\mathfrak{G} \times \mathfrak{G}} \mathbf{d}^p(x, y) \, d\sigma(x, y) \right\},$$

where the minimum (called *optimal transport plan*) is over all Borel probability measures  $\sigma$  on  $\mathfrak{G} \times \mathfrak{G}$  with respective marginals  $\mu$  and  $\nu$ .

For  $p \geq 1$ , the Wasserstein distance  $W_p$  metrises the topology of weak convergence of Borel probability measures on  $\mathfrak{G}$ . The resulting metric space of probability measures is then called  $L^p$ -Wasserstein space over  $\mathfrak{G}$

In [MRT15] this Wasserstein distance was already studied on metric graphs for the case of  $p = 1$ , making use of the additive property  $\mathbf{d}^p(x, z) = \mathbf{d}^p(x, y) + \mathbf{d}^p(y, z)$ , whenever a point  $y$  lies on a shortest path between  $x$  and  $z$ . Clearly, for any  $p > 1$  this property does not hold anymore and the approach of [MRT15] is not at one's disposal.

Nevertheless, for  $p \geq 1$ , the  $L^p$ -Wasserstein space is a geodesic space, i.e. any two Borel probability measures  $\mu_0$  and  $\mu_1$  on  $\mathfrak{G}$  can be joined by a constant-speed geodesic; that is a curve of probability measures  $(\mu_t)_{t \in [0,1]}$  satisfying

$$W_p(\mu_s, \mu_t) = |s - t| W_p(\mu_0, \mu_1) \quad \forall s, t \in [0, 1].$$

A dynamic characterisation of the Wasserstein distance between Borel probability measures on Euclidean space, going back to the works of Benamou and Brenier [BB99], [BB00], makes use of the geodesic structure of the underlying metric space  $X$ . This allows one to write

$$W_2^2(\mu, \nu) = \min_{\mu_t} \left\{ \int_0^1 |\dot{\mu}_t|^2 \, dx \, dt \right\}$$

with a minimum over all 2-absolutely continuous curves  $(\mu_t)_{t \in [0,1]}$  in the  $L^2$ -Wasserstein space over  $\mathfrak{G}$ , which means that the metric derivative  $t \mapsto |\dot{\rho}_t|$  exists as a function

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in  $L^2(0, 1)$ , connecting  $\mu$  to  $\nu$ . The so-called *Benamou-Brenier formula* asserts for a.e. time  $t$  that  $|\dot{\rho}_t| \leq \|v_t\|_{L^2(\mu_t)}$  for every vectorfield  $(v_t)_{t \in [0,1]}$  solving the continuity equation

$$\frac{d}{dt}\mu_t + \nabla \cdot (v_t \mu_t) = 0 \quad (1)$$

with no-flux boundary conditions in the distributional sense. In addition, there exists a vectorfield achieving a.e. equality  $|\dot{\rho}_t| = \|v_t\|_{L^2(\mu_t)}$ ; thus,

$$W_2^2(\mu, \nu) = \min_{(\mu_t, v_t)} \left\{ \int_0^1 \|v_t\|_{L^2(\mu_t)}^2 dx \right\} \quad (2)$$

with a minimum over all pairs  $(\mu_t, v_t)_{t \in [0,1]}$  solving (1). The standard proofs of this formula make use of the fact that under suitable regularity assumptions on the initial measure  $\mu_0$ , the (then unique) solution  $(\mu_t, v_t)_{t \in [0,1]}$  for (1) is completely characterised by  $\mu_0$  and a flow  $T$  on  $\mathbb{R}^n$ , giving rise to the pair of solutions via the relations

$$T(t, \cdot) \# \mu_0 = \mu_t, \quad \frac{d}{dt}T(t, x) = v_t, \quad T(0, x) = x.$$

Conversely, on a metric such a flow  $T$  typically fails to exist as a solution to the continuity equation (1) is not even uniquely determined by an initial condition  $\mu_0$  and a given vectorfield  $(v_t)_{t \in [0,1]}$  (note that on a metric graph the no-flux boundary conditions have to be replaced by suitable conditions posed on every node in  $V$ ).

All the more so, on a metric graph  $\mathfrak{G}$ , a shortest path between any two points need not be uniquely determined by its endpoints. This behaviour translates to constant-speed geodesics of probability measures. In fact, even the more general notion of *non-branching geodesics* typically fails for Wasserstein spaces over metric graphs in the sense that one might find two distinct constant speed geodesics  $(\mu_t)_{t \in [0,1]}$  and  $(\nu_t)_{t \in [0,1]}$ , taking the same values for all times  $t \in [0, t_0]$  up to some  $t_0 \in (0, 1)$ .

Despite this pathological behaviour of geodesics in Wasserstein spaces over metric graphs, a Benamou-Brenier formula (2) is not forfeit. Indeed, in [GH15] Gigli and Han established a notion for the continuity equation on metric measure spaces. Transferred to the setting of metric graphs, those abstract results imply that solutions  $(\mu_t, v_t)_{t \in [0,1]}$  of the continuity equation (1) satisfy the inequality  $|\dot{\rho}_t| \leq \|v_t\|_{L^2(\mu_t)}$ , under the additional assumption that  $\mu_t$  is absolutely continuous with respect to the one-dimensional Lebesgue measure on  $\mathfrak{G}$  for all times  $t \in [0, 1]$ .

Whereas we show that geodesics satisfy this assumption as long as one verifies that both end-points  $\mu_0$  and  $\mu_1$  are absolutely continuous with respect to the Lebesgue measure, thus establishing the Benamou-Brenier formula between any two absolutely continuous probability measures on  $\mathfrak{G}$ , we can push thing further: In fact, a delicate regularisation step, tuned in line with the node-conditions which accompany the continuity equation (1) on a metric graph, allows for a Benamou-Brenier formula (2) of full generality, i.e. valid between arbitrary Borel probability measures on a metric graph.

The continuity equation which forms the backbone of this Benamou-Brenier formula will also serve as a crucial ingredient to investigate the convergence of the so-called JKO scheme (named after Jordan, Kinderlehrer, and Otto for their seminal paper [JKO98]) for the combined energy functional  $\mathcal{F} = \text{Ent} + \mathcal{V}$  consisting of a logarithmic entropy functional  $\text{Ent}(\mu) = \int_{\mathfrak{G}} \rho \log \rho dx$  and an internal energy functional  $\mathcal{V}(\mu) = \int_{\mathfrak{G}} V \rho dx$ , whenever  $\mu$  is absolutely continuous such that  $d\mu = \rho dx$ . Then the JKO-scheme is



defined by recursively solving the minimisation problem

$$\mu_{k+1} \in \operatorname{argmin}_{\mu} \mathcal{F}(\mu) + \frac{1}{2\tau} W_2^2(\mu, \mu_k)$$

for all  $k \in \mathbb{N}$ , some initial condition  $\mu_0$ , and a fixed parameter  $\tau > 0$ .

The JKO-scheme is a crucial tool in the framework of generation results for gradient flows in metric spaces as employed in [AGS08]. Typically, geodesic convexity of the functional  $\mathcal{F}$ , i.e. convexity of the function  $t \mapsto \mathcal{F}(\mu_t)$  along geodesics  $(\mu_t)_{t \in [0,1]}$ , is exploited to show convergence of the JKO-scheme to a gradient flow for  $\mathcal{F}$ .

However, on a Wasserstein space over a metric graph, functionals like the entropy Ent or the squared metric  $W_2^2(\mu, \cdot)$  need not be geodesically (semi-)convex as we shall see in several examples. Thus, the abstract generation results in [AGS08] are of limited use in a metric graph setting. We will circumvent this issue by following a more direct approach, already successfully employed in [San15] or [IPS19]. Hence, by means of geodesic interpolation of the JKO-scheme  $(\mu_k)_{k \in \mathbb{N}}$ , we may extract a limit curve which may be identified as a solution to a particular continuity equation corresponding to a Fokker-Planck equation

$$\frac{d\mu_t}{dt} \mu_t = \Delta \mu_t + \nabla \cdot (\nabla V \mu), \quad (3)$$

together with suitable node conditions.

The goal of the final section is to identify solutions of the Fokker-Planck equation (3) as gradient flows for the functional  $\mathcal{F}$  on the  $L^2$ -Wasserstein space over  $\mathfrak{G}$ . Inspired by ideas from [Erb16], this may be done without relying on results derived from the JKO-scheme in the previous section. Instead, we make use of a weak chain rule for the derivative  $t \mapsto \mathcal{F}(\mu_t)$  along 2-absolutely continuous curves  $(\mu_t)_{t \in [0,T]}$  in the  $L^2$ -Wasserstein space over  $\mathfrak{G}$ , proved by means of a regularised continuity equation.

In particular, a careful analysis based on interpolation arguments from [AG13] and [AGS08], as well as results from semigroup theory on metric graphs (see e.g. [Mug14]) allow us to identify the limit curve as a gradient flow in the EDE (energy dissipation equality) sense, a notion which does not rely on geodesic convexity of the involved functional.

**Organisation of the Paper.** In Section 2 we recall the notion of absolutely continuous curves taking values in metric spaces, accompanied by definitions for the metric differential and the metric slope. This is followed by an introduction of Wasserstein distances via the Kantorovich transport problem and its dual formulation as well as a recap of geodesics in Wasserstein spaces.

Section 3 is about to the concept of metric graphs and the (non-)existence of transport maps.

Section 4 is devoted to the continuity equation and the Benamou-Brenier formula on metric graphs. To this aim, a regularisation procedure for solutions of the continuity equation, defined in a way to be compatible with the node conditions of said continuity equation, is introduced as well.

The concise Section 5 contains several counter-examples where geodesic convexity along the entropy and the squared Wasserstein distance is not satisfied.

Section 7 covers gradient flows on metric graphs. We prove convergence of the JKO-scheme for a typical energy functional consisting of a logarithmic entropy plus a potential energy to a solution of the corresponding Fokker-Planck equation.

Finally, in the last section solutions of the Fokker-Planck equation are identified as EDE gradient flows for the aforementioned energy functional  $\mathcal{F}$ .

## 2. PRELIMINARIES ON OPTIMAL TRANSPORT

## 2.1. Absolutely continuous curves and gradient flows in metric spaces.

**Definition 2.1.** Let  $(X, d)$  be a metric space and  $(0, T)$  be an open interval. We say that a curve  $\gamma : (0, T) \rightarrow X$  is *absolutely continuous* if there exists a function  $g \in L^1(0, T)$  such that

$$d(\gamma_s, \gamma_t) \leq \int_s^t g(r) \, dr \quad \forall s, t \in (0, T) : s \leq t, \quad (4)$$

where we adopted the notation  $\gamma_r := \gamma(r)$ .

It turns out that for every absolutely continuous function there is a natural choice of  $g$  which minimises the right-hand side of (4), the so-called metric derivative of  $\gamma$ .

**Proposition 2.2.** *For every absolutely continuous curve  $\gamma : (0, T) \rightarrow X$ , the metric derivative defined by the limit*

$$|\dot{\gamma}_t| := \lim_{s \rightarrow t} \frac{d(\gamma_s, \gamma_t)}{|s - t|}$$

*exists for a.e.  $t \in (0, T)$  and belongs to  $L^1(0, T)$ . The metric derivative  $|\dot{\gamma}_t|$  may be chosen as admissible integrand for the right-hand side of (4), minimal in the sense that*

$$|\dot{\gamma}_t| \leq g(t) \quad \text{a.e. } t \in (0, T)$$

*for every  $g \in L^1(0, T)$  satisfying (4).*

*Proof.* See for instance Theorem 1.1.2 in [AGS08]. □

In addition to the metric derivative, we also introduce the notion of a metric slope.

**Definition 2.3.** Given a functional  $F : X \rightarrow \mathbb{R} \cup \{+\infty\}$ , we define the *effective domain* of  $F$  as

$$\text{dom } F := \{x \in X : F(x) < +\infty\}.$$

The (*descending*) *slope* of  $F$  is defined as

$$|\partial F|(x) := \begin{cases} \limsup_{y \rightarrow x} \frac{(F(x) - F(y))^+}{d(x, y)} & \text{if } x \in \text{dom } F, \\ 0 & \text{if } x \text{ is an isolated point in } X, \\ +\infty & \text{otherwise,} \end{cases}$$

where  $(\cdot)^+ := \max\{\cdot, 0\}$  denotes the positive part of a function.

Now we are in the position to introduce two closely related notions of gradient flows in a metric space.

**Definition 2.4.** Let  $F : X \rightarrow \mathbb{R} \cup \{+\infty\}$  be a functional with non-empty effective domain.

- (1) We say that an absolutely continuous curve  $(\gamma_t)_{t \geq 0}$  starting from  $\gamma_0 \in \text{dom } F$  satisfies the *energy dissipation inequality* if

$$F(\gamma_t) + \frac{1}{2} \int_s^t |\dot{\gamma}_r|^2 \, dr + \frac{1}{2} \int_s^t |\partial F|^2(\gamma_r) \, dr \leq F(\gamma_s)$$

for  $s = 0$  and all  $t \geq 0$  as well as for a.e.  $s > 0$  and all  $t \geq s$ .

(2) We say that  $(\gamma_t)_{t \geq 0}$  satisfies the *energy dissipation equality* if

$$F(\gamma_t) + \frac{1}{2} \int_s^t |\dot{\gamma}_r|^2 dr + \frac{1}{2} \int_s^t |\partial F|^2(\gamma_r) dr = F(\gamma_s)$$

for all  $0 \leq s \leq t$ .

**2.2. Wasserstein spaces.** In this section we collect some basic facts on the family of  $L^p$ -Wasserstein distances on spaces of probability measures. We refer to Chapter 5 in [San15], Chapter 2 in [AG13], or Chapter 6 in [Vil08] for more details.

Let  $(X, d)$  be a Polish space, which we assume to be compact for simplicity. The space of Borel probability measures on  $X$  is denoted by  $\mathcal{P}(X)$ . The pushforward measure  $T\#\mu$  induced by a Borel map  $T : X \rightarrow Y$  between two Polish spaces is defined by  $(T\#\mu)(A) := \mu(T^{-1}(A))$ .

**Definition 2.5** (Transport plans and maps). (1) A (*transport*) *plan* between probability measures  $\mu, \nu \in \mathcal{P}(X)$  is a probability measure  $\sigma \in \mathcal{P}(X \times X)$  with respective marginals  $\mu$  and  $\nu$ , i.e.

$$(\text{proj}_1)\#\sigma = \mu \quad \text{and} \quad (\text{proj}_2)\#\sigma = \nu,$$

where  $\text{proj}_i(x_1, x_2) := x_i$  for  $i = 1, 2$ . The set of all transport plans between  $\mu$  and  $\nu$  is denoted by  $\Pi(\mu, \nu)$ .

(2) A transport plan  $\sigma \in \Pi(\mu, \nu)$  is said to be induced by a Borel measurable *transport map*  $T : X \rightarrow X$  if  $\sigma = (\text{Id}, T)\#\mu$ , where  $(\text{Id}, T)$  denotes the mapping  $x \mapsto (x, T(x))$ .

**Definition 2.6** (Kantorovich-Rubinstein-Wasserstein distance). For  $p \geq 1$ , the  $L^p$ -Kantorovich-Rubinstein-Wasserstein distance between probability measures  $\mu, \nu \in \mathcal{P}(X)$  is defined by an optimal transport problem with respect to the cost function  $d^p$  viz.

$$W_p(\mu, \nu) := \inf \left\{ \left( \int_{X \times X} d^p(x, y) d\sigma(x, y) \right)^{1/p} : \sigma \in \Pi(\mu, \nu) \right\}. \quad (5)$$

The infimum above is always attained by some  $\sigma_{\min} \in \Pi(\mu, \nu)$ ; we call any such  $\sigma_{\min}$  *optimal (transport) plan* between  $\mu$  and  $\nu$ . If a transport map  $T$  induces an optimal transport plan, we call  $T$  *optimal* as well.

By compactness of  $(X, d)$ , the  $L^p$ -Wasserstein distance metrises the weak convergence in  $\mathcal{P}(X)$  for any  $p \geq 1$ . Moreover,  $(\mathcal{P}(X), W_p)$  is a compact metric space as well.

The following result, due to Brenier [Bre91], shows the uniqueness of an optimal transport plan for a large class of measures in a Euclidean setting. We state it in a simplified form.

**Theorem 2.7** (Brenier's Theorem). *Let  $\Omega \subset \mathbb{R}^n$  be a compact and convex domain and let  $\mu, \nu \in \mathcal{P}(\Omega)$ . If  $\mu \ll \mathcal{L}^n$ , then for  $p = 2$ , the optimal transport plan  $\sigma_{\min}$  between  $\mu$  and  $\nu$  in (5) is unique and of the form  $\sigma_{\min} = (\text{Id}, T)\#\mu$  for some  $\mu$ -a.e. uniquely determined map  $T : \Omega \rightarrow \Omega$  which can be written as  $T = \nabla \phi$  for some convex function  $\phi$  on  $\Omega$ .*

We conclude this section with a dual formula for the Wasserstein distance (see, e.g. [San15, Section 1.6.2]). To this aim, we recall that for  $c(x, y) := d^p(x, y)$ , the *c-transform* of a function  $\varphi : X \rightarrow \mathbb{R} \cup \{+\infty\}$  is defined by  $\varphi^c(y) := \inf_{x \in X} c(x, y) - \varphi(x)$ . A function  $\psi : X \rightarrow \mathbb{R} \cup \{+\infty\}$  is called *c-concave* if there exists a function  $\varphi : X \rightarrow \mathbb{R} \cup \{+\infty\}$  such that  $\psi = \varphi^c$ .

**Proposition 2.8** (Kantorovich duality). *For any two probability measures  $\mu, \nu \in \mathcal{P}(X)$  we have*

$$W_p^p(\mu, \nu) = \sup_{\varphi, \psi \in C(X)} \left\{ \int_X \varphi d\mu + \int_X \psi d\nu : \varphi(x) + \psi(y) \leq d^p(x, y) \quad \forall x, y \in X \right\}.$$

Moreover, the supremum is attained by a maximising pair of the form  $(\varphi, \psi) = (\varphi, \varphi^c)$ , where  $\varphi$  is a  $c$ -concave function.

The maximiser  $\varphi$  is then called a *Kantorovich potential*.

### 3. OPTIMAL TRANSPORT ON METRIC GRAPHS

**3.1. Metric graphs and function spaces on metric graphs.** In this section, we introduce the basic concepts around the notion of a metric graph, commonly found in standard references like [MRT15], [BK13] or [Kuc08].

**Definition 3.1.** Let  $G = (V, E, m)$  be a orientated, weighted graph. We identify each edge  $e = (e_{\text{init}}, e_{\text{term}}) \in E$  with an interval  $(0, m_e)$  and the corresponding nodes  $e_{\text{init}}, e_{\text{term}} \in V$  with the respective end-points of the interval. Note that the orientation of  $e$  plays a role in this definition.

The *spaces of open and closed metric edges* over  $G$  are defined as the respective topological disjoint unions

$$\mathfrak{E} := \coprod_{e \in E} (0, m_e) \quad \text{and} \quad \bar{\mathfrak{E}} := \coprod_{e \in E} [0, m_e],$$

together with the respective canonical injections  $\iota_e : (0, m_e) \rightarrow \mathfrak{E}$  and  $\bar{\iota}_e : [0, m_e] \rightarrow \bar{\mathfrak{E}}$ . For a function  $\varphi$  on  $\mathfrak{E}$  or  $\bar{\mathfrak{E}}$ , we will adopt the short-hand notations  $\varphi_e := \varphi \circ \iota_e$  or  $\varphi_e := \varphi \circ \bar{\iota}_e$ , respectively.

We define the metric graph over  $G$  as the topological quotient space

$$\mathfrak{G} := \bar{\mathfrak{E}} / \sim,$$

where we identify points  $x \sim y$  whenever  $x = \iota_e(w_e)$  and  $y = \iota_f(w_f)$  for end-points  $w_e, w_f$  corresponding to a common node  $w \in V$  of respective edges  $e, f \in E_w$ .

In addition, we introduce orientation coefficients as follows: For  $w \in V$  and  $e \in E_w$  we set  $\sigma_e(w) = 1$  if  $\bar{\iota}_e(0) = w$  and  $\sigma_e(w) = -1$  if  $\bar{\iota}_e(m_e) = w$ .

**Definition 3.2.** For any point  $x \in \mathfrak{G}$  with  $x$  belonging to an open metric edge  $(0, m_e)$  for some  $e \in E$ , we call a graph  $\tilde{G}$  the *subdivision* of  $G = (V, E, m)$  at  $x$  if  $\tilde{G} = (\tilde{V}, \tilde{E}, \tilde{m})$  with node set  $\tilde{V} := V \cup \{x\}$ , edge set  $\tilde{E} := (E \setminus \{e\}) \cup \{(e_{\text{init}}, x), (x, e_{\text{term}})\}$ , and weight function  $\tilde{m} : E \rightarrow \mathbb{R}^+$  defined on each edge  $f \in E$  by

$$\tilde{m}_f := \begin{cases} m_f & \text{if } f \neq e, \\ x & \text{if } f = (e_{\text{init}}, x) \\ m_e - x & \text{if } f = (x, e_{\text{term}}). \end{cases}$$

In case that  $x$  corresponds to a node in  $G$ , we simply set  $\tilde{G} := G$ .

Note that the spaces of metric edges over  $\tilde{G}$  differ from the corresponding spaces over  $G$ . On the other hand, the metric graph  $\mathfrak{G}$  is invariant under subdivisions of the underlying graph  $G$ .

Consecutive subdivisions at points  $x_1, x_2, \dots, x_k \in \mathfrak{G}$  always result in the same graph, independent of the order of subdivisions.

The notion of subdivision of a metric graph allows us to metrise  $\mathfrak{G}$ .

**Definition 3.3.** For any two points  $x, y \in \mathfrak{G}$ , denote by  $d(x, y)$  the node distance of  $x$  and  $y$  in the underlying graph  $\tilde{G}$  obtained by subdivision of  $\mathfrak{G}$  at  $x$  and  $y$ .

By construction, the distance function  $d$  metrises the topology of  $\mathfrak{G}$ .

In the following, we introduce several classes of function spaces on metric graphs. Recall that the *local Lipschitz constant* of a function  $f : X \rightarrow \mathbb{R}$  is defined by

$$\text{lip}(f)(x) := \limsup_{y \rightarrow x} \frac{|f(y) - f(x)|}{d(x, y)},$$

whenever  $x$  is not isolated and 0 otherwise. We write  $\text{lip}_x(f)(x, t)$  for the local Lipschitz constant with respect to the spatial variable  $x$  of  $\psi$ .

The (*global*) *Lipschitz constant* is defined by

$$\text{Lip}(f) := \sup_{y \neq x} \frac{|f(y) - f(x)|}{d(x, y)}.$$

Note that  $\text{Lip}(f) = \sup_x \text{lip}(f)(x)$ , provided that  $X$  is a geodesic space.

**Definition 3.4.** We denote by  $C(\mathfrak{G})$  the space of continuous real-valued functions on  $\mathfrak{G}$ , endowed with the uniform norm  $\|\cdot\|_\infty$ .

Likewise, we denote by  $\text{Lip}(\mathfrak{G})$  the space of all Lipschitz functions on  $\mathfrak{G}$  and by  $C^k(\bar{\mathfrak{E}})$  the space of all functions  $\varphi$  on  $\bar{\mathfrak{E}}$  such that  $\varphi_e$  has continuous derivatives up to order  $k \in \mathbb{N}$  for each edge  $e \in E$ .

By  $\lambda$  we denote the 1-dimensional Lebesgue measure, lifted to the corresponding spaces of metric edges  $\mathfrak{E}$  and  $\bar{\mathfrak{E}}$  as pushforward measure with respect to the canonical injections  $\iota_e$  and  $\bar{\iota}_e$ , respectively. In a similar fashion,  $\lambda$  lifts to the metric graph  $\mathfrak{G}$  as well.

Denote by  $L^p(\mathfrak{G})$  the  $p$ -Lebesgue space over the measure space  $(\mathfrak{G}, \lambda)$ .

For  $p \in [1, \infty]$  and  $k \in \mathbb{N}$ , we introduce the *Sobolev space*  $W^{k,p}(\mathfrak{G})$  as completion of  $C(\mathfrak{G}) \cap C^k(\bar{\mathfrak{E}})$  with respect to the norm

$$\|u\|_{W^{k,p}} := \begin{cases} \left( \sum_{l=0}^k \|u^{(l)}\|_{L^p}^p \right)^{1/p} & \text{if } p < \infty, \\ \max_{l \leq k} \|u^{(l)}\|_{L^\infty} & \text{if } p = \infty. \end{cases}$$

Furthermore, we consider the set of test functions

$$\mathcal{D}(\mathfrak{G}) := \{ \phi \in C^1(\bar{\mathfrak{E}}) : \phi \text{ consistent with } \sim \},$$

as well as the set of space-time test functions

$$\mathcal{D}((0, T) \times \mathfrak{G}) := \{ \phi \in C_c^1((0, T) \times \bar{\mathfrak{E}}) : \phi, \partial_t \phi \text{ consistent with } \sim \}.$$

We will view functions in  $\mathcal{D}(\mathfrak{G})$  and  $\mathcal{D}((0, T) \times \mathfrak{G})$  also as a function on  $\mathfrak{G} = \bar{\mathfrak{E}} / \sim$  and  $(0, T) \times \mathfrak{G}$ , respectively.

### 3.2. Geodesics in Wasserstein Spaces.

**Definition 3.5.** We call a curve  $\gamma : [0, 1] \rightarrow X$  a (*constant-speed*) *geodesic* if

$$d(\gamma_s, \gamma_t) = |s - t|d(\gamma_0, \gamma_1) \quad \forall s, t \in [0, 1].$$

A metric space  $(X, d)$  is called *geodesic* if every pair of points in  $X$  can be connected by a constant-speed geodesic.

Denote by  $\text{Geod}(X) \subseteq C([0, 1]; X)$  the space of all constant-speed geodesics in  $X$ . The *evaluation maps*  $\text{eval}_t : \text{Geod}(X) \rightarrow X$  are defined by  $\text{eval}_t(\gamma) := \gamma_t$  for every time  $t \in [0, 1]$ .

In addition, we introduce a Borel measurable *geodesic selection map*  $\text{GeodSel} : X \times X \rightarrow \text{Geod}(X)$ , which assigns each pair of points  $(x, y)$  a geodesic connecting  $x$  to  $y$ .

Existence of the map  $\text{GeodSel}$  follows from an application of the Kuratowski and Ryll-Nardzewski measurable selection theorem (see e.g. Theorem 6.9.3 in [Bog07]) to the multivalued function corresponding to the graph

$$\Gamma := \{((x, y), \gamma) : \gamma \text{ is a constant-speed geodesic connecting } x \text{ to } y \text{ in } X\},$$

noting that  $\text{Geod}(X)$  is a compact metric space (see e.g. Section 2.3 in [Pap05]) and  $\Gamma$  is closed in  $X^2 \times \text{Geod}(X)$ .

The following result relates geodesics in the Wasserstein space to geodesics in the underlying metric space (see Theorem 2.10 in [AG13] or Corollary 7.22 in [Vil08] for a proof).

**Proposition 3.6.** *If  $(X, d)$  is a compact geodesic space, then, for  $p > 1$ , the  $L^p$ -Wasserstein space  $(\mathcal{P}(X), W_p)$  is a compact geodesic space as well. Any optimal transport plan  $\sigma$  between  $\mu$  and  $\nu$  induces a constant-speed geodesic  $(\mu_t)_{t \in [0, 1]}$  from  $\mu$  to  $\nu$  viz*

$$\mu_t = (\text{eval}_t)_\# \boldsymbol{\mu}, \tag{6}$$

where  $\boldsymbol{\mu} := (\text{GeodSel})_\# \sigma$  denotes the lift of the plan  $\sigma$  to the space of geodesics  $\text{Geod}(X)$  via the Borel map  $\text{GeodSel}$ .

Conversely, every constant-speed geodesic  $(\mu_t)_{t \in [0, 1]}$  in  $\mathcal{P}(X)$  is of form (6) for some geodesic selection map  $\text{GeodSel}$  and some optimal transport plan  $\sigma \in \Pi(\mu_0, \mu_1)$ .

**3.3. The Monge problem for Wasserstein spaces over metric graphs.** Throughout the remainder of this article, we will make the following assumptions on the underlying discrete graph.

**Assumptions 3.7.** The oriented, weighted graph  $G = (V, E, m)$  is finite, connected and contains neither loops nor multiple edges.

*Remark 3.8.* Note that the metric graph over some graph  $G$  stays invariant under subdivisions of edges in  $G$ . Therefore, we may always introduce additional subdivisions, in order to resolve loops and multiple edges in a given graph, thus, fulfilling the assumptions stated above.

Due to our assumptions, the metric space  $\mathfrak{G}$  is compact, Polish, and geodesic. Since Wasserstein spaces inherit those properties, the same holds true for  $(\mathcal{P}(\mathfrak{G}), W_p)$ . However, geodesics are not uniquely determined by their end-points and may *branch*, i.e. there may exist two distinct geodesics  $(\mu_t)_{t \in [0, 1]}$  and  $(\nu_t)_{t \in [0, 1]}$ , taking the same values for all times  $t \in [0, t_0]$  up to some  $t_0 \in (0, 1)$ .

The following simple example shows that one cannot expect optimal transport maps to exist between measures which are absolutely continuous w.r.t.  $\lambda$  on  $\mathfrak{G}$ .

**Example 3.9.** Consider a metric graph as shown in Figure 1 with uniform weight  $m = 1$  on each edge.

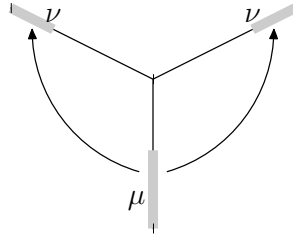


FIGURE 1. The support of probability measures  $\mu$  and  $\nu$  on a metric graph induced by a star with 3 leaves.

Denote by  $\mu$  and  $\nu$  uniform probability measures on the designated edge segments above. Due to a split of mass, there exists no optimal transport map from  $\mu$  to  $\nu$  for any  $p > 1$ .

Nevertheless, it is possible to characterise the Kantorovich transport problem on a metric graph as a superposition of Monge transport problems, provided that we assume some regularity on the probability measures as typically done on an Euclidean domain. Indeed, we observe that, as soon as two probability measures  $\mu$  and  $\nu$  are concentrated on a geodesic curve in  $\mathfrak{G}$ , the Kantorovich problem between  $\mu$  and  $\nu$  reduces to the usual transport problem on the real line. In particular, monotone transport along the geodesic curve provides an optimal solution which is described by an optimal transport map whenever  $\mu \ll \lambda$ .

We introduce the following notation.

**Definition 3.10.** Consider two edges  $e, f \in E$  as well as a shortest path  $\{\gamma_i\}_{i=1}^N$  of edges  $\gamma_i \in E$  connecting an end-node of  $e$  to an end-node of  $f$ . Denote by

$$\mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_N} = (V_{e,f}^{\gamma_1 \dots \gamma_N}, E_{e,f}^{\gamma_1 \dots \gamma_N})$$

the subgraph of  $\mathfrak{G}$  with edge set

$$E_{e,f} := \{e, f\} \cup \gamma_1 \cup \dots \cup \gamma_N,$$

and node set  $V_{e,f}^{\gamma_1 \dots \gamma_N}$  consisting of all end-nodes of edges in  $E_{e,f}^{\gamma_1 \dots \gamma_N}$ .

Note that the definition above covers the case when the edges  $e$  and  $f$  agree.

Below as well as throughout the remainder of this article, we will usually consider the  $p$ -Wasserstein distance for  $p > 1$ ; we refer to [MRT15] for an extensive investigation of the 1-Wasserstein distance on metric graphs.

**Proposition 3.11.** *Let  $\mu, \nu$  be two probability measures on  $\mathfrak{G}$  such that  $\mu \ll \lambda$ . For  $p > 1$ , the  $p$ -Wasserstein distance between  $\mu$  and  $\nu$  is given by a superposition of Monge transport problems viz.*

$$W_p^p(\mu, \nu) = \min \left\{ \sum_i \int_e d^p(x, T_i(x)) d\mu_i(x) \right\}, \quad (7)$$

where the minimum is over all finite families  $(\mu_i, T_i)_{i \in I}$  of sub-measures  $\mu_i$  of  $\mu$  and transport maps  $T_i : \text{supp } \mu_i \rightarrow f$  satisfying

$$\sum_i \mu_i = \mu \quad \text{and} \quad \sum_i (T_i)_\# \mu_i = \nu. \quad (8)$$

*Proof.* To show that the right-hand side of (7) is an upper bound for  $W_p^p(\mu, \nu)$  it is enough to note that, by virtue of (8), the probability measure  $\sigma \in \mathcal{P}(\mathfrak{G} \times \mathfrak{G})$  given by

$$\sigma := \sum_i (\text{Id}, T_i)_{\#} \mu_i$$

is an admissible plan between  $\mu$  and  $\nu$ .

In order to find an optimal family  $(\mu_i, T_i)_{i \in I}$  which achieves equality in (7), we make use of Proposition 3.6 to represent a constant-speed geodesic  $(\mu_t)_{t \in [0,1]}$  from  $\mu$  to  $\nu$  as

$$\mu_t = (\text{eval}_t)_{\#} \boldsymbol{\mu} \quad \text{and} \quad \boldsymbol{\mu} := (\text{GeodSel})_{\#} \sigma$$

for a fixed geodesic selection map  $\text{GeodSel} : \mathfrak{G} \times \mathfrak{G} \rightarrow \mathfrak{G}$  and an optimal plan  $\sigma$  between  $\mu$  and  $\nu$ .

For every choice of edges  $e, f \in E$  and every shortest path  $\gamma_{e \rightarrow f} := \{\gamma_i\}_{i=1}^N$  in  $G$ , connecting an end-node of  $e$  to an end-node of  $f$ , we denote by  $\mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}}$  the corresponding subgraph as defined in Definition 3.10.

Consider the set of all constant-speed geodesics in  $\mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}}$  connecting points on the metric edge  $e$  to points on the metric edge  $f$  via the path  $\gamma_{e \rightarrow f}$ . In order to avoid measurability issues, we introduce this set as a measurable subset of  $\text{Geod}(\mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}})$ , given by

$$\text{Geod}_{e,f}^{\gamma_{e \rightarrow f}} := \text{eval}_0^{-1}(e) \cap \text{eval}_1^{-1}(f) \cap \bigcap_{t \in \mathbb{Q} \cap (0,1)} \text{eval}_t^{-1}(\mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}}). \quad (9)$$

Note that this set may be identified as a measurable subset of  $\text{Geod}(\mathfrak{G})$  as well.

Introduce the interpolation curve

$$\mu_t^{\gamma_{e \rightarrow f}} := (\text{eval}_t)_{\#} \boldsymbol{\mu} \big|_{\text{Geod}_{e,f}^{\gamma_{e \rightarrow f}}},$$

which is of constant mass on  $\mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}}$  for each time  $t \in [0, 1]$ . In particular, the measures  $\mu_0^{\gamma_{e \rightarrow f}}$  and  $\mu_1^{\gamma_{e \rightarrow f}}$  are concentrated on the metric edges  $e$  and  $f$ , respectively. The curve  $(\mu_t^{\gamma_{e \rightarrow f}})_{t \in [0,1]}$  is a constant-speed geodesic between those two measures.

For  $e \neq f$ , the subgraph  $\mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}}$  is isometrically isomorph to a compact interval on the real line. Therefore, the existence of a unique optimal transport map  $T^{\gamma_{e \rightarrow f}}$  for the transport problem between the measures  $\mu_0^{\gamma_{e \rightarrow f}}$  and  $\mu_1^{\gamma_{e \rightarrow f}}$  with respect to the cost function  $\mathbf{d}^p$  follows immediately (cf. e.g. Theorem 2.9 in [San15]).

In case  $e = f$ , the subgraph  $\mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}}$  is isometrically isomorph to a 1-dimensional torus. Again, we may appeal to classic results (cf. Theorem 1.25 in [San15]) to obtain existence of a unique optimal transport map  $T^{\gamma_{e \rightarrow f}}$  for the transport problem between the measures  $\mu_0^{\gamma_{e \rightarrow f}}$  and  $\mu_1^{\gamma_{e \rightarrow f}}$  with respect to the cost function  $\mathbf{d}^p$ .

As a result, the finite family

$$\{(\mu_0^{\gamma_{e \rightarrow f}}, T^{\gamma_{e \rightarrow f}}) : \forall \gamma_{e \rightarrow f} \text{ s.t. } e, f \in E\},$$

where  $\gamma_{e \rightarrow f}$  denotes every shortest path in  $G$ , connecting an end-nodes of  $e$  to an end-node of  $f$ , attains the minimum in (7).  $\square$

In addition to the families of sub-measures which appeared in Proposition 3.11, we can also consider sub-measures which do not depend on any choice of a geodesic selection map: Given two probability measures  $\mu, \nu \in W_2(\mathfrak{G})$  and an optimal transport plan  $\sigma$  between  $\mu$  and  $\nu$  with respect to  $\mathbf{d}^p$ , set

$$\mu_f := \sigma(\cdot, f) \quad \text{and} \quad \nu_e := \sigma(e, \cdot) \quad e, f \in E.$$



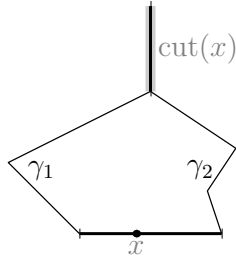


FIGURE 2. A subgraph consisting of a pair of disjoint edges connected by two shortest paths  $\gamma_1$  and  $\gamma_2$ . The pair of edges does not satisfy the (CUT) condition, unless we impose a subdivision at the point  $x$ .

Note that we have

$$\sum_{f \in E} \mu_f = \mu \quad \text{and} \quad \sum_{e \in E} \nu_e = \nu,$$

as well as  $\mu_f(e) = \nu_e(f)$  for all metric edges  $e, f$  in  $\mathfrak{E}$ . That means that (up to a rescaling of  $\mu$  and  $\nu$  to probability measures)  $\sigma|_{e \times f}$  describes the optimal transport between  $\mu_f|_e$  and  $\nu_e|_f$ .

To study the Monge transport problem between  $\mu_f|_e$  and  $\nu_e|_f$ , i.e. to investigate whether  $\sigma|_{e \times f}$  may be represented by a (single) transport map, we introduce the following geometric condition.

To this aim, recall that the *cut locus*  $\text{cut}(x)$  of a point  $x$  in a geodesic space  $X$  is the set consisting of all points  $y \in X$  such that there exist at least two distinct constant-speed geodesics connecting  $x$  to  $y$ .

**Definition 3.12.** For a pair of edges  $e, f \in E$ , we denote by  $\mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_4}$  the metric graph corresponding to a subgraph of  $G$ , consisting of the edges  $e$  and  $f$  together with four shortest paths  $\gamma_1, \dots, \gamma_4$  in  $G$ , each connecting one of the four respective pair of endpoints in  $\{e_{\text{init}}, e_{\text{term}}\} \times \{f_{\text{init}}, f_{\text{term}}\}$ .

We say that a pair of *open* metric edges  $e$  and  $f$  in  $\mathfrak{E}$  (also denoted by  $e \rightarrow f$  below) satisfies the (CUT) condition if there does not exist any point  $x$  on  $f$  such that  $\lambda(\text{cut}(x) \cap e) > 0$ , where  $\text{cut}(x)$  denotes the cut locus of the point  $x$  in the geodesic space  $\mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_4}$ ; see also Figure 2.

The metric graph  $\mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_4}$  in the definition above does not depend on any particular choice of geodesic paths between each pair of end-nodes of  $e$  and  $f$ .

*Remark 3.13.* For any point  $x \in \mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_4}$ , the cut locus  $\text{cut}(x)$  on  $\mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_4}$  consists of the union of single points and line segments, each where at least one end-point is a node.

Thus, whenever a graph does not satisfy (CUT), we may introduce a subdivision at each point  $x \in \text{int } f$  where  $\lambda(\text{cut}(x) \cap e) > 0$  on  $\mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_4}$  (the number of those points is finite). As a result, we obtain a new graph satisfying (CUT). By construction, both the old and the new graph give rise to the same metric graph.

We collect some observations regarding the (CUT) condition.

**Proposition 3.14.** *On a metric graph  $\mathfrak{G}$ , let  $e, f$  be metric edges in  $\mathfrak{E}$  such that  $e \rightarrow f$  satisfies the (CUT) condition. Consider probability measures  $\mu$  and  $\nu$  on  $e$  and  $f$ , respectively, such that  $\mu \ll \lambda$ . Then there exists a unique optimal transport plan between  $\mu$  and  $\nu$  for every  $p > 1$ . This plan arises from a transport map  $T^{e \rightarrow f}$ .*

*For  $\lambda$ -a.e.  $x$  on  $e$ , the point  $T^{e \rightarrow f}(x)$  does not belong to  $\text{cut}(x)$  on  $\mathfrak{G}$ .*

*Proof.* Note that the cut locus on  $\mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_4}$  takes one of the following two forms:

**Case 1:**  $\text{cut}(x) \cap \text{int } e$  is empty for all  $x \in f$ . We may remove edges from  $\mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_4}$  to end up with a path graph  $\mathfrak{G}_{\text{path}}$  whose distance function agrees with the one on  $\mathfrak{G}$  between points  $x$  on  $e$  and  $y$  on  $f$ .

By identifying  $\mathfrak{G}_{\text{path}}$  with a compact interval, we may invoke existence results on the real line (cf. e.g. Theorem 2.9 in [San15]). In particular, there exists a unique optimal transport plan between  $\mu$  and  $\nu$  for the cost function  $\mathbf{d}^p$  with  $p > 1$ .

On the compact interval identified with  $\mathfrak{G}_{\text{path}}$ , this plan arises from a monotone transport map  $T^{e \rightarrow f} = F_\nu^{[-1]} \circ F_\mu$  in terms of the cumulative distribution function  $F_\mu$  for  $\mu$  and the pseudo-inverse  $F_\nu^{[-1]}$  of the cumulative distribution function for  $\nu$ .

**Case 2:**  $\text{cut}(x) \cap \text{int } e$  is not empty for some  $x \in f$ . In this case, the set  $\text{cut}(x) \cap \text{int } e$  is either empty or a singleton for each  $x \in f$ . Hence, we may remove edges from  $\mathfrak{G}_{e,f}^{\gamma_1 \dots \gamma_4}$  to end up at a 4-cycle  $\mathfrak{G}_{\text{cycle}}$  whose distance function agrees with the one on  $\mathfrak{G}$  between points  $x$  on  $e$  and  $y$  on  $f$ .

By identifying  $\mathfrak{G}_{\text{cycle}}$  with a 1-dimensional torus, we may again appeal to corresponding existence results (cf. e.g. Theorem 1.25 in [San15]). In particular, there exists a unique optimal transport plan between  $\mu$  and  $\nu$  for the cost function  $\mathbf{d}^p$  with  $p > 1$ . Moreover, this plan arises from an optimal transport map  $T^{e \rightarrow f}(x) = \nabla \varphi(x)$  for  $\lambda$ -a.e.  $x$  on  $e$  for some geodesically convex function  $\varphi$  on  $\mathfrak{G}_{\text{cycle}}$ .  $\square$

Proposition 3.14 immediately implies the following characterisation of the  $L^p$ -Wasserstein distance by means of a family of transport maps.

**Corollary 3.15.** *Let  $\sigma$  be an optimal transport plan between two probability measures  $\mu$  and  $\nu$  on  $\mathfrak{G}$  for  $p > 1$ . Assume that  $\mathfrak{G}$  satisfies the (CUT) condition and  $\mu \ll \lambda$ . Then the  $L^p$ -Wasserstein distance between  $\mu$  and  $\nu$  may be written as a superposition of Monge transport problems viz.*

$$W_p^p(\mu, \nu) = \min \left\{ \sum_{f \in E} \int_{\mathfrak{G}} \mathbf{d}^p(x, T_f(x)) \, \mathrm{d}\mu_f(x) \right\}, \quad (10)$$

where the minimum runs over all families  $(\mu_f, T_f)_{f \in E}$  of submeasures  $\mu_f$  of  $\mu$  and transport maps  $T_f : \mathfrak{G} \rightarrow f$  such that

$$\sum_{f \in E} \mu_f = \mu \quad \text{and} \quad \sum_{f \in E} (T_f)_\# \mu_f = \nu.$$

For every  $f \in E$  and  $\lambda$ -a.e.  $x \in \mathfrak{G}$ , the point  $T^f(x)$  does not belong to  $\text{cut}(x)$  on  $\mathfrak{G}$ .

*Remark 3.16.* (i) Instead of  $\mathbf{d}^p$ , one can also consider a cost function on  $\mathfrak{G} \times \mathfrak{G}$  which is strictly convex along geodesics.

(ii) The optimal transport plans considered in the results above are usually not unique. In particular, the underlying monotone transport maps depend on the amount of mass to be transported between each pair of metric edges  $e, f$  in  $E$  as prescribed by the optimal transport plan.

In the last part of this section we will address the issue whether the set of absolutely continuous measures on a metric graph is geodesically convex. This question has been answered positively for absolutely continuous measures on a manifold via the construction of suitable locally Lipschitz continuous transport maps (see e.g. Corollary 2.24 in [AG13]). Let us recall this approach in the following setting of a constant speed geodesic with initial absolutely continuous measure on the real line, which will be of subsequent use.

**Lemma 3.17.** *Let  $(\mu_t)_{t \in [0,1]}$  be a constant-speed geodesic in  $\mathcal{P}_p(\mathbb{R})$  such that  $\mu_0 \ll \lambda$ . Then for any times  $t \in (0,1)$ , the unique optimal transport plan from  $\mu_t$  to  $\mu_0$  is induced by a locally Lipschitz continuous transport map.*

*Proof.* Recall that the absolute continuity of  $\mu_0$  implies that the unique optimal transport plan from  $\mu_0$  to  $\mu_1$  is induced by the nondecreasing monotone transport map  $T_{0 \rightarrow 1} := F_{\mu_1}^{[-1]} \circ F_{\mu_0}$  in terms of cumulative distribution functions and their pseudo-inverses. In particular, the constant-speed geodesic  $(\mu_t)_{t \in [0,1]}$  takes the form

$$\mu_t = ((1-t)\text{Id} + tT_{0 \rightarrow 1})_{\#} \mu_0 \quad \forall t \in [0,1].$$

In order to obtain an optimal transport map from  $\mu_t$  to  $\mu_0$ , it remains to show that  $((1-t)\text{Id} + tT_{0 \rightarrow 1})^{-1}$  is a single-valued Lipschitz map with constant bounded from above by  $1/(1-t)$ . Indeed, this claim follows directly from the monotonicity of  $T_{0 \rightarrow 1}$  via the estimate

$$\begin{aligned} & |(1-t)x + tT_{0 \rightarrow 1}(x) - (1-t)y - tT_{0 \rightarrow 1}(y)|^2 \\ &= (1-t)^2|x-y|^2 + t^2|T_{0 \rightarrow 1}(x) - T_{0 \rightarrow 1}(y)|^2 + 2t(1-t)(x-y)(T_{0 \rightarrow 1}(x) - T_{0 \rightarrow 1}(y)) \\ &\geq (1-t)^2|x-y|^2 \end{aligned}$$

for all  $x, y \in \mathbb{R}$ , which allows us to conclude.  $\square$

*Remark 3.18.* It is easy to adapt the result above to probability measures on the 1-dimensional torus  $\mathbb{R} \setminus (r\mathbb{Z})$  with perimeter  $r > 0$ , noting that the unique optimal transport plan is induced by a geodesically convex transport map (see Section 1.3.2 in [San15]).

The construction in the proof of Proposition 3.11 allows us to answer whether constant-speed geodesics inherit absolute continuity from their end-points.

**Proposition 3.19.** *Let  $\sigma$  be an optimal transport plan between two probability measures  $\mu$  and  $\nu$  on  $\mathfrak{G}$  for  $p > 1$  such that  $\mu \ll \lambda$ . Then every constant-speed geodesic  $(\mu_t)_{t \in [0,1]}$  from  $\mu$  to  $\nu$  satisfies  $\mu_t \ll \lambda$  for each time  $t \in (0,1)$ .*

*Proof.* Fix a geodesic selection map  $\text{GeodSel}$  and a transport plan  $\sigma$  such that the constant-speed geodesic  $(\mu_t)_{t \in [0,1]}$  is represented by formula (6). Following the proof of Proposition 3.11, for every shortest path  $\gamma_{e \rightarrow f} := \{\gamma_i\}_{i=1}^N$  in  $G$ , connecting an end-node of  $e$  to an end-node of  $f$ , we obtain a constant speed geodesic  $(\mu_t^{\gamma_{e \rightarrow f}})_{t \in [0,1]}$  on the metric graph  $\mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}}$ , satisfying

$$\sum_{\substack{e,f \in E \\ \gamma_{e \rightarrow f}}} \mu_t^{\gamma_{e \rightarrow f}} = \mu_t \quad \forall t \in [0,1]. \quad (11)$$

In case  $e \neq f$ , the metric graph  $\mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}}$  is isometrically isomorph to a compact interval on the real line and we may apply Lemma 3.17 to obtain the existence of a unique optimal transport map  $T_{s \rightarrow t}^{\gamma_{e \rightarrow f}}$  from  $\mu_t^{\gamma_{e \rightarrow f}}$  to  $\mu_s^{\gamma_{e \rightarrow f}}$ , which is Lipschitz continuous with a constant  $1/(1-t)$  for any times  $t \in (0,1)$  and  $s \in [0,1]$ .

If  $e = f$ , the existence of such a unique Lipschitz continuous optimal transport map follows from Remark 3.18.

Note that for any Borel set  $A \subseteq \mathfrak{G}_{e,f}^{\gamma_{e \rightarrow f}}$ , the inclusion  $A \subseteq (T_{s \rightarrow t}^{\gamma_{e \rightarrow f}})^{-1}(T_{s \rightarrow t}^{\gamma_{e \rightarrow f}}(A))$  implies the inequality

$$\mu_t^{\gamma_{e \rightarrow f}}(A) \leq \mu_t^{\gamma_{e \rightarrow f}}(T_{s \rightarrow t}^{\gamma_{e \rightarrow f}})^{-1}(T_{s \rightarrow t}^{\gamma_{e \rightarrow f}}(A)) = \mu_s^{\gamma_{e \rightarrow f}}(T_{s \rightarrow t}^{\gamma_{e \rightarrow f}}(A)). \quad (12)$$

Recall that the Lipschitz continuity of the transport maps yields that every Borel null set  $A$  is mapped again to a Borel null set  $T_{s \rightarrow t}^{\gamma_{e \rightarrow f}}(A)$ . In particular for  $s = 0$ , (12) and the absolute continuity of  $\mu_0^{\gamma_{e \rightarrow f}}$  imply that  $\mu_t^{\gamma_{e \rightarrow f}}$  is absolutely continuous as well; by (11), we conclude.  $\square$

#### 4. THE CONTINUITY EQUATION ON A METRIC GRAPH

In this section we fix a metric graph  $\mathfrak{G}$  and perform a detailed study of the continuity equation

$$\partial_t \mu_t + \nabla \cdot J_t = 0 \quad (13)$$

in this context.

**Definition 4.1** (Strong solution). A pair of measurable functions  $(\rho, U)$  with  $\rho : (0, T) \times \mathfrak{G} \rightarrow \mathbb{R}_+$  and  $U : (0, T) \times \bar{\mathfrak{E}} \rightarrow \mathbb{R}_+$  is said to be a strong solution to (13) if

- (i)  $t \mapsto \rho(t, x)$  is continuously differentiable for every  $x \in \mathfrak{G}$ ;
- (ii)  $x \mapsto U(t, x)$  belongs to  $\mathcal{D}(\mathfrak{G})$  for every  $t \in (0, T)$ ;
- (iii) the continuity equation  $\frac{d}{dt} \rho_t + \nabla \cdot U_t = 0$  holds for every  $t \in (0, T)$  and  $x \in \mathfrak{E}$ ;
- (iv) for every  $t \in (0, T)$  and  $w \in V$  we have  $\sum_{e \in E_w} \sigma_e(w) U_t(w_e) = 0$ .

Here, we write  $\rho_t := \rho(t, \cdot)$  and  $U_t := U(t, \cdot)$ .  $E_w$  denotes the set of all edges adjacent to the node  $w \in V$  and  $w_e$  denotes the corresponding end-point of the metric edge  $e$  which is identified with  $w$ .

To motivate the definition of weak solutions, suppose that we have a strong solution  $(\rho_t, U_t)_{t \in (0, T)}$  to the continuity equation (13). Let  $\psi \in \mathcal{D}(\mathfrak{G})$  be a test function. Integrating by parts we obtain on every metric edge  $e$  gives

$$\frac{d}{dt} \int_0^{m_e} \psi \rho_t dx = \int_0^{m_e} \nabla \psi \cdot U_t dx + \psi U_t \Big|_0^{m_e}.$$

Then summation over all  $e \in E$  yields

$$\frac{d}{dt} \int_{\mathfrak{G}} \psi \rho_t dx = \int_{\bar{\mathfrak{E}}} \nabla \psi \cdot U_t dx + \sum_{w \in V} \psi(w) \sum_{e \in E_w} \sigma_e(w) U_t(w_e) = \int_{\bar{\mathfrak{E}}} \nabla \psi \cdot U_t dx,$$

where we used the continuity of  $\psi$  on  $\mathfrak{G}$  as well as the node condition (iv) above in the last step. This ensures that the net ingoing momentum vanishes at every node in  $V$ . In particular, choosing  $\psi \equiv 1$  yields

$$\int_{\mathfrak{G}} \rho_s dx = \int_{\mathfrak{G}} \rho_t dx,$$

for all  $s, t \in (0, T)$ , i.e. solutions to the continuity equation are mass-preserving. Here condition (iv) is crucial to ensure that no creation or annihilation of mass occurs at the nodes.

**Definition 4.2** (Weak solution). A pair  $(\mu_t, J_t)_{t \in (0, T)}$  consisting of Borel families of probability measures  $\mu_t$  on  $\mathfrak{G}$  and signed measures  $J_t$  on  $\bar{\mathfrak{E}}$  is said to be a weak solution to (13) if

- (i)  $t \mapsto \int_{\mathfrak{G}} \psi d\mu_t$  is absolutely continuous for every test function  $\psi \in \mathcal{D}$ ;
- (ii)  $\int_0^T |J_t|(\bar{\mathfrak{E}}) dt < \infty$ ;
- (iii) for a.e.  $t \in (0, T)$ , we have

$$\frac{d}{dt} \int_{\mathfrak{G}} \psi d\mu_t = \int_{\bar{\mathfrak{E}}} \nabla \psi \cdot dJ_t. \quad (14)$$

Whenever there exists a family  $(v_t)_{t \in (0, T)}$  of vectorfields  $v_t$  on  $\bar{\mathfrak{E}}$  such that  $J_t = v_t \cdot \mu_t$ , then we will speak of  $(\mu_t, v_t)_{t \in (0, T)}$  as a weak solution to (13) as well.

*Remark 4.3.* If  $(\mu_t, J_t)_{t \in (0, T)}$  is a weak solution to the continuity equation, then  $t \mapsto \mu_t$  is weakly continuous. Thus, we can continuously extend  $(\mu_t)_t$  to the interval  $[0, T]$ .

*Remark 4.4.* Note that  $(\mu_t, J_t)_{t \in (0, T)}$  is a weak solution if and only if the following conditions hold: (i)  $t \mapsto \mu_t$  is weakly continuous; (ii) from Definition 4.2 holds; and

(iii) for every  $\phi \in \mathcal{D}((0, T) \times \mathfrak{G})$ , we have

$$\int_0^T \left( \int_{\mathfrak{G}} \partial_t \phi \, d\mu_t \, dt + \int_{\bar{\mathfrak{E}}} \nabla \phi \cdot dJ_t \right) dt = 0. \quad (15)$$

The next result asserts that the momentum field does not give mass to vertices for a.e. time point. Hence, we can equivalently restrict the integral in (14) and (15) to the space of open edges  $\mathfrak{E}$ .

**Lemma 4.5.** *Let  $B := \bar{\mathfrak{E}} \setminus \mathfrak{E}$  denote the set of all boundary points of edges. For any weak solution to the continuity equation  $(\mu_t, J_t)_{t \in (0, T)}$ , we have*

$$\int_0^T |J_t|(B) \, dt = 0.$$

*Proof.* Fix a metric edge  $e$  in  $\bar{\mathfrak{E}}$  and take any  $w \in \{e_{\text{init}}, e_{\text{term}}\}$ . Fix a function  $\eta \in C_c^1(\mathbb{R})$  satisfying  $\eta(0) = 0$  and  $\eta'(0) = 1$ . For  $\varepsilon > 0$ , we define  $\varphi^\varepsilon : \bar{\mathfrak{E}} \rightarrow \mathbb{R}$  by  $\varphi^\varepsilon(x) := \mathbb{1}_e(x) \varepsilon \eta(d(x, w)/\varepsilon)$ . Note that  $\varphi^\varepsilon$  belongs to  $\mathcal{D}(\mathfrak{G})$  for  $\varepsilon$  small enough. Moreover,  $|\nabla \varphi^\varepsilon(w)| = 1$ . On the other hand,  $\varphi^\varepsilon \rightarrow 0$  uniformly on  $\mathfrak{G}$  and  $\nabla \varphi^\varepsilon(x) \rightarrow 0$  for any  $x \neq w$  as  $\varepsilon \searrow 0$ . Choosing  $\varphi = \varphi^\varepsilon$  in (15), we obtain by passing to the limit that  $\int_0^T J_t(\{w\}) \, dt = 0$ .  $\square$

**Lemma 4.6** (Weak and strong solutions). *The following assertions hold:*

- (1) *If  $(\rho_t, U_t)_{t \in (0, T)}$  is a strong solution to the continuity equation, then the pair  $(\mu_t, J_t)_{t \in (0, T)}$  defined by  $\mu_t = \rho_t \cdot \lambda$  and  $J_t = U_t \cdot \lambda$  is a weak solution to the continuity equation.*
- (2) *If  $(\mu_t, J_t)_{t \in (0, T)}$  is a weak solution to the the continuity equation (14) such that the densities  $\rho_t$  and  $U_t$  exist for all times  $t \in (0, T)$  and satisfy the regularity conditions (i) and (ii) of Definition 4.1. Then  $(\rho_t, U_t)_{t \in (0, T)}$  is a strong solution to the continuity equation.*

*Proof.* Both claims are straightforward consequences of integration-by-parts on each metric edge in  $\mathfrak{E}$ .  $\square$

The next result relates the metric differential of  $t \mapsto \mu_t$  to the corresponding  $L^2$ -norm of the vectorfields  $v_t$ .

**Theorem 4.7** (Characterisation of absolutely continuous curves). *The following statements hold:*

- (i) *If  $(\mu_t)_{t \in (0, T)}$  is absolutely continuous in  $(\mathcal{P}(\mathfrak{G}), W_2)$ , then for a.e.  $t \in (0, T)$ , there exists a vectorfield  $v_t \in L^2(\mu_t)$  such that  $\|v_t\|_{L^2(\mu_t)} \leq |\dot{\mu}_t|$  and  $(\mu_t, v_t)_{t \in (0, T)}$  is a weak solution to the continuity equation (14).*
- (ii) *Conversely, if  $(\mu_t, v_t)_{t \in (0, T)}$  is a weak solution to the continuity equation (14) satisfying  $\int_0^1 \|v_t\|_{L^2(\mu_t)} \, dt < +\infty$ , then  $(\mu_t)_{t \in (0, T)}$  is absolutely continuous in  $(\mathcal{P}(\mathfrak{G}), W_2)$  and  $|\dot{\mu}|(t) \leq \|v_t\|_{L^2(\mu_t)}$  for a.e.  $t \in (0, T)$ .*

*Proof of (i).* For this part of the proof, we follow a strategy employed in Theorem 8.3.1 of [AGS08], modified accordingly to our setting of metric graphs.

The idea of the proof is as follows: On the space-time domain  $Q := (0, T) \times \mathfrak{G}$  we consider the Borel measure  $\boldsymbol{\mu} := \int_0^T \delta_t \otimes \mu_t dt$  whose disintegration with respect to the Lebesgue measure on  $(0, T)$  is given by  $(\mu_t)_{t \in (0, T)}$ . To deal with the fact that gradients of smooth functions are multi-valued at the nodes, we define  $\bar{\mu}_t \in \mathcal{M}_+(\bar{\mathfrak{E}})$  by  $\bar{\mu}_t(A) := \sum_{e \in E} \mu_t(A \cap \bar{e})$  for every Borel set  $A \subseteq \bar{\mathfrak{E}}$ . We then set  $\bar{Q} := (0, T) \times \bar{\mathfrak{E}}$  and define  $\bar{\boldsymbol{\mu}} \in \mathcal{M}_+(\bar{Q})$  by  $\bar{\boldsymbol{\mu}} := \int_0^T \delta_t \otimes \bar{\mu}_t dt$ . Consider the linear spaces of functions  $\mathcal{T}$  and  $\mathcal{V}$  given by

$$\begin{aligned} \mathcal{T} &:= \text{span} \left\{ (0, T) \times \mathfrak{G} \ni (t, x) \mapsto a(t)\varphi(x) : a \in C_c^1(0, T), \varphi \in C(\mathfrak{G}) \cap C^1(\bar{\mathfrak{E}}) \right\}, \\ \mathcal{V} &:= \left\{ (0, T) \times \bar{\mathfrak{E}} \ni (t, x) \mapsto \nabla_x \Phi(t, x) : \Phi \in \mathcal{T} \right\}. \end{aligned}$$

The strategy is to show that the linear functional  $L : \mathcal{V} \rightarrow \mathbb{R}$  given by

$$L(a \otimes \nabla \varphi) := - \int_Q \dot{a}(t)\varphi(x) d\boldsymbol{\mu}(x, t),$$

is well-defined and  $L^2(\bar{Q}, \bar{\boldsymbol{\mu}})$ -bounded with  $\|L\|^2 \leq \int_0^T |\dot{\mu}_t|^2 dt$ . The existence of a velocity vectorfield  $\boldsymbol{v} \in L^2(\bar{Q}, \bar{\boldsymbol{\mu}})$  follows then by the Riesz representation theorem. Once this is done, we show that the momentum vectorfield  $\boldsymbol{J} := \boldsymbol{v} \cdot \boldsymbol{\mu}$  does not assign mass to boundary points in  $\bar{\mathfrak{E}}$ , so that  $\boldsymbol{v}$  can be interpreted as an element in  $L^2(Q, \boldsymbol{\mu})$  and the integration over vectorfields can be restricted to  $\mathfrak{E}$ .

*Step 1.* Fix a test function  $\varphi \in C(\mathfrak{G}) \cap C^1(\bar{\mathfrak{E}})$  and consider the bounded and upper semicontinuous function  $H : \mathfrak{G} \times \mathfrak{G} \rightarrow \mathbb{R}$  given by

$$H(x, y) := \begin{cases} \text{lip}(\varphi)(x) & \text{if } x = y, \\ \frac{|\varphi(x) - \varphi(y)|}{d(x, y)} & \text{if } x \neq y, \end{cases}$$

for  $x, y \in \mathfrak{G}$ . For  $s, t \in (0, T)$ , let  $\sigma^{s \rightarrow t} \in \Pi(\mu_s, \mu_t)$  be an optimal plan. The Cauchy-Schwarz inequality yields

$$\begin{aligned} \left| \int_{\mathfrak{G}} \varphi d\mu_s - \int_{\mathfrak{G}} \varphi d\mu_t \right| &\leq \int_{\mathfrak{G} \times \mathfrak{G}} d(x, y) H(x, y) d\sigma^{s \rightarrow t}(x, y) \\ &\leq W_2(\mu_s, \mu_t) \left( \int_{\mathfrak{G} \times \mathfrak{G}} H^2(x, y) d\sigma^{s \rightarrow t}(x, y) \right)^{1/2}. \end{aligned} \tag{16}$$

As  $\varphi$  is globally Lipschitz on  $\mathfrak{G}$ , we obtain

$$\left| \int_{\mathfrak{G}} \varphi d\mu_s - \int_{\mathfrak{G}} \varphi d\mu_t \right| \leq \text{Lip}(\varphi) W_2(\mu_s, \mu_t)$$

and infer that the mapping  $t \mapsto \int_{\mathfrak{G}} \varphi d\mu_t$  is absolutely continuous, hence, differentiable up to a null set  $N_\varphi \subseteq (0, T)$ .

Fix  $t \in (0, T)$  and take a sequence  $\{s_n\}_{n \in \mathbb{N}}$  converging to  $t$ . Since  $\{\mu_{s_n}\}$  is weakly convergent, this sequence is tight. Consequently,  $\{\sigma^{s_n \rightarrow t}\}_{n \in \mathbb{N}}$  is tight as well, and we may extract a subsequence converging weakly to some  $\hat{\sigma} \in \mathcal{P}(\mathfrak{G} \times \mathfrak{G})$ . It readily follows

that  $\hat{\sigma} \in \Pi(\mu_t, \mu_t)$ . Moreover, along the convergent subsequence, we have

$$\int_{\mathfrak{G} \times \mathfrak{G}} d^2(x, y) d\hat{\sigma}(x, y) \leq \liminf_{n \rightarrow \infty} \int_{\mathfrak{G} \times \mathfrak{G}} d^2(x, y) d\sigma^{s_n \rightarrow t}(x, y) = \liminf_{n \rightarrow \infty} W_2^2(\mu_{s_n}, \mu_t) = 0,$$

which implies that  $\hat{\sigma} = (\text{Id}, \text{Id})_{\#} \mu_t$ .

Using this result and the upper-semicontinuity of  $H$ , it follows from (16) that

$$\begin{aligned} \limsup_{s \rightarrow t} \left| \frac{\int_{\mathfrak{G}} \varphi d\mu_s - \int_{\mathfrak{G}} \varphi d\mu_t}{s - t} \right| &\leq |\dot{\mu}_t| \limsup_{s \rightarrow t} \left( \int_{\mathfrak{G} \times \mathfrak{G}} H^2(x, y) d\sigma^{s \rightarrow t}(x, y) \right)^{1/2} \\ &\leq |\dot{\mu}_t| \cdot \|\text{lip}(\varphi)\|_{L^2(\mu_t)}. \end{aligned} \quad (17)$$

*Step 2.* Take  $\Phi \in \mathcal{T}$ . Using dominated convergence, Fatou's Lemma, and (17), we obtain

$$\begin{aligned} \left| \int_Q \frac{d}{dt} \Phi(x, t) d\boldsymbol{\mu}(x, t) \right| &= \lim_{h \searrow 0} \left| \frac{1}{h} \int_Q \Phi(x, t - h) - \Phi(x, t) d\boldsymbol{\mu}(x, t) \right| \\ &= \lim_{h \searrow 0} \left| \frac{1}{h} \int_0^T \left( \int_{\mathfrak{G}} \Phi(x, t) d\mu_{t+h}(x) - \int_{\mathfrak{G}} \Phi(x, t) d\mu_t(x) \right) dt \right| \\ &\leq \int_0^T |\dot{\mu}_t| \cdot \|\text{lip}_x(\Phi)(\cdot, t)\|_{L^2(\mu_t)} dt \\ &\leq \left( \int_0^T |\dot{\mu}_t|^2 dt \right)^{1/2} \left( \int_Q |\text{lip}_x(\Phi)(x, t)|^2 d\boldsymbol{\mu}(x, t) \right)^{1/2}. \end{aligned} \quad (18)$$

Since  $\int_Q |\text{lip}_x(\Phi)(x, t)|^2 d\boldsymbol{\mu}(x, t) \leq \int_{\bar{Q}} |\nabla \Phi(x, t)|^2 d\bar{\boldsymbol{\mu}}(x, t)$ , we infer that  $L$  is well-defined and extends to a bounded linear functional on the closure of  $\mathcal{V}$  in  $L^2(\bar{Q}, \bar{\boldsymbol{\mu}})$  with  $\|L\|^2 \leq \int_0^T |\dot{\mu}_t|^2 dt$ .

The Riesz representation theorem yields the existence of a vectorfield  $\boldsymbol{v}$  in  $\bar{\mathcal{V}} \subseteq L^2(\bar{Q}, \bar{\boldsymbol{\mu}})$  such that  $\|\boldsymbol{v}\|_{L^2(\bar{\boldsymbol{\mu}})}^2 \leq \int_0^T |\dot{\mu}_t|^2 dt$  and

$$- \int_0^T \dot{a}(t) \int_{\mathfrak{G}} \varphi(x) d\mu_t(x) dt = L(a \otimes \nabla \varphi) = \int_0^T a(t) \int_{\bar{\mathfrak{E}}} \nabla \varphi(x) v_t(x) d\bar{\boldsymbol{\mu}}_t(x) dt \quad (19)$$

for  $v_t := \boldsymbol{v}(t, \cdot)$  and all  $a \in C_c^1(0, T)$  and  $\varphi \in C(\mathfrak{G}) \cap C^1(\bar{\mathfrak{E}})$ .

Lemma 4.5 implies that for a.e.  $t$  the momentum field  $J_t := v_t \cdot \bar{\boldsymbol{\mu}}_t$  does not give mass to any boundary point in  $\bar{\mathfrak{E}}$ . Consequently, the spatial domain of integration on the right-hand side of (19) may be restricted to  $\mathfrak{E}$ .

In particular, (19) implies that  $t \mapsto \int_{\mathfrak{E}} \nabla \varphi \cdot v_t d\mu_t$  is a distributional derivative for  $t \mapsto \int_{\mathfrak{G}} \varphi d\mu_t$ . Since the latter function is absolutely continuous and, therefore, belongs to the Sobolev space  $W^{1,1}(0, T)$ , we obtain

$$\frac{d}{dt} \int_{\mathfrak{G}} \varphi d\mu_t = \int_{\mathfrak{E}} \nabla \varphi \cdot v_t d\mu_t \quad \text{for a.e. } t \in (0, T). \quad (20)$$

We conclude that  $(\mu_t, v_t)_{t \in (0, T)}$  solves the continuity equation in the weak sense.

*Step 4.* It remains to verify (by a standard argument) the inequality relating the  $L^2(\mu_t)$ -norm of the vectorfield  $v_t$  to the metric differential of  $\mu_t$ .

To gain insight of this, fix a sequence  $(\boldsymbol{\varpi}_i)_{i \in \mathbb{N}}$  of functions  $\boldsymbol{\varpi}_i \in \mathcal{V}$  converging to  $\boldsymbol{v}$  in  $L^2(\bar{\boldsymbol{\mu}})$  as  $i \rightarrow \infty$ . Then for every compact interval  $I \subseteq (0, T)$  and  $a \in C^1(0, T)$

satisfying  $0 \leq a \leq 1$  and  $\text{supp } a = I$ , we have

$$\begin{aligned} \int_Q a(t) |\mathbf{v}(x, t)|^2 d\boldsymbol{\mu}(x, t) &= \lim_{i \rightarrow \infty} \int_Q a(t) \boldsymbol{\varpi}_i(x, t) \mathbf{v}(x, t) d\boldsymbol{\mu}(x, t) \\ &= \lim_{i \rightarrow \infty} L(a\boldsymbol{\varpi}_i) \leq \left( \int_0^T \mathbb{1}_I |\dot{\mu}_t|^2 dt \right)^{1/2} \lim_{i \rightarrow \infty} \left( \int_Q \mathbb{1}_I |\boldsymbol{\varpi}_i|^2 d\boldsymbol{\mu} \right)^{1/2} \\ &= \left( \int_0^T \mathbb{1}_I |\dot{\mu}_t|^2 dt \right)^{1/2} \left( \int_Q \mathbb{1}_I |v|^2 d\boldsymbol{\mu} \right)^{1/2}. \end{aligned}$$

Letting  $\|a - \mathbb{1}_I\|_\infty \rightarrow 0$ , this inequality implies

$$\int_I \int_{\mathbb{E}} |v_t|^2 d\mu_t dt \leq \int_I |\dot{\mu}_t|^2 dt.$$

Since  $I \subseteq (0, T)$  is arbitrary, this implies that  $\|v_t\|_{L^2(\mu_t)} \leq |\dot{\mu}_t|$  for a.e.  $t \in (0, T)$ .  $\square$

**4.1. Regularisation of solutions to the continuity equation.** For the proof of the second part of Theorem 4.7, we need to make use of the Hopf-Lax formula on abstract metric spaces and its relation to the dual problem of optimal transportation.

**Definition 4.8** (Hopf-Lax formula). For a real-valued function  $f$  on a Polish space  $(X, d)$ , we define  $Q_t f : X \rightarrow \mathbb{R} \cup \{-\infty\}$  by

$$Q_t f(x) := \inf_{y \in X} f(y) + \frac{1}{2t} d^2(x, y)$$

for all  $t > 0$  as well as  $Q_0 f := f$ .

The Hopf-Lax formula satisfies the following basic properties which were proven in [AGS14].

**Proposition 4.9** (Properties of the Hopf-Lax semigroup). *For any Lipschitz function  $f : X \rightarrow \mathbb{R}$  the following statements hold:*

- (i) For every  $t \geq 0$ , we have  $\text{Lip}(Q_t f) \leq 2\text{Lip}(f)$ .
- (ii) For every  $x \in X$ , the mapping  $t \mapsto Q_t f(x)$  is continuous on  $\mathbb{R}_0^+$ , locally semi-concave on  $\mathbb{R}^+$  and the inequality

$$\frac{d}{dt} Q_t f(x) + \frac{1}{2} \text{lip}(Q_t f)^2(x) \leq 0 \tag{21}$$

holds for  $t \geq 0$  up to a countable number of exceptions.

- (iii) The mapping  $(t, x) \mapsto \text{lip}(Q_t f)(x)$  is upper semicontinuous on  $\mathbb{R}^+ \times X$ .

In addition to the Hopf-Lax formula, we also need to regularise the solutions of the continuity equation. To this aim, we adapt the standard procedure widely used for regularisation for solutions of measures on bounded Euclidean domains to the settings of metric graphs.

The node conditions in Definition 4.1.iv imply that we usually cannot expect the momentum field  $J_t = v_t \cdot \mu_t$  of any solution of the continuity equation  $(\mu_t, v_t)_{t \in (0, T)}$  to be continuous at nodes, regardless of regularity of  $\mu_t$  and  $v_t$  in the interior of each edge.

Below, we develop a regularisation scheme for solutions of the continuity equation under the following assumption on the regularisation parameter  $\varepsilon$ .

**Assumption 4.10.** In this section  $\varepsilon > 0$  is chosen small enough such that  $2\varepsilon$  is a strict lower bound for both the length of any edge in  $E$  and the injectivity radius at any point in  $\mathfrak{G}$ .



Recall that on a metric graph The injectivity radius corresponds to half the total length of the shortest embedded cycle.

This means that for any two points  $x, y \in \mathfrak{G}$  of distance less than  $2\varepsilon$ , the geodesic connecting  $x$  to  $y$  is uniquely defined.

We consider the supergraph  $\mathfrak{G}_{\text{ext}} \supseteq \mathfrak{G}$  defined by adjoining an additional auxiliary edge  $e_v^{\text{ext}}$  of length  $\varepsilon$  to each node  $v \in V$  (see Figure 3). The corresponding set of metric edges will be denoted by  $\mathfrak{L}_{\text{ext}} \supset \mathfrak{L}$ . For the purpose of this definition below, we identify each edge  $e = (e_{\text{init}}, e_{\text{term}}) \in E$  with the interval  $(-\frac{m_e}{2}, \frac{m_e}{2})$  instead of  $(0, m_e)$ . Again, the nodes  $e_{\text{init}}, e_{\text{term}} \in V$  correspond to the respective end-points of the interval. For each fixed edge  $e \in E$  we identify the auxiliary edges  $e_{e_{\text{init}}}^{\text{ext}}$  and  $e_{e_{\text{term}}}^{\text{ext}}$  with the intervals  $(-\frac{m_e}{2} - 2\varepsilon, -\frac{m_e}{2})$  and  $(\frac{m_e}{2}, \frac{m_e}{2} + 2\varepsilon)$ , respectively.

We next define a regularisation procedure for functions based on averaging. To obtain a continuous function, it will be crucial to use non-centred averages. For this purpose, we set  $\alpha_e^\varepsilon := (m_e + 2\varepsilon)/m_e$  and  $\alpha^\varepsilon(x) := \alpha_e^\varepsilon$ , whenever  $x$  is a point on the metric edge  $e$  in  $\mathfrak{L}$ .

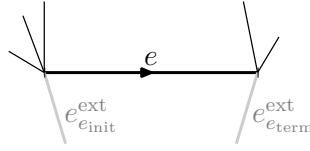


FIGURE 3. The construction of the supergraph  $\mathfrak{G}_{\text{ext}}$  by means of adjoining an additional leaf at every node in  $V$ .

**Definition 4.11** (Regularisation of functions). For  $\varphi \in L^1(\mathfrak{G}_{\text{ext}})$ , we define  $\varphi^\varepsilon : \mathfrak{G} \rightarrow \mathbb{R}$  by

$$\varphi^\varepsilon(x) := \frac{1}{2\varepsilon} \int_{\alpha_e^\varepsilon x - \varepsilon}^{\alpha_e^\varepsilon x + \varepsilon} \varphi(y) dy \quad \text{for } x \in [-\frac{m_e}{2}, \frac{m_e}{2}]. \quad (22)$$

Note that the value of  $\varphi^\varepsilon$  in the nodes does not depend on the choice of the edge, so that  $\varphi^\varepsilon$  indeed defines a function on  $\mathfrak{G}$ . We collect some basic properties of this regularisation in the following result.

**Proposition 4.12.** *The following properties hold for every  $\varepsilon > 0$  be sufficiently small:*

(i) *Regularising effect: For any  $\varphi \in C(\mathfrak{G}_{\text{ext}})$  we have  $\varphi^\varepsilon \in C(\mathfrak{G}) \cap C^1(\bar{\mathfrak{E}})$  and*

$$\nabla \varphi^\varepsilon(y) = \frac{\alpha_e^\varepsilon}{2\varepsilon} (\varphi(\alpha_e^\varepsilon y + \varepsilon) - \varphi(\alpha_e^\varepsilon y - \varepsilon)) \quad (23)$$

*for  $y \in [-m_e/2, m_e/2]$ .*

(ii) *If  $\varphi$  belongs to  $C(\mathfrak{G}_{\text{ext}})$ , then  $\varphi^\varepsilon$  converges uniformly to  $\varphi|_{\mathfrak{G}}$  as  $\varepsilon \searrow 0$ .*

*Proof.* The claim in (i) follows by a direct computation; the one in (ii) follows using the uniform continuity of  $\varphi$  on  $\mathfrak{G}_{\text{ext}}$ .  $\square$

As a first application of the regularisation procedure above, we state a useful lemma.

**Lemma 4.13** (Weak continuity). *Let  $(\rho_t, J_t)_{t \in (0, T)}$  be a weak solution to the continuity equation on  $\mathfrak{G}$ . Then  $t \mapsto \int_{\mathfrak{G}} \varphi d\mu_t$  is continuous for every  $\varphi \in C(\mathfrak{G})$ .*

*Proof.* Take a continuous extension of  $\varphi$  to  $\mathfrak{G}_{\text{ext}}$  and define  $\varphi^\varepsilon$  accordingly. Proposition 4.12.ii then implies that  $\varphi^\varepsilon$  converges uniformly to  $\varphi$  on  $\mathfrak{G}$  as  $\varepsilon \searrow 0$ . As a result, the function  $t \mapsto \int_{\mathfrak{G}} \varphi^\varepsilon d\mu_t$  converges uniformly to  $t \mapsto \int_{\mathfrak{G}} \varphi d\mu_t$ . Since  $\varphi^\varepsilon$  belongs to

$C(\mathfrak{G}) \cap C^1(\overline{\mathfrak{E}})$  by Proposition 4.12.i, we conclude that the mapping  $t \mapsto \int_{\mathfrak{G}} \varphi d\mu_t$  is continuous, being a uniform limit of continuous functions.  $\square$

By duality, we obtain a natural regularisation for measures.

**Definition 4.14** (Regularisation of measures). For  $\mu \in \mathcal{M}(\mathfrak{G})$  we define  $\mu^\varepsilon \in \mathcal{M}(\mathfrak{G}_{\text{ext}})$  by

$$\int_{\mathfrak{G}_{\text{ext}}} \varphi d\mu^\varepsilon := \int_{\mathfrak{G}} \varphi^\varepsilon d\mu. \quad (24)$$

It is readily checked that the right-hand side defines a positive linear functional on  $C(\mathfrak{G}_{\text{ext}})$ , so that  $\mu^\varepsilon$  is indeed a well-defined measure.

**Proposition 4.15.** *The following properties hold for any  $\varepsilon > 0$ :*

- (i) *Mass preservation:*  $\mu^\varepsilon(\mathfrak{G}_{\text{ext}}) = \mu(\mathfrak{G})$  for any  $\mu \in \mathcal{M}(\mathfrak{G})$ .
- (ii) *Regularising effect:* For any  $\mu \in \mathcal{P}(\mathfrak{G})$ , the measure  $\mu^\varepsilon$  is absolutely continuous with respect to  $\lambda$  with density

$$\rho^\varepsilon(x) = \begin{cases} \frac{1}{2\varepsilon} \mu(e \cap I_e(x)), & \text{for } x \text{ on } e \text{ in } \mathfrak{E}, \\ \frac{1}{2\varepsilon} \left( \mathbb{1}_{\{d(x,w) \leq 2\varepsilon\}} \mu(\{w\}) + \sum_{e \in E: w \in e} \mu(e \cap I_e(x)) \right) & \text{for } x \text{ on } e_w^{\text{ext}}, w \in V, \end{cases}$$

where

$$I_e(x) := \left( \frac{x - \varepsilon}{a_e^\varepsilon}, \frac{x + \varepsilon}{a_e^\varepsilon} \right).$$

In particular,  $\rho^\varepsilon(x) \leq \frac{1}{2\varepsilon}$  for all  $x \in \mathfrak{G}_{\text{ext}}$ .

- (iii) *Kinetic energy bound:* For  $\mu \in \mathcal{P}(\mathfrak{G})$  and  $v \in L^2(\mu)$ , define  $J = v \cdot \mu \in \mathcal{M}(\mathfrak{G})$ . Consider the regularised measures  $\mu^\varepsilon \in \mathcal{P}(\mathfrak{G}_{\text{ext}})$  and  $J^\varepsilon \in \mathcal{M}(\mathfrak{G}_{\text{ext}})$ . Then  $J^\varepsilon = v^\varepsilon \cdot \mu^\varepsilon$  for some  $v^\varepsilon \in L^2(\mu^\varepsilon)$  and we have

$$\int_{\mathfrak{E}_{\text{ext}}} |v^\varepsilon|^2 d\mu^\varepsilon \leq \int_{\mathfrak{E}} |v|^2 d\mu. \quad (25)$$

- (iv) For any  $\mu \in \mathcal{P}(\mathfrak{G})$  we have weak convergence  $\mu^\varepsilon \rightharpoonup \mu$  in  $\mathcal{P}(\mathfrak{G}_{\text{ext}})$  as  $\varepsilon \rightarrow 0$ .
- (v) For any  $\mu \in \mathcal{P}(\mathfrak{G})$ , absolutely continuous with respect to  $\lambda$  such that  $\mu = \rho \cdot \lambda$ , we have convergence  $\rho^\varepsilon \rightarrow \rho$  in  $L^1(\mathfrak{G}_{\text{ext}})$  as  $\varepsilon \rightarrow 0$ .
- (vi) Let  $(\mu_t, v_t)_{t \in (0, T)}$  be a weak solution to the continuity equation (14). Then the regularised pair  $(\mu_t^\varepsilon, \alpha^\varepsilon v_t^\varepsilon)_{t \in (0, T)}$ , where the vectorfield  $v_t^\varepsilon$  is defined as in (iii) above, satisfies a weak continuity equation on  $\mathfrak{G}_{\text{ext}}$  in the following sense: For every absolutely continuous function  $\varphi$  on  $\mathfrak{G}_{\text{ext}}$ , the function  $t \mapsto \int_{\mathfrak{G}_{\text{ext}}} \varphi d\mu_t^\varepsilon$  is absolutely continuous and for a.e.  $t \in (0, T)$  we have

$$\frac{d}{dt} \int_{\mathfrak{G}_{\text{ext}}} \varphi d\mu_t^\varepsilon = \int_{\mathfrak{E}_{\text{ext}}} \nabla \varphi \cdot (\alpha^\varepsilon v_t^\varepsilon) d\mu_t^\varepsilon. \quad (26)$$

In order to prove (iii), we will make use of the so-called Benamou-Brenier functional (cf. e.g. Section 5.3.1 in [San15] for corresponding results in a Euclidean setting).

**Definition 4.16.** Denote the set  $K_2 := \{(a, b) \in \mathbb{R} \times \mathbb{R} : a + b^2/2 \leq 0\}$ . The Benamou-Brenier functional  $\mathcal{B}_2 : \mathcal{M}(\mathfrak{G}) \times \mathcal{M}(\mathfrak{E}) \rightarrow \mathbb{R} \cup \{+\infty\}$  is defined by

$$\mathcal{B}_2(\mu, J) := \sup_{(a, b) \in C_b(\mathfrak{G}, K_2)} \left\{ \int_{\mathfrak{G}} a d\mu + \int_{\mathfrak{E}} b dJ \right\}.$$

**Lemma 4.17.** *The following statements hold:*

(i) The pointwise supremum over the set  $K_{\mathfrak{G}}$  is characterised by the identity

$$\sup_{(a,b) \in K_2} \{az + by\} = \begin{cases} \frac{|y|^2}{2z} & \text{if } z > 0, \\ 0 & \text{if } z = 0 \text{ and } y = 0, \\ +\infty & \text{otherwise.} \end{cases} \quad (27)$$

(ii) We have

$$\mathcal{B}_2(\mu, J) = \sup_{(a,b) \in L^\infty(\mathfrak{G}, K_2)} \left\{ \int_{\mathfrak{G}} a \, d\mu + \int_{\mathfrak{E}} b \, dJ \right\}, \quad (28)$$

where  $L^\infty(\mathfrak{G}, K_2)$  denotes (by abuse of notation) the set of all bounded measurable functions  $a, b : \mathfrak{G} \rightarrow \mathbb{R}$  such that  $a + b^2/2 \leq 0$ .

(iii) The functional  $\mathcal{B}_2$  is convex and lower semicontinuous with respect to the topology of weak convergence on  $\mathcal{M}(\mathfrak{G}) \times \mathcal{M}(\mathfrak{E})$ .

(iv) If  $\mu$  is non-negative such that  $J \ll \mu$ , we may write  $J = v \cdot \mu$  and

$$\mathcal{B}_2(\mu, J) = \frac{1}{2} \int_{\mathfrak{E}} |v|^2 \, d\mu. \quad (29)$$

Otherwise, we have  $\mathcal{B}_2(\mu, J) = +\infty$ .

*Proof.* For (i) we refer to the proof of Lemma 5.17 in [San15].

Regarding (ii), we note that the right-hand side of (28) is clearly bounded from above by  $\mathcal{B}_2(\mu, J)$ . In order to prove equality of both sides, we show that any pair of bounded measurable functions  $a, b : \mathfrak{G} \rightarrow \mathbb{R}$  satisfying  $a + b^2/2 \leq 0$  can be approximated by bounded continuous functions in a suitable way. Indeed, we may appeal to Lusin's theorem (see e.g. Theorem 7.1.13 in [Bog07]) to obtain functions  $a_\delta, b_\delta \in C_b(\mathfrak{G}, K_2)$  such that

$$\mu(\{a \neq a_\delta\}) \leq \frac{\delta}{2}, \quad \sup |a_\delta| \leq \sup |a| \quad \text{and} \quad |J|(\{b \neq b_\delta\}) \leq \frac{\delta}{2}, \quad \sup |b_\delta| \leq \sup |b|.$$

Define  $\tilde{a}_\delta := \min\{a_\delta, -|b_\delta|^2/2\}$  such that the inequality  $\tilde{a}_\delta + b_\delta^2/2 \leq 0$  is satisfied. Hence, the pair  $(\tilde{a}_\delta, b_\delta)$  is admissible for the supremum of the right-hand side of (28).

Since  $\int_{\mathfrak{G}} \tilde{a}_\delta \, d\mu + \int_{\mathfrak{E}} b_\delta \, dJ$  converges to  $\int_{\mathfrak{G}} a \, d\mu + \int_{\mathfrak{E}} b \, dJ$  as  $\delta \searrow 0$ , we infer that equality holds in (28).

Now the convexity and lower semicontinuity in (iii) are an immediate consequence of the definition of  $\mathcal{B}_2$  as supremum over linear functionals.

It remains to prove (iv): At first, assume that  $\mu$  is non-negative such that  $E \ll \mu$  with  $J = v \cdot \mu$ . Then we may infer the existence of a so-called lattice supremum in  $\mathcal{F} := \{a + bv : (a, b) \in L^\infty(\mathfrak{G}, K_2)\}$ ; that is a measurable function  $\vee \mathcal{F} : \mathfrak{G} \rightarrow \mathbb{R}$  satisfying

$$\vee \mathcal{F}(x) = \sup_{f \in \mathcal{F}} \{f(x)\} \quad \mu\text{-a.e. } x \in \mathfrak{G},$$

(cf. e.g. Theorem 5.7.1 in [Bog07] for a general existence result). Note that the pointwise supremum on the right-hand side of this equation need not be a measurable function in  $x$ .

Taking (28) and (27) into account, the considerations above yield

$$\mathcal{B}_2(\mu, J) = \sup_{(a,b) \in L^\infty(\mathfrak{G}, K_2)} \left\{ \int_{\mathfrak{G}} a + bv \, d\mu \right\} = \int_{\mathfrak{G}} \vee \mathcal{F} \, d\mu = \frac{1}{2} \int_{\mathfrak{E}} |v|^2 \, d\mu,$$

where we used that  $\mathcal{B}_2(\mu|_V, J) \equiv 0$  to pass from the first to the second equality above.

Finally, we show that  $\mathcal{B}_2(\mu, J) = +\infty$  whenever the above assumptions are not met. Indeed, if there exists a Borel set  $A \subseteq \mathfrak{G}$  such that  $\mu(A) < 0$ , then we may choose  $a = k\mathbb{1}_A$  and  $b \equiv 0$  for any  $k \leq 0$ . Then the resulting bound  $\mathcal{B}_2(\mu, J) \geq k\mu(A)$  gives the claim as  $k \rightarrow -\infty$ .

In the remaining case, the signed measure  $J$  is not absolutely continuous with respect to  $\mu$ , i.e. there exists a  $\mu$ -null set  $A \subseteq \mathfrak{G}$  such that  $E(A) \neq 0$ . Then we may take  $a = -\frac{k^2}{2}\mathbb{1}_A$  and  $b = k\mathbb{1}_A$  for any  $k \in \mathbb{R}$ . We infer  $\mathcal{B}_2(\mu, J) \geq -\frac{k^2}{2}J(A) \rightarrow +\infty$  as  $k \rightarrow \infty$ , which allows us to conclude.  $\square$

*Proof of Proposition 4.15.* The claims in (i) and (ii) follow readily from the definitions.

To prove (iii), we first note that  $J^\varepsilon \ll \mu^\varepsilon$  implies the existence of a vectorfield  $v \in L^2(\mu^\varepsilon)$  such that  $J^\varepsilon = v^\varepsilon \cdot \mu^\varepsilon$ .

We know from the results stated in Lemma 4.17 that the  $L^2$ -norm of the vectorfield  $v$  is related to the so-called *Benamou-Brenier functional* by means of the identity

$$\frac{1}{2} \int_{\mathfrak{E}} |v|^2 d\mu = \sup \left\{ \int_{\mathfrak{G}} a d\mu + \int_{\mathfrak{E}} b dJ \right\}, \quad (30)$$

where the supremum is over all bounded measurable functions  $a, b : \mathfrak{G} \rightarrow \mathbb{R}$  such that  $a + b^2/2 \leq 0$ .

For any two such  $a$  and  $b$  defined on  $\mathfrak{G}_{\text{ext}}$ , we consider regularised functions  $a^\varepsilon$  and  $b^\varepsilon$  as done for a function  $\varphi$  in (22). Using Jensen's inequality and the fact that the regularisation is linear and positivity-preserving, we obtain

$$a^\varepsilon(x) + \frac{1}{2}|b^\varepsilon(x)|^2 \leq \left(a + \frac{1}{2}|b|^2\right)^\varepsilon(x) \leq 0 \quad \forall x \in \mathfrak{G}$$

Consequently, the functions  $a^\varepsilon$  and  $b^\varepsilon$  belong to the admissible set for the supremum on the right-hand side of (30); thus

$$\int_{\mathfrak{G}} a^\varepsilon d\mu + \int_{\mathfrak{E}} b^\varepsilon dJ \leq \frac{1}{2} \int_{\mathfrak{E}} |v|^2 d\mu. \quad (31)$$

At the same time, the identity

$$\int_{\mathfrak{G}_{\text{ext}}} a d\mu^\varepsilon + \int_{\mathfrak{E}_{\text{ext}}} b dJ^\varepsilon = \int_{\mathfrak{G}} a^\varepsilon d\mu + \int_{\mathfrak{E}} b^\varepsilon dJ \quad (32)$$

allows us to pass to supremum over all admissible functions  $a$  and  $b$  in (31) to arrive at (25).

(iv) is a direct consequence of the duality formula (24), together with the uniform convergence of  $(\varphi^\varepsilon)_{\varepsilon>0}$  on  $\mathfrak{G}$ , established in Proposition 4.12.ii.

The claim in (v) follows from the representation of the regularised densities  $\rho^\varepsilon$  as shown in Proposition 4.15.ii above, together with an  $L^p$ -version of the Lebesgue differentiation theorem (see e.g. Theorem 1.34 in [EG15]), applied to each metric edge in  $\mathfrak{E}_{\text{ext}}$  separately.

It remains to prove (vi). Since  $\varphi$  is absolutely continuous,  $\varphi$  is differentiable a.e. in  $\mathfrak{E}_{\text{ext}}$ . Moreover, we recall from Proposition 4.12.i that the regularised function  $\varphi^\varepsilon$  actually belongs to  $C(\mathfrak{G}) \cap C^1(\mathfrak{E})$  and satisfies the identity

$$\nabla \varphi^\varepsilon(x) = \alpha^\varepsilon(x)(\nabla \varphi)^\varepsilon(x) \quad \forall x \in \mathfrak{E}. \quad (33)$$

In particular, we may test the pair  $(\mu_t, v_t)_{t \in (0, T)}$  against  $\varphi^\varepsilon$ , resulting in the claim as a consequence of the computation

$$\frac{d}{dt} \int_{\mathfrak{G}_{\text{ext}}} \varphi d\mu_t^\varepsilon = \frac{d}{dt} \int_{\mathfrak{G}} \varphi^\varepsilon d\mu_t = \int_{\mathfrak{E}} \nabla \varphi^\varepsilon \cdot v_t d\mu_t = \int_{\mathfrak{E}_{\text{ext}}} \nabla \varphi \cdot (\alpha^\varepsilon v_t^\varepsilon) d\mu_t^\varepsilon, \quad (34)$$

where we used that  $\alpha^\varepsilon$  is constant on each metric edge in  $\mathfrak{E}$  in the rightmost equality above.  $\square$

Now we are ready to prove the second part of Theorem 4.7, adapting an approach from [GH15]. In that work the authors prove an analogous result in more general metric measure spaces, but they require a stronger assumption on the measures (namely, a uniform bound on their densities with respect to the reference measure). Here we consider more general measures as well using the regularisation procedure described above.

*Proof of (i) in Theorem 4.7.* For simplicity, we consider only the case  $T = 1$  as the proof for arbitrary  $T > 0$  follows along the very same lines below.

The main step of the proof is to show that

$$W_2^2(\mu_0, \mu_1) \leq \int_0^1 \|v_r\|_{L^2(\mu_r)}^2 dr. \quad (35)$$

From there, a simple reparametrisation argument (see Lemma 1.1.4 and Lemma 8.1.3 in [AGS08]) yields

$$W_2^2(\mu_t, \mu_s) \leq \frac{1}{|s-t|} \int_s^t \|v_r\|_{L^2(\mu_r)}^2 dr$$

for all  $0 \leq s < t \leq 1$ , which implies the absolute continuity of the curve  $(\mu_t)_{t \in (0, 1)}$  in  $W_2(\mathfrak{G})$  as well as the desired bound  $|\dot{\mu}|(t) \leq \|v_t\|_{L^2(\mu_t)}$  for every Lebesgue point  $t \in (0, 1)$  of the mapping  $t \mapsto \|v_t\|_{L^2(\mu_t)}^2$ .

Thus, we have to show (35): To this aim, we will work on a supergraph  $\mathfrak{G}_{\text{ext}} \supseteq \mathfrak{G}$  satisfying Assumptions 4.10 for  $\varepsilon > 0$  small enough.

By Kantorovich duality (Proposition 2.8), there exists  $\varphi \in C(\mathfrak{G})$  satisfying

$$\frac{1}{2} W_2^2(\mu_0, \mu_1) = \int_{\mathfrak{G}} Q_1 \varphi d\mu_1 - \int_{\mathfrak{G}} \varphi d\mu_0. \quad (36)$$

We consider continuous extensions of  $\varphi$  and  $Q_1 \varphi$  to  $\mathfrak{G}_{\text{ext}}$ , both constant on each auxiliary metric edge in  $\bar{\mathfrak{E}}_{\text{ext}}$ . In particular,  $\varphi$  and  $Q_1 \varphi$  are continuous on  $\mathfrak{G}_{\text{ext}}$ .

Set  $J_t := v_t \cdot \mu_t$  and consider a regularised pair  $(\mu_t^\varepsilon, J_t^\varepsilon)_{t \in (0, 1)}$  as defined by (24). We write

$$\begin{aligned} \int_{\mathfrak{G}_{\text{ext}}} Q_1 \varphi d\mu_1^\varepsilon - \int_{\mathfrak{G}_{\text{ext}}} \varphi d\mu_0^\varepsilon &= \sum_{i=0}^{n-1} \left( \int_{\mathfrak{G}_{\text{ext}}} Q_{(i+1)/n} \varphi - Q_{i/n} \varphi d\mu_{(i+1)/n}^\varepsilon \right. \\ &\quad \left. + \int_{\mathfrak{G}_{\text{ext}}} Q_{i/n} \varphi d(\mu_{(i+1)/n}^\varepsilon - \mu_{i/n}^\varepsilon) \right), \end{aligned} \quad (37)$$

and bound the two terms on the right-hand side separately.

*Bound 1.* To estimate the first term on the right-hand side of (37), we use (21) to obtain

$$\begin{aligned}
\sum_{i=0}^{n-1} \int_{\mathfrak{G}_{\text{ext}}} Q_{(i+1)/n} \varphi - Q_{i/n} \varphi \, d\mu_{(i+1)/n}^\varepsilon &\leq -\frac{1}{2} \sum_{i=0}^{n-1} \int_{\mathfrak{G}_{\text{ext}}} \int_{i/n}^{(i+1)/n} \text{lip}^2(Q_t \varphi) \, dt \, d\mu_{(i+1)/n}^\varepsilon \\
&= -\frac{1}{2} \int_{\mathfrak{G}_{\text{ext}} \times (0,1)} \text{lip}^2(Q_t \varphi)(x) \, d\mu_n^\varepsilon(x, t),
\end{aligned} \tag{38}$$

where the measures  $\mu_n^\varepsilon := \sum_{i=0}^{n-1} \mu_{(i+1)/n}^\varepsilon \otimes \mathcal{L}^1|_{(i/n, (i+1)/n)}$  are defined on  $\mathfrak{G}_{\text{ext}} \times (0, 1)$ .

To show weak convergence of the sequence  $(\mu_n^\varepsilon)_{n \in \mathbb{N}}$ , we take  $\psi \in C(\mathfrak{G}_{\text{ext}} \times [0, 1])$ . Note that  $t \mapsto \mu_t$  is weakly continuous by Lemma 4.13, hence  $t \mapsto \mu_t^\varepsilon$  is weakly continuous as well. Consequently,  $\int_{\mathfrak{G}_{\text{ext}}} \psi(\cdot, t) \, d\mu_{\lfloor tn \rfloor/n}^\varepsilon \rightarrow \int_{\mathfrak{G}_{\text{ext}}} \psi(\cdot, t) \, d\mu_t^\varepsilon$  for every fixed  $t$ . Integrating in time over  $(0, 1)$ , we infer, using dominated convergence, that  $\mu_n^\varepsilon$  converges weakly to  $\mu^\varepsilon := \int_0^1 \mu_t^\varepsilon \otimes \delta_t \, dt$  as  $n \rightarrow \infty$ .

As  $\text{lip}^2(Q_t \varphi)$  is not necessarily continuous, an additional argument is required to pass to the limit in (38). For this purpose, we observe that Proposition 4.15.ii yields  $\mu_n^\varepsilon \ll \lambda \otimes \mathcal{L}^1$  with a density  $\rho_n^\varepsilon(x, t) \leq 1/(2\varepsilon)$  for  $x \in \mathfrak{G}_{\text{ext}}$  and  $t \in (0, 1)$ . In particular, the family  $(\rho_n^\varepsilon)_{n \in \mathbb{N}}$  is uniformly integrable with respect to  $\lambda \otimes \mathcal{L}^1$ . Consequently, the Dunford-Pettis theorem (see e.g. Theorem 4.7.18 in [Bog07]) implies that  $(\rho_n^\varepsilon)_{n \in \mathbb{N}}$  has weak\*-compact closure in  $L^1(\mathfrak{G}_{\text{ext}} \times (0, 1))$ . Since  $\text{lip}^2(Q_t \varphi)$  is bounded, we may, therefore, pass to the limit in (38) and infer that

$$\begin{aligned}
\limsup_{n \rightarrow \infty} \sum_{i=0}^{n-1} \int_{\mathfrak{G}_{\text{ext}}} Q_{(i+1)/n} \varphi - Q_{i/n} \varphi \, d\mu_{(i+1)/n}^\varepsilon &\leq -\frac{1}{2} \int_{\mathfrak{G}_{\text{ext}} \times (0,1)} \text{lip}^2(Q_t \varphi)(x) \, d\mu^\varepsilon(x, t) \\
&= -\frac{1}{2} \int_0^1 \int_{\mathfrak{E}_{\text{ext}}} \text{lip}^2(Q_t \varphi) \, d\mu_t^\varepsilon \, dt,
\end{aligned} \tag{39}$$

where we used that  $\mu_t^\varepsilon \ll \lambda$  on  $\mathfrak{G}_{\text{ext}}$  to remove the set of nodes  $V$  from the domain of integration.

*Bound 2.* To treat the second term in (37), take a Lipschitz function  $\varphi : \mathfrak{G} \rightarrow \mathbb{R}$ .

As  $(\mu_t)_{t \in (0,1)}$  belongs to a weak solution to the continuity equation and we know from Proposition 4.12.i that  $(Q_{i/n} \varphi)^\varepsilon$  belongs to  $C(\mathfrak{G}) \cap C^1(\bar{\mathfrak{E}})$ , we infer that the mapping  $t \mapsto \int_{\mathfrak{G}} (Q_{i/n} \varphi)^\varepsilon \, d\mu_t$  is absolutely continuous. Therefore,

$$\begin{aligned}
\sum_{i=0}^{n-1} \int_{\mathfrak{G}_{\text{ext}}} Q_{i/n} \varphi \, d(\mu_{(i+1)/n}^\varepsilon - \mu_{i/n}^\varepsilon) &= \sum_{i=0}^{n-1} \int_{\mathfrak{G}} (Q_{i/n} \varphi)^\varepsilon \, d(\mu_{(i+1)/n} - \mu_{i/n}) \\
&= \sum_{i=0}^{n-1} \int_{i/n}^{(i+1)/n} \left( \int_{\mathfrak{E}} \nabla(Q_{i/n} \varphi)^\varepsilon v_t \, d\mu_t \right) dt \\
&= \sum_{i=0}^{n-1} \int_{i/n}^{(i+1)/n} \left( \sum_{e \in E} \alpha_e^\varepsilon \int_e (\nabla Q_{i/n} \varphi)^\varepsilon v_t \, d\mu_t \right) dt \\
&= \sum_{i=0}^{n-1} \int_{i/n}^{(i+1)/n} \left( \sum_{e \in E} \alpha_e^\varepsilon \int_e \nabla Q_{i/n} \varphi \cdot v_t^\varepsilon \, d\mu_t^\varepsilon \right) dt \\
&\leq \frac{\alpha_{\max}^\varepsilon}{2} \sum_{i=0}^{n-1} \int_{i/n}^{(i+1)/n} \int_{\mathfrak{E}_{\text{ext}}} |\nabla Q_{i/n} \varphi|^2 \, d\mu_t^\varepsilon \, dt + \frac{\alpha_{\max}^\varepsilon}{2} \int_0^1 \int_{\mathfrak{E}_{\text{ext}}} |v_t^\varepsilon|^2 \, d\mu_t^\varepsilon \, dt,
\end{aligned} \tag{40}$$

where  $\alpha_{\max}^\varepsilon := \max_{e \in E} \alpha_e^\varepsilon$ .

By Proposition 4.9.iii, we have the bound  $\limsup_{n \rightarrow \infty} \text{lip}^2(Q_{\lfloor nt \rfloor / n} \varphi) \leq \text{lip}^2(Q_t \varphi)$ . As  $\varphi$  is Lipschitz continuous, (i) in the same proposition shows that  $\sup_{t,x} \text{lip}(Q_t \varphi)(x) < \infty$ . Thus, we may invoke Fatou's lemma to obtain

$$\limsup_{n \rightarrow \infty} \sum_{i=0}^{n-1} \int_{i/n}^{(i+1)/n} \int_{\mathbb{E}_{\text{ext}}} |\nabla Q_{i/n} \varphi|^2 d\mu_t^\varepsilon dt \leq \int_0^1 \int_{\mathbb{E}_{\text{ext}}} \text{lip}^2(Q_t \varphi) d\mu_t^\varepsilon dt.$$

Using this estimate together with Proposition 4.15.iii, we obtain

$$\begin{aligned} \limsup_{n \rightarrow \infty} \sum_{i=0}^{n-1} \int_{\mathbb{G}_{\text{ext}}} Q_{i/n} \varphi d(\mu_{(i+1)/n}^\varepsilon - \mu_{i/n}^\varepsilon) &\leq \frac{\alpha_{\max}^\varepsilon}{2} \int_0^1 \int_{\mathbb{G}_{\text{ext}}} \text{lip}^2(Q_t \varphi) d\mu_t^\varepsilon dt \\ &+ \frac{\alpha_{\max}^\varepsilon}{2} \int_0^1 \int_{\mathbb{E}} |v_t|^2 d\mu_t dt. \end{aligned} \quad (41)$$

*Combination of both bounds.* Recalling (37), we use (39) and (41) to obtain

$$\int_{\mathbb{G}_{\text{ext}}} Q_1 \varphi d\mu_1^\varepsilon - \int_{\mathbb{G}_{\text{ext}}} \varphi d\mu_0^\varepsilon \leq \frac{\alpha_{\max}^\varepsilon}{2} \int_0^1 \int_{\mathbb{E}} |v_t|^2 d\mu_t dt + \frac{1 - \alpha_{\max}^\varepsilon}{2} \int_{\mathbb{G}_{\text{ext}}} \int_0^1 \text{lip}^2(Q_t \varphi) d\mu_t^\varepsilon dt$$

Using Proposition 4.15(iv), the fact that  $\alpha_{\max}^\varepsilon \rightarrow 1$ , and the bound  $\sup_t \text{Lip}(Q_t \varphi) < \infty$ , we may pass to the limit to obtain

$$\int_{\mathbb{G}} Q_1 \varphi d\mu_1 - \int_{\mathbb{G}} \varphi d\mu_0 \leq \frac{1}{2} \int_0^1 \int_{\mathbb{E}} |v_t|^2 d\mu_t dt. \quad (42)$$

In view of (36), this yields the result.  $\square$

**Corollary 4.18** (Benamou–Brenier formula). *For any  $\mu, \nu \in \mathcal{P}(\mathbb{G})$ , we have*

$$W_2^2(\mu, \nu) = \min \left\{ \int_0^1 \int_{\mathbb{E}} |v_t|^2 d\mu_t dt \right\}, \quad (43)$$

where the minimum runs over all weak solutions to the continuity equation  $(\mu_t, v_t)_{t \in [0,1]}$  satisfying  $\mu_0 = \mu$  and  $\mu_1 = \nu$ .

*Proof.* As  $(\mathcal{P}(\mathbb{G}), W_2)$  is a geodesic space, we may write

$$W_2^2(\mu, \nu) = \min \left\{ \int_0^1 |\dot{\mu}|(t) dt \right\},$$

where the minimum is taken over all absolutely continuous curves  $(\mu_t)_{t \in [0,1]}$  connecting  $\mu$  to  $\nu$ . By Theorem 4.7, we may replace  $|\dot{\mu}|(t)$  with  $\|v_t\|_{L^2(\mu_t)}$  in the formula above, which allows us to conclude.  $\square$

**Proposition 4.19.** *For  $i \in \{1, 2\}$ , let  $(\mu_t^i, v_t^i)_{t \in (0, T)}$  be two solutions to the continuity equation on  $\mathbb{G}$  in the weak sense. Under the assumption that both  $(\mu_t^i)_{t \in (0, T)}$  are absolutely continuous curves in  $W_2(\mathbb{G})$  such that  $\mu_t^i \ll \lambda$  with uniformly bounded densities for all times  $t \in (0, T)$ , we have*

$$\frac{1}{2} \frac{d}{dt} W_2^2(\mu_t^1, \mu_t^2) = \int_{\mathbb{G}} \nabla \varphi_t \cdot v_t^1 d\mu_t^1 + \int_{\mathbb{G}} \nabla \psi_t \cdot v_t^2 d\mu_t^2 \quad \text{for a.e. } t \in (0, T),$$

where  $(\varphi_t, \psi_t)$  denotes any pair of Kantorovich potentials for the dual transport problem between  $\mu_t^1$  and  $\mu_t^2$  for the cost function  $\frac{1}{2} d^2(\cdot, \cdot)$  on  $\mathbb{G}$ .

For the proof we make use of the following lemma (see e.g. Lemma 2.3 in [DMM16] or Proposition 3.6 in [GH15]).

**Lemma 4.20.** *Let  $(\mu_t, v_t)_{t \in (0, T)}$  be a solution to the continuity equation such that  $t \mapsto \|v_t\|_{L^2(\mu_t)}$  belongs to  $L^1(0, T)$  and  $\mu_t^i \ll \lambda$  with uniformly bounded densities for all times  $t \in (0, T)$ . Then there exists a null set  $\mathcal{N} \subset (0, T)$  such that*

$$\frac{d}{dt} \int_{\mathfrak{G}} \varphi d\mu_t = \int_{\mathfrak{G}} \nabla \varphi \cdot v_t d\mu_t \quad \forall t \in (0, T) \setminus \mathcal{N}, \forall \varphi \in W^{1,2}(\mathfrak{G}). \quad (44)$$

*Proof.* For every time  $t \in (0, T)$ , denote by  $L_t$  the linear functional on  $W^{1,2}(\mathfrak{G})$  given by the right-hand side of (44), i.e.

$$L_t(\varphi) := \int_{\mathfrak{G}} \nabla \varphi \cdot v_t d\mu_t \quad \forall \varphi \in W^{1,2}(\mathfrak{G}).$$

By definition of  $L_t$  and Hölder's inequality, we have the bound  $\|L_t\| \leq \|v_t\|_{L^2(\mu_t)}$ , which is finite for a.e.  $t \in (0, T)$ . Fix a countable dense family  $\{\varphi_n\}_{n \in \mathbb{N}}$  of functions  $\varphi_n \in C(\mathfrak{G}) \cap C^1(\bar{\mathfrak{E}})$  in  $W^{1,2}(\mathfrak{G})$ .

For every  $n \in \mathbb{N}$ , denote by  $I_n$  the set of Lebesgue points of the mapping  $t \mapsto L_t(\varphi_n)$ . Then  $\mathcal{N} := (0, T) \setminus \bigcap_{n \in \mathbb{N}} I_n$  is a null set. We may assume that every time  $s \in (0, T) \setminus \mathcal{N}$  is a Lebesgue point for  $t \mapsto \|v_t\|_{L^2(\mu_t)}$  as well.

By assumption, we may test each  $\varphi_n$  against the weak continuity equation which, when integrated over a time interval  $(s, s+h) \subset (0, T)$ , takes the form

$$\int_{\mathfrak{G}} \varphi_n d\mu_{s+h} - \int_{\mathfrak{G}} \varphi_n d\mu_s = \int_s^{s+h} L_r(\varphi_n) dr \quad \forall n \in \mathbb{N}.$$

Since the family  $\{\varphi_n\}_{n \in \mathbb{N}}$  is dense in  $W^{1,2}(\mathfrak{G})$ , for every  $\varphi \in W^{1,2}(\mathfrak{G})$  and the densities of  $\mu_t$  are uniformly bounded in  $t$ , we may find a sequence  $(\varphi_{n_k})_{k \in \mathbb{N}}$  such that  $\varphi_{n_k} \rightarrow \varphi$  and  $\nabla \varphi_{n_k} \rightarrow \nabla \varphi$  in  $L^2(\mu_t)$ . In particular, we may pass to the limit in the equality above to arrive at

$$\int_{\mathfrak{G}} \varphi d\mu_{s+h} - \int_{\mathfrak{G}} \varphi d\mu_s = \int_s^{s+h} L_r(\varphi) dr \quad \forall \varphi \in W^{1,2}(\mathfrak{G}). \quad (45)$$

Moreover, for every  $\varphi \in W^{1,2}(\mathfrak{G})$ , there is an index  $n \in \mathbb{N}$  such that  $\|\varphi - \varphi_n\|_{W^{1,2}} < \varepsilon$ . For  $s \in (0, T) \setminus \mathcal{N}$  and  $h > 0$  small enough, we compute

$$\begin{aligned} & \frac{1}{h} \int_s^{s+h} |L_r(\varphi) - L_s(\varphi)| dr \\ & \leq \varepsilon \left( \|L_s\| + \frac{1}{h} \int_s^{s+h} \|L_r\| dr \right) + \frac{1}{h} \int_s^{s+h} |L_r(\varphi_n) - L_s(\varphi_n)| dr \\ & \leq \varepsilon \left( \|v_s\|_{L^2(\mu_s)} + \frac{1}{h} \int_s^{s+h} \|v_r\|_{L^2(\mu_r)} dr + \frac{1}{h} \|L_s\| \right). \end{aligned}$$

By arbitrariness of  $\varepsilon > 0$  and boundedness of all terms in the parenthesis in the last line, we conclude that  $s \in (0, T) \setminus \mathcal{N}$  is a Lebesgue point for  $t \mapsto L_t(\varphi)$ . Therefore, we may differentiate with respect to time in (45) at each such  $s$ , in order to arrive at (44).  $\square$

For the following proof we will follow along some lines of the one of Theorem 2.4 in [DMM16].



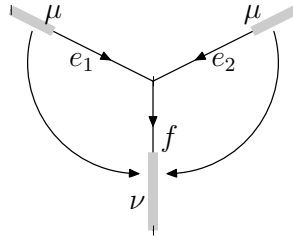


FIGURE 4. The support of probability measures  $\mu$  and  $\nu$  on a metric graph induced by a oriented star with 3 leaves.

*Proof of Proposition 4.19.* Note that the pair  $(\varphi_{t_0}, \psi_{t_0})$  of Kantorovich potentials for some fixed time  $t_0 \in (0, T)$  is at least admissible for the dual transport problem between  $\mu_t^1$  and  $\mu_t^2$  for any other time  $t \in (0, T)$ ; therefore,

$$\frac{1}{2}W_2^2(\mu_t^1, \mu_t^2) - \int_{\mathfrak{G}} \varphi_{t_0} d\mu_t^1 - \int_{\mathfrak{G}} \psi_{t_0} d\mu_t^2 \geq 0. \quad (46)$$

In particular, we have equality above when  $t = t_0$ .

Fix  $t_0$  such that  $t \mapsto W_2^2(\mu_t^1, \mu_t^2)$  differentiable at  $t_0$ . By Lemma 4.20, we may assume that  $t \mapsto \int_{\mathfrak{G}} \varphi_{t_0} d\mu_t^1$  and  $t \mapsto \int_{\mathfrak{G}} \psi_{t_0} d\mu_t^2$  are differentiable at  $t_0$  as well. This means that the left-hand side of (46) is differentiable at  $t_0$ ; by optimality, its derivative vanishes at  $t_0$ . Henceforth, we have established the equality

$$\frac{1}{2} \frac{d}{dt_0} W_2^2(\mu_{t_0}^1, \mu_{t_0}^2) = \frac{d}{dt_0} \int_{\mathfrak{G}} \varphi_{t_0} d\mu_{t_0}^1 + \frac{d}{dt_0} \int_{\mathfrak{G}} \psi_{t_0} d\mu_{t_0}^2 \quad \text{for a.e. } t_0 \in (0, T).$$

In order to conclude, we apply the continuity equation in the weak sense to the right-hand side above.  $\square$

## 5. GEODESIC CONVEXITY OF THE ENTROPY AND CURVATURE IN THE SENSE OF ALEXANDROV ON $W_2(\mathfrak{G})$

In this section we consider entropy functionals on  $\mathcal{P}(\mathfrak{G})$  of the form

$$\text{Ent}(\mu) := \begin{cases} \int_{\mathfrak{G}} \rho \log \rho dx & \text{if } \mu = \rho \cdot \lambda, \\ +\infty & \text{otherwise.} \end{cases} \quad (47)$$

The results for semicontinuity of functionals of this type also hold for metric graphs (cf. Proposition 7.2 below); in particular, the entropy functional  $\text{Ent}$  is lower semicontinuous on  $W_2(\mathfrak{G})$ .

The following example shows that for  $p \geq 1$ , the entropy functional  $\text{Ent}$  on the metric space  $(\mathcal{P}(\mathfrak{G}), W_p)$  over a metric graph  $\mathfrak{G}$  induced by a graph with maximum degree larger than 2 is *not* geodesically  $K$ -convex for any  $K \in \mathbb{R}$ .

**Example 5.1.** Consider a metric graph induced by a graph with 3 leaves as shown in Figure 4. We assume an edge weight of 1 on each of the edges  $e_1, e_2, f$ , as well as two probability measures

$$\mu := \frac{1}{2\varepsilon} (\mathbb{1}_{[0,\varepsilon]}|_{e_1} + \mathbb{1}_{[0,\varepsilon]}|_{e_2}) \quad \text{and} \quad \nu := \frac{1}{\varepsilon} \mathbb{1}_{[1-\varepsilon,1]}|_f.$$

It is straightforward to find an optimal transport map from  $\mu$  to  $\nu$ . Indeed, it is optimal to transfer mass in a monotonic way from  $\mu$  on each of the edges  $e_1$  and  $e_2$  to



FIGURE 5. On the left a geodesic triangle between the highlighted nodes of the metric graph and on the right the corresponding comparison triangle in the Euclidean plane.

$\nu$ . Hence, the constant speed-geodesic from  $\mu$  to  $\nu$  is given by  $(T_{t\#\mu})_{t \in [0,1]}$  with

$$T_t(x) := \begin{cases} x + (2 - \varepsilon)t \in e_i & \text{if } x \leq 1 - (2 - \varepsilon)t \\ x + (2 - \varepsilon)t - 1 \in f & \text{if } x \geq 1 - (2 - \varepsilon)t \end{cases}$$

for  $x \in e_i$ ,  $i \in \{1, 2\}$ .

Now, the relative entropy of  $\mu_t$  reads as follows on each edge:

$$\text{Ent}(\mu_t|_{e_i}) = \begin{cases} \frac{1}{2} \log\left(\frac{1}{2\varepsilon}\right) & \text{if } (2 - \varepsilon)t \leq 1 - \varepsilon \\ (1 - (2 - \varepsilon)t)\frac{1}{2} \log\left(\frac{1}{2\varepsilon}\right) & \text{if } 1 - \varepsilon \leq (2 - \varepsilon)t \leq 1 \\ 0 & \text{if } 1 \leq (2 - \varepsilon)t \end{cases}$$

$$\text{Ent}(\mu_t|_f) = \begin{cases} 0 & \text{if } (2 - \varepsilon)t \leq 1 - \varepsilon \\ (2 - \varepsilon)t \log\left(\frac{1}{\varepsilon}\right) & \text{if } 1 - \varepsilon \leq (2 - \varepsilon)t \leq 1 \\ \log\left(\frac{1}{\varepsilon}\right) & \text{if } 1 \leq (2 - \varepsilon)t. \end{cases}$$

Note that the derivative along  $t \mapsto \text{Ent}(\mu_t)$  diverges to  $+\infty$  for  $\varepsilon \searrow 0$  and any time  $1 - \varepsilon < (2 - \varepsilon)t < 1$ , whereas the derivative along  $t \mapsto \text{Ent}(\mu_t)$  vanishes for a.e. any other time  $t$ . We conclude that  $t \mapsto \text{Ent}(\mu_t)$  is not  $K$ -convex for any  $K \in \mathbb{R}$ .

In the next example, we investigate whether  $\mathfrak{G}$  and  $W_2(\mathfrak{G})$  are CAT[0] spaces. To this end, recall that we call a geodesic space  $(X, d)$  *non-positively curved* aka CAT[0] if  $d(\cdot, z)$  is 2-convex along geodesics in  $X$  for all  $z \in X$ . This is characterised by the property that every geodesic triangle in  $X$  is *thin* when compared to an isometric triangle in Euclidean space.

If  $d(\cdot, z)$  is 2-concave along geodesics in  $X$  for all  $z \in X$ , then  $X$  is called *positively curved*. This corresponds to the property that geodesic triangles in  $X$  are *fat*.

The comparison of geodesic triangles in Figure 5 shows that metric graphs are usually neither positively nor non-positively curved. A similar behaviour is observed for  $W_2(\mathfrak{G})$ .

**Example 5.2.** Consider a metric graph with atomic probability measures as described in Figure 6. Then  $t \mapsto W_2^2(\mu_t, \nu)$  is not convex. Hence,  $W_2(\mathfrak{G})$  cannot be CAT[0].

Similarly, we can consider a metric graph induced by a triangle with uniform edge weights, which is then positively curved. Since this property is inherited by Wasserstein spaces (cf. e.g. Theorem 2.20 in [AG13]), this means that the 2-Wasserstein space of this uniform triangle is positively curved as well.

In particular, any metric graph which contains embeddings of both examples of metric graphs above gives rise to a corresponding 2-Wasserstein space that is neither positively nor non-positively curved.

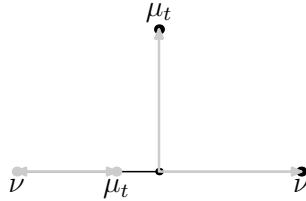


FIGURE 6. A probability measure  $\nu$  is concentrated with equal mass on bottom left and bottom right node. For each time  $t \in [0, 1]$ , the probability measure  $\mu_t$  is concentrated with equal mass on the top node and  $\{\gamma_t\}$ , where  $\gamma : [0, 1] \rightarrow \mathfrak{G}$  is a constant-speed geodesic connecting the bottom left to the bottom right node.

## 6. CONVERGENCE OF THE JKO-SCHEME

**6.1. Optimality conditions of the JKO-scheme at each time step.** In this section we show convergence of the JKO-scheme for the combination  $\mathcal{F} := \text{Ent} + \mathcal{V}$  of an entropy functional as in (47) and a potential energy functional

$$\mathcal{V}(\mu) := \int_X V \, d\mu \quad \forall \mu \in \mathcal{P}(\mathfrak{G})$$

with respect to some potential  $V$  on  $\mathfrak{G}$ . In addition, we identify the limit curve as a solution to the corresponding Fokker-Planck equation.

**Assumptions 6.1.** Throughout this section, we make the following assumptions:

- (i) The potential function  $V : \mathfrak{G} \rightarrow \mathbb{R}$  is Lipschitz continuous.
- (ii) The initial measure  $\rho_0 \in \mathcal{P}(\mathfrak{G})$  satisfies  $\mathcal{F}(\rho_0) < +\infty$ .

Below, we will denote, by abuse of notation, with  $L^\infty(\mathfrak{G}) \cap \mathcal{P}(\mathfrak{G})$  the space of all Borel probability measures which are absolutely continuous with respect to  $\lambda$  with densities belonging to  $L^\infty(\mathfrak{G})$ .

*Throughout this section, any (probability) measure, absolutely continuous w.r.t.  $\lambda$ , will be identified with its density function.*

**Definition 6.2.** We call  $\rho \in \mathcal{P}(\mathfrak{G})$  *regular* for a functional  $F : \mathcal{P}(\mathfrak{G}) \rightarrow \mathbb{R} \cup \{+\infty\}$  if  $F$  takes finite values only along any convex combination between  $\rho$  and  $\tilde{\rho} \in L^\infty(\mathfrak{G}) \cap \mathcal{P}(\mathfrak{G})$ . In this case, we call every measurable function  $\frac{\delta F}{\delta \rho}(\rho)$ , given by

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} F(\rho + \varepsilon\chi) = \int_{\mathfrak{G}} \frac{\delta F}{\delta \rho}(\rho) \, d\chi \quad \text{with } \chi = \tilde{\rho} - \rho \text{ for some } \tilde{\rho} \in L^\infty(\mathfrak{G}) \cap \mathcal{P}(\mathfrak{G}),$$

the *first variation* of  $F$  at  $\rho$ .

**Proposition 6.3.** *Let  $p > 1$  and  $\nu \in \mathcal{P}(\mathfrak{G})$ .*

- (i) *The functional  $\mu \mapsto W_p^p(\mu, \nu)$  is convex on  $\mathcal{P}(\mathfrak{G})$ .*
- (ii) *The subdifferential of  $\mu \mapsto W_p^p(\mu, \nu)$  at  $\mu_0$  coincides with the set of Kantorovich potentials for the dual transport problem from  $\mu_0$  to  $\nu$  with respect to the cost  $\frac{1}{2}d^2$ .*
- (iii) *In case, there is only one such Kantorovich potential  $\bar{\varphi}$  which is  $d^p$ -concave (up to additive constants), we also have the first variation formula*

$$\frac{\delta W_p^p(\cdot, \nu)}{\delta \rho}(\mu) := \left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} W_p^p(\mu + \varepsilon\chi) = \bar{\varphi}$$

*for any perturbation  $\chi = \tilde{\mu} - \mu$  with  $\tilde{\mu} \in L^\infty(\mathfrak{G}) \cap \mathcal{P}(\mathfrak{G})$ .*

This is the case, when at least one of the measures  $\mu$  or  $\nu$  has full support on  $\mathfrak{G}$ .

*Proof.* See the proofs of Propositions 7.17 and 7.18 in [San15] in a Euclidean setting, which carry over straightforwardly.  $\square$

**Proposition 6.4.** *Let  $F : \mathcal{P}(\mathfrak{G}) \rightarrow \mathbb{R} \cup \{+\infty\}$  be a functional, minimised by  $\rho_0$ , regular for  $F$  such that the first variation of  $F$  at  $\rho_0$  exists.*

(i) *If  $\frac{\delta F}{\delta \rho}(\rho_0)$  is a continuous function on  $\mathfrak{G}$ , then*

$$\frac{\delta F}{\delta \rho}(\rho_0) \leq \text{ess inf} \frac{\delta F}{\delta \rho}(\rho_0) \quad (48)$$

*everywhere with equality on  $\text{supp } \rho_0$ .*

(ii) *If  $\rho_0 \ll \lambda$ , then (48) holds  $\lambda$ -a.e. with equality at  $\lambda$ -a.e. point where  $\rho_0$  does not vanish.*

*Proof.* See the proof of Proposition 7.20 in [San15] in a Euclidean setting, which carries over mutatis mutandis.  $\square$

**Proposition 6.5.** *For each  $\tau > 0$  and every initial measure  $\rho_0^\tau := \rho_0$  satisfying Assumption 6.1.ii, the recursively defined optimisation problem*

$$\rho_{k+1}^\tau \in \underset{\rho \in \mathcal{P}(\mathfrak{G})}{\text{argmin}} \mathcal{F}(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_k^\tau) \quad (49)$$

*has a unique minimiser at each step  $k \in \mathbb{N}_0$ .*

*Proof.* Existence of a minimiser follows by the direct method in the calculus of variation, using that  $\mathcal{F}$  is a lower semicontinuous functional on the compact space  $(\mathcal{P}(\mathfrak{G}), W_2)$ .

Uniqueness of the minimiser is implied by convexity of  $W_2^2(\cdot, \rho_k^\tau)$ , together with strict convexity of  $\mathcal{F}$  (which is a sum of the a strictly convex functional  $\text{Ent}$  and linear functional  $\mathcal{V}$ ); see also Proposition 7.2.  $\square$

In the next result we collect some properties of the minimiser in (49).

**Proposition 6.6.** *For every  $k \in \mathbb{N}_0$ , the unique minimiser  $\rho_{k+1}^\tau$  in (49) is absolutely continuous with respect to  $\lambda$ . Identified with its density function,  $\rho_{k+1}^\tau$  satisfies the following properties:*

(i)  $\rho_{k+1}^\tau > 0$   $\lambda$ -a.e. and  $\log \rho_{k+1}^\tau \in L^1(\mathfrak{G})$ .

(ii) *Denote by  $\overline{\varphi}_{k+1 \rightarrow k}^\tau$  the (up to constants) unique Kantorovich potential from  $\rho_{k+1}^\tau$  to  $\rho_k^\tau$  with respect to  $\frac{1}{2}d^2$ . Then*

$$\frac{\overline{\varphi}_{k+1 \rightarrow k}^\tau}{\tau} + \log \rho_{k+1}^\tau + V = \text{constant } \lambda\text{-a.e.} \quad (50)$$

*In particular,  $\log \rho_{k+1}^\tau$  is Lipschitz continuous on  $\mathfrak{G}$ .*

(iii) *We have the identity*

$$\frac{\overline{\varphi}_{k+1 \rightarrow k}^\tau}{\tau} = -\nabla(\log \rho_{k+1}^\tau + V) \quad \lambda\text{-a.e.} \quad (51)$$

*Proof.* For (i) see the proof of Lemma 8.6 in [San15], which carries over to the setting of metric graphs without any major modifications to speak of.

Regarding (ii), we compute the first variation of  $\rho \rightarrow \mathcal{F}(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_k^\tau)$  at  $\rho = \rho_{k+1}^\tau$ : Write  $\rho_\varepsilon := (1 - \varepsilon)\rho_{k+1}^\tau + \varepsilon\tilde{\rho}$  for some probability density  $\tilde{\rho} \in L^\infty(\mathfrak{G})$ . By definition,  $\text{Ent}(\rho) < \infty$  for  $\rho \in \{\rho_{k+1}^\tau, \tilde{\rho}\}$ . Due to the convexity of the entropy functional (which

follows from the convexity of  $x \mapsto x \log x$ ,  $\text{Ent}(\rho_\varepsilon)$  takes finite values along  $t \in [0, 1]$  as well. Therefore, the first variation of the entropy functional is expressed in terms of

$$\int_{\mathfrak{G}} \frac{\delta \text{Ent}}{\delta \rho}(\rho_{k+1}^\tau) d(\rho_{k+1}^\tau - \tilde{\rho}) := \frac{d}{d\varepsilon} \Big|_{\varepsilon=0} \int_{\mathfrak{G}} \rho_\varepsilon \log \rho_\varepsilon dx = \int_{\mathfrak{G}} \log \rho_{k+1}^\tau + 1 d(\rho_{k+1}^\tau - \tilde{\rho}), \quad (52)$$

where we used dominated convergence in form of

$$\left| \frac{d}{d\varepsilon}(\rho_\varepsilon \log \rho_\varepsilon) \right| \leq (\rho_{k+1}^\tau + \log \|\tilde{\rho}\|_\infty)(|\log \rho_{k+1}^\tau| + \log \|\tilde{\rho}\|_\infty + 1) \in L^1(\mathfrak{G})$$

to differentiate under the integral sign in (52).

In a similar fashion, we obtain  $\frac{\delta V}{\delta \rho}(\rho_{k+1}^\tau) = V$ , whereas the the first variation of  $\rho \mapsto \frac{1}{2}W_2^2(\rho, \rho_k^\tau)$  is known from Proposition 6.3 to be the (unique) Kantorovich potential  $\bar{\varphi} := \bar{\varphi}_{k+1 \rightarrow k}^\tau$  from  $\rho_k^\tau$  to  $\rho_{k+1}^\tau$ .

Altogether, the first variation of all terms involved takes the form

$$\frac{\delta}{\delta \rho} \left( \mathcal{F}(\rho) + \frac{1}{2\tau} W_2^2(\rho, \rho_k^\tau) \right) (\rho_{k+1}^\tau) = \log \rho_{k+1}^\tau + 1 + V + \frac{\bar{\varphi}}{\tau}. \quad (53)$$

Due to Proposition 6.4, this expression is a.e. constant; hence (50) follows.

Since both  $\bar{\varphi}$  and  $V$  are Lipschitz continuous functions on  $\mathfrak{G}$ , (50) implies that  $\rho_{k+1}^\tau$  and, therefore, also  $\log \rho_{k+1}^\tau$  has a Lipschitz representative in  $L^1(\mathfrak{G})$ . In particular, we may assume that (50) is constant everywhere on  $\mathfrak{G}$ . Now (51) follows by taking the derivative of both sides of this equality.  $\square$

## 6.2. Interpolation between time steps.

**Definition 6.7.** We define the *piecewise constant interpolation curves* for a time-discrete sequence  $(\rho_k^\tau)_{k \in \mathbb{N}}$  of minimisers in (49) and corresponding  $c$ -concave Kantorovich potentials from  $\rho_{k+1}^\tau$  to  $\rho_k^\tau$  with respect to the cost function  $c := \frac{1}{2}d^2$  by

$$\rho_t^\tau := \rho_{k+1}^\tau, \quad v_t^\tau := \frac{\nabla \bar{\varphi}_{k+1 \rightarrow k}^\tau}{\tau}, \quad J_t^\tau := v_t^\tau \rho_t^\tau \quad \text{for } t \in (k\tau, (k+1)\tau].$$

Likewise, we define the *geodesic interpolation curves* for a fixed geodesics selection map  $\text{GeodSel}$  and optimal transport plans  $\pi_{k+1 \rightarrow k}^\tau$  from  $\rho_{k+1}^\tau$  to  $\rho_k^\tau$  by

$$\tilde{\rho}_t^\tau := (\text{GeodSel}_{\tilde{t}})_{\#} \pi_{k+1 \rightarrow k}^\tau, \quad \tilde{v}_t^\tau := \frac{\nabla \phi_{\tilde{t}}}{\tau}, \quad \tilde{J}_t^\tau := \tilde{v}_t^\tau \tilde{\rho}_t^\tau$$

for times

$$\tilde{t} = \frac{(k+1)\tau - t}{\tau}, \quad t \in (k\tau, (k+1)\tau]$$

and a potential function given by  $\phi_{\tilde{t}} := -Q_{1-\tilde{t}}(-\bar{\varphi}_{k+1 \rightarrow k}^\tau)^c$ , where  $Q$  denotes the Hopf-Lax semigroup as given in Definition 4.8 and  $(\cdot)^c$  denotes the  $c$ -transform for the cost  $c := \frac{1}{2}d^2$ .

We collect some basic facts about  $(\rho_k^\tau)_{k \in \mathbb{N}_0}$  and the interpolants introduced above.

**Lemma 6.8.** (i) *The densities  $\rho_k^\tau$  satisfy the following bounds in terms of the  $L^2$ -Wasserstein distance:*

$$\frac{W_2^2(\rho_{k+1}^\tau, \rho_k^\tau)}{2\tau} \leq \mathcal{F}(\rho_k^\tau) - \mathcal{F}(\rho_{k+1}^\tau) \quad \forall k \in \mathbb{N}_0 \quad (54)$$

and

$$\sum_k \frac{W_2^2(\rho_{k+1}^\tau, \rho_k^\tau)}{\tau} \leq 2(\mathcal{F}(\rho_0^\tau) - \inf_{\rho} \mathcal{F}(\rho)). \quad (55)$$

- (ii) The family of interpolation densities  $(\rho^\tau)_{\tau>0}$  is equi-integrable on  $[0, T] \times \mathfrak{G}$ .
- (iii) Both, the  $c$ -transform  $(-\bar{\varphi}_{k+1 \rightarrow k}^\tau)^c$  and the potential function  $\phi_{\tilde{t}}$  are Lipschitz continuous, uniformly with respect to  $t$ . In particular,  $\int_0^T \|\tilde{v}_t^\tau\|_{L^2(\tilde{\rho}_t^\tau)} dt < \infty$  for all  $T > 0$ .
- (iv) The pair  $(\tilde{\rho}_t^\tau, \tilde{v}_t^\tau)_{t \in [0, T]}$  satisfies the continuity equation in the weak sense for every  $T > 0$ .

*Proof.* The first bound in (i) follows from a comparison of two successive optimisers in (49). Then we may sum over  $k \in \mathbb{N}_0$  in (54) and use that the resulting right-hand side is a telescopic sum to obtain the second bound (55).

For the proof of (ii), recall that (54) implies  $\mathcal{F}(\rho_{k+1}^\tau) \leq \mathcal{F}(\rho_k^\tau)$  which, by iteration over  $k \in \mathbb{N}_0$ , gives the uniform bound  $\mathcal{F}(\rho_k^\tau) \leq \mathcal{F}(\rho_0) < +\infty$ . By definition of the piecewise constant interpolation, this implies  $\mathcal{F}(\rho_t^\tau) \leq \mathcal{F}(\rho_0)$ ; in particular, we have  $\text{Ent}(\rho_t^\tau) \leq \mathcal{F}(\rho_0)$ .

Note that  $f(x) := x \log x$  is actually a super-linear function, i.e. for every  $\varepsilon > 0$  there exists a constant  $M > 0$  such that  $f(x)/x = \log(x) > 1/\varepsilon$  for all  $x > M$ . In particular, we may assume that

$$\frac{f(x)}{x} = \log x > \frac{2}{\varepsilon} \mathcal{F}(\rho_0) \quad \forall x > M.$$

Therefore, for every set  $A \subseteq [0, T] \times \mathfrak{G}$  such that  $(\mathcal{L}^1 \times \lambda)(A) \leq \varepsilon/(2M)$ , we obtain the estimate

$$\begin{aligned} \int_A \rho_t^\tau(x) d(t, x) &= \int_{A \cap \{\rho_t^\tau \leq M\}} \rho_t^\tau(x) d(t, x) + \int_{A \cap \{\rho_t^\tau > M\}} \frac{\rho_t^\tau(x)}{f(\rho_t^\tau(x))} f(\rho_t^\tau(x)) d(t, x) \\ &\leq (\mathcal{L}^1 \times \lambda)(A) + \frac{\varepsilon}{2\mathcal{F}(\rho_0)} \mathcal{F}(\rho_0) dt \leq \varepsilon, \end{aligned}$$

uniformly for all  $\tau > 0$ ; we conclude that the family  $(\rho^\tau)_{\tau>0}$  is equi-integrable.

Regarding (iii), the Lipschitz continuity of  $(-\bar{\varphi}_{k+1 \rightarrow k}^\tau)^c$  is inherited from the one of the cost function  $c = \frac{1}{2}d^2$ . Now the Lipschitz continuity of  $\phi_{\tilde{t}}$  is a direct consequence of Proposition 4.9.

For the proof of the claim in (iv), we first note that every  $c$ -concave Kantorovich potential  $\bar{\varphi}$  satisfies

$$\nabla \bar{\varphi}(x_0) = \frac{1}{2} \nabla_{x_0} d^2(x_0, y) = - \frac{d}{dt} \Big|_{t_0=0} \text{GeodSel}_{t_0}(x_0, y) \quad (56)$$

for  $(\lambda \times \lambda)$ -a.e.  $(x_0, y)$  in the support of an optimal transport plan corresponding to  $\bar{\varphi}$ . In particular, for the choice  $\bar{\varphi} = (1 - \tilde{t})\phi_{\tilde{t}}$  (which is a Kantorovich potential from  $\tilde{\rho}_t^\tau$  to  $\tilde{\rho}_{k\tau}^\tau$ ), the formula above implies the continuity equation

$$\begin{aligned} \frac{d}{dt} \int_{\mathfrak{G}} \varphi d\tilde{\rho}_t^\tau &= \frac{d}{dt} \int_{\mathfrak{G} \times \mathfrak{G}} \varphi(\text{GeodSel}_{\tilde{t}}(x, y)) d\pi_{k+1 \rightarrow k}^\tau \\ &= - \frac{1}{(1 - \tilde{t})\tau} \frac{d}{dt} \Big|_{t_0=0} \int_{\mathfrak{G} \times \mathfrak{G}} \varphi(\text{GeodSel}_{\tilde{t}+t_0(1-\tilde{t})}(x, y)) d\pi_{k+1 \rightarrow k}^\tau \\ &= \frac{1}{\tau} \int_{\mathfrak{G} \times \mathfrak{G}} \nabla \varphi(\text{GeodSel}_t(x, y)) \cdot \nabla \phi_t(\text{GeodSel}_t(x, y)) d\pi_{k+1 \rightarrow k}^\tau \\ &= \int_{\mathfrak{G}} \nabla \varphi \cdot \tilde{v}_t^\tau d\tilde{\rho}_t^\tau, \end{aligned}$$

where we used that  $\tilde{\rho}_t^\tau \ll \lambda$  and  $\pi_{k+1 \rightarrow k}^\tau \ll \lambda \times \lambda$ ; the former, due to Proposition 3.19 and the latter, due to both margins of  $\pi_{k+1 \rightarrow k}^\tau$  being absolutely continuous with respect to  $\lambda$ .  $\square$

**Lemma 6.9.** *Up to subsequences, the interpolants  $\rho_t^\tau, \tilde{\rho}_t^\tau$  and  $J_t^\tau, \tilde{J}_t^\tau$  introduced above converge weakly in the following sense as  $\tau \rightarrow 0$ :*

- (i)  $J^\tau \rightharpoonup J$  and  $\tilde{J}^\tau \rightharpoonup J$  in  $\mathcal{M}([0, T] \times \mathfrak{G})$  for some signed limit measure  $J$  on space-time.
- (ii)  $W_2(\rho_t^\tau, \rho_t) \rightarrow 0$  and  $W_2(\tilde{\rho}_t^\tau, \rho_t) \rightarrow 0$  uniformly in  $t \in [0, T]$  for some limit curve  $(\rho_t)_{t \in [0, T]}$ , both absolutely continuous and  $1/2$ -Hölder continuous with respect to  $W_2$ .

*Proof.* We start with the proof of (i): As  $(\tilde{\rho}_t^\tau)_{t \in [0, T]}$  is defined via a geodesic interpolation, its metric derivative is piecewise constant and equals to

$$|\dot{\tilde{\rho}}_t^\tau| = \frac{1}{\tau} W_2(\tilde{\rho}_{k+1}^\tau, \tilde{\rho}_k^\tau) = \frac{1}{\tau} \int_{\mathfrak{G}} \mathbf{d}^2(x, y) d\tilde{\rho}_{k+1}^\tau = \|v_t^\tau\|_{L^2(\tilde{\rho}_t^\tau)} \quad \text{a.e. } t \in (k\tau, (k+1)\tau), \quad (57)$$

where we used the identity

$$|\nabla \overline{\varphi(x_0)}|^2 = |\nabla_{x_0} \mathbf{d}^2(x_0, y)/2|^2 = \mathbf{d}^2(x_0, y) \quad (\lambda \times \lambda)\text{-a.e. } (x_0, y) \in \text{supp } \pi_{k+1 \rightarrow k}^\tau, \quad (58)$$

which, in turn, is a consequence of (56).

Note that (57), together with (55), implies the total variation bound

$$\begin{aligned} |J^\tau|([0, T] \times \mathfrak{G}) &= \int_0^T \int_{\mathfrak{G}} |v_t^\tau| d\rho_t^\tau dt \leq \int_0^T \|v_t^\tau\|_{L^2(\rho_t^\tau)} dt \\ &\leq \sqrt{T} \int_0^T \|v_t^\tau\|_{L^2(\rho_t^\tau)}^2 dt = \sqrt{T} \sum_{k=0}^{\infty} \tau \left( \frac{1}{\tau} W_2(\rho_{k+1}^\tau, \rho_k^\tau) \right)^2 \leq \sqrt{TC} \end{aligned}$$

for some constant  $C > 0$ .

By means of Theorem 4.7,  $|\dot{\tilde{\rho}}_t^\tau| = \|\tilde{v}_t^\tau\|_{L^2(\tilde{\rho}_t^\tau)}$  for a.e.  $t \in [0, T]$ . Hence, we also get

$$\begin{aligned} |\tilde{J}^\tau|([0, T] \times \mathfrak{G}) &= \int_0^T \int_{\mathfrak{G}} |\tilde{v}_t^\tau| d\tilde{\rho}_t^\tau dt \leq \sqrt{T} \int_0^T \|\tilde{v}_t^\tau\|_{L^2(\tilde{\rho}_t^\tau)}^2 dt \\ &= \sqrt{T} \int_0^T \|v_t^\tau\|_{L^2(\rho_t^\tau)}^2 dt \leq \sqrt{TC}. \end{aligned}$$

As a result, both  $(J^\tau)_{\tau > 0}$  and  $(\tilde{J}^\tau)_{\tau > 0}$  are relative compact families of signed measures in space-time with respect to the topology of weak convergence.

For this part of the proof it remains to show that the limit curves for  $(J^\tau)_{\tau > 0}$  and  $(\tilde{J}^\tau)_{\tau > 0}$  agree. To this aim, let  $f : [0, T] \times \mathfrak{G} \rightarrow \mathbb{R}$  be a Lipschitz function and set

$$\chi_{\tilde{t}}(x, y) := f(x)v_{\tilde{t}}^\tau(x) - f(\text{GeodSel}_{\tilde{t}}(x, y))\tilde{v}_{\tilde{t}}^\tau(\text{GeodSel}_{\tilde{t}}).$$

We compute

$$\left| \int_0^T \int_{\mathfrak{G}} f d(J_t^\tau - \tilde{J}_t^\tau) dt \right| = \left| \sum_k \int_{k\tau}^{(k+1)\tau} \int_{\mathfrak{G} \times \mathfrak{G}} \chi_{\tilde{t}}(x, y) d\pi_{k+1 \rightarrow k}^\tau(x, y) dt \right|$$

$$\leq \sum_k \int_{k\tau}^{(k+1)\tau} \int_{\mathfrak{G} \times \mathfrak{G}} \mathbb{1}_{d^2(x,y) > \tau}(x,y) |\chi_{\tilde{t}}(x,y)| d\pi_{k+1 \rightarrow k}^\tau(x,y) \quad (59a)$$

$$+ \int_{\mathfrak{G} \times \mathfrak{G}} \mathbb{1}_{d^2(x,V) < \tau/2}(x,y) |\chi_{\tilde{t}}(x,y)| d\pi_{k+1 \rightarrow k}^\tau(x,y) \quad (59b)$$

$$+ \int_{\mathfrak{G} \times \mathfrak{G}} \mathbb{1}_{\text{GeodSel}(x,y) \subseteq e}(x,y) |\chi_{\tilde{t}}(x,y)| d\pi_{k+1 \rightarrow k}^\tau(x,y) dt \quad (59c)$$

Recalling the estimates above, we have  $\int_0^T \|\tilde{v}_t^\tau\|_{L^2(\rho_t^\tau)}^2 dt = \int_0^T \|v_t^\tau\|_{L^2(\rho_t^\tau)}^2 dt \leq C$ , which in turn implies the bound

$$\sum_k \int_{k\tau}^{(k+1)\tau} \int_{\mathfrak{G} \times \mathfrak{G}} |\chi_{\tilde{t}}(x,y)|^2 d\pi_{k+1 \rightarrow k}^\tau(x,y) dt \leq 4\|f\|_\infty^2 C.$$

In particular, invoking Hölder's inequality, this implies for the term in (59a) the estimate

$$\begin{aligned} & \sum_k \int_{k\tau}^{(k+1)\tau} \int_{\mathfrak{G} \times \mathfrak{G}} \mathbb{1}_{d^2(x,y) > \tau}(x,y) |\chi_{\tilde{t}}(x,y)| d\pi_{k+1 \rightarrow k}^\tau(x,y) \\ & \leq 2\|f\|_\infty \sqrt{C} \left( \sum_k \int_{\mathfrak{G} \times \mathfrak{G}} \tau \mathbb{1}_{d^2(x,y) > \tau}(x,y) d\pi_{k+1 \rightarrow k}^\tau(x,y) \right)^{1/2} \\ & \leq 2\|f\|_\infty \sqrt{C} \left( \sum_k W_2^2(\rho_{k+1}^\tau, \rho_k^\tau) \right)^{1/2}, \end{aligned}$$

which vanishes as  $\tau \rightarrow 0$ , due to (55).

In a similar fashion, we may estimate the term in (59b):

$$\begin{aligned} & \sum_k \int_{k\tau}^{(k+1)\tau} \int_{\mathfrak{G} \times \mathfrak{G}} \mathbb{1}_{d^2(x,V) < \tau/2}(x,y) |\chi_{\tilde{t}}(x,y)| d\pi_{k+1 \rightarrow k}^\tau(x,y) \\ & \leq 2\|f\|_\infty \sqrt{C} \left( \sum_k \tau \int_{\mathfrak{G} \times \mathfrak{G}} \mathbb{1}_{d^2(x,V) < \tau/2}(x,y) d\pi_{k+1 \rightarrow k}^\tau(x,y) \right)^{1/2} \\ & = 2\|f\|_\infty \sqrt{C} \left( \int_0^T \int_{\mathfrak{G}} \mathbb{1}_{d^2(x,V) < \tau/2}(x) d\rho_t^\tau(x) dt \right)^{1/2}. \end{aligned}$$

Recalling from Lemma 6.8.i that the family of densities  $(\rho_t^\tau)_{\tau > 0}$  is equi-integrable on  $[0, T] \times \mathfrak{G}$ , we may pass to the limit in the estimate above to conclude that the term (59b) vanishes as  $\tau \rightarrow 0$ .

Turning to (59c), we first note that as long as  $\text{GeodSel}(x,y)$  belongs to a single edge  $e \in E$ , corresponding geodesics are uniquely determined by convex combinations, i.e.  $\text{GeodSel}_{\tilde{t}} = (1-\tilde{t})x + \tilde{t}y$ . In particular, the speed  $\frac{d}{dt} \text{GeodSel}_{\tilde{t}}(x,y)$  equals to a constant for all  $\tilde{t} \in [0, 1]$ . Moreover, invoking (56) for the Kantorovich potential  $\bar{\varphi} = (1-\tilde{t})\phi_{\tilde{t}}$  at  $x_0 = \text{GeodSel}_{\tilde{t}}(x,y)$  yields

$$\begin{aligned} (1-\tilde{t})\nabla\phi_{\tilde{t}}(\text{GeodSel}_{\tilde{t}}(x,y)) &= \frac{1}{2}\nabla_{x_0} d^2(\text{GeodSel}_{\tilde{t}}(x,y), y) \\ &= \frac{1-\tilde{t}}{2}\nabla_x d^2(x,y) = (1-\tilde{t})\frac{d}{dt} \text{GeodSel}_{\tilde{t}}(x,y) \end{aligned}$$



for every pair of end-points  $(x, y)$  in the support of  $\pi_{k+1 \rightarrow k}^\tau$  such that  $\text{GeodSel}(x, y)$  belongs to a single edge. Likewise, (56) holds for  $\bar{\varphi} = \bar{\varphi}_{k+1 \rightarrow k}^\tau$  at  $x_0 = x$ , which, combined with the formula above, results in

$$\nabla \phi_{\bar{t}}(\text{GeodSel}_{\bar{t}}(x, y)) = \frac{d}{d\bar{t}} \text{GeodSel}_{\bar{t}}(x, y) = \nabla \bar{\varphi}_{k+1 \rightarrow k}^\tau(x).$$

Thus, we may estimate the term  $|\chi_{\bar{t}}(x, y)|$  for all  $(x, y) \in \text{supp } \pi_{k+1 \rightarrow k}^\tau$  such that  $\text{GeodSel}(x, y)$  belongs to a single edge as follows

$$\begin{aligned} |\chi_{\bar{t}}(x, y)| &= |f(x) - f(\text{GeodSel}_{\bar{t}}(x, y))| \cdot |v_{\bar{t}}^\tau(x)| \\ &\leq \text{Lip}(f) d(x, \text{GeodSel}_{\bar{t}}(x, y)) |v_{\bar{t}}^\tau(x)| = \tau \text{Lip}(f) |v_{\bar{t}}^\tau(x)|^2, \end{aligned}$$

where we used (58) in form of the identity  $\frac{1}{\tau} d(x, y) = |v_{\bar{t}}^\tau(x)|$ .

With those considerations in mind, we may estimate (59c) as

$$\begin{aligned} &\sum_k \int_{k\tau}^{(k+1)\tau} \int_{\mathfrak{G} \times \mathfrak{G}} \mathbb{1}_{\text{GeodSel}(x, y) \subseteq e} | \chi_{\bar{t}}(x, y) | d\pi_{k+1 \rightarrow k}^\tau(x, y) dt \\ &\leq \tau \text{Lip}(f) \int_0^T \|v_{\bar{t}}^\tau\|_{L^2(\rho_{\bar{t}}^\tau)}^2 dt \leq \tau \text{Lip}(f) \sqrt{TC}, \end{aligned}$$

which allows us to conclude that  $\int_0^T \int_{\mathfrak{G}} f d(J_t^\tau - \tilde{J}_t^\tau) dt$  vanishes as  $\tau \rightarrow 0$ .

Moving on to (ii), the computations above also imply the bound  $\int_0^T |\dot{\rho}_r^\tau|^2 dr \leq \sqrt{TC}$ . Thus, for all  $s, t \in [0, T]$  such that  $s < t$ , we obtain

$$W_2(\tilde{\rho}_s^\tau, \tilde{\rho}_t^\tau) \leq \int_s^t |\dot{\rho}_r^\tau| dr \leq (t-s)^{1/2} \left( \int_s^t |\dot{\rho}_r^\tau|^2 dr \right)^{1/2} \leq \tilde{C}(t-s)^{1/2} \quad (60)$$

for some constant  $\tilde{C} > 0$ . In other words, the curve  $(\tilde{\rho}_t^\tau)_{t \in [0, T]}$  is uniformly 1/2-Hölder continuous with respect to  $\tau > 0$ . Since  $(\tilde{\rho}_t^\tau)_{t \in [0, T]}$  takes values in the compact space  $(\mathcal{P}(\mathfrak{G}), W_2)$ , we may invoke a metric version of the Arzelá-Ascoli theorem (see e.g. Proposition 3.3.1 in [AGS08]) to extract the required subsequence, converging to a limit curve  $(\rho_t)_{t \in [0, T]}$ , both absolutely continuous and 1/2-Hölder continuous with respect to  $W_2$ .

Choosing  $s = k\tau$  in (60), we obtain the bound  $W_2(\rho_t^\tau, \tilde{\rho}_t^\tau) \leq \tilde{C}\sqrt{\tau}$ , we conclude that (up to a subsequence)  $\rho_t^\tau$  converges as well uniformly in time to  $\rho_t$  as  $\tau \rightarrow 0$ .  $\square$

### 6.3. Passing to the limiting equation.

**Proposition 6.10.** *The piece-wise constant interpolants  $\rho^\tau$  and  $J^\tau$  converge weakly (up to some subsequences) to limit measures  $\rho$  and  $J$ , respectively, on space-time. The pair  $(\rho_t, J_t)_{t \in [0, T]}$  satisfies in the weak sense of Definition 4.2 the continuity equation  $\frac{d}{dt}\rho + \nabla \cdot J = 0$  with  $J = -\nabla\rho - \rho\nabla V$ .*

*In particular, for any initial value  $\rho_0 \in \mathcal{P}(\mathfrak{G})$  with  $\mathcal{F}(\rho_0) < +\infty$ , the curve  $t \mapsto \rho_t$  provides a weak solution to the Fokker-Planck equation  $\frac{d}{dt}\rho = \Delta\rho + \nabla \cdot (\rho\nabla V)$ .*

*Proof.* The weak convergence of  $(\rho^\tau, J^\tau)$  to  $(\rho, J)$  and the absolute continuity of  $\rho$  with respect to  $W_2$  are consequences of Lemma 6.9.

Note that, according to Remark 4.4, the weak continuity equation may be equivalently expressed in the following distributional form

$$\int_0^T \int_{\mathfrak{G}} \dot{\phi} d\rho_t^\tau + \int_{\mathfrak{E}} \nabla \phi \cdot dJ_t^\tau dt = 0 \quad \forall \phi \in \mathcal{D}((0, T) \times \mathfrak{G}). \quad (61)$$

Hence, the weak convergence of  $(\rho^\tau, J^\tau)$  implies that we (61) as  $\tau \rightarrow 0$ .

It remains to show that  $J = -\nabla\rho - \rho\nabla V$  in the sense of distributions: To this aim, recall from Proposition 6.6 that  $J^\tau = v^\tau\rho^\tau = -\nabla\rho^\tau - \rho^\tau\nabla V$ , again in the sense of distributions since both  $\rho^\tau$  and  $\rho^\tau\nabla V$  are  $L^1$ -functions:

$$\int_0^T \int_{\mathfrak{G}} \phi \cdot dJ_t^\tau dt = \int_0^T \int_{\mathfrak{G}} \nabla \cdot \phi - \phi \cdot \nabla V d\rho_t^\tau dt \quad \forall \phi \in \mathcal{D}((0, T) \times \mathfrak{G}). \quad (62)$$

In order to conclude, we need pass to the limit in this equation as  $\tau \rightarrow 0$ . To this aim, we already noted in Lemma 6.8 that the family of densities  $(\rho^\tau)_{\tau>0}$  is equi-integrable. Therefore, we may invoke the Dunford-Pettis theorem (cf. e.g. Theorem 4.7.25 in [Bog07]) to infer that (up to a subsequence)  $\rho^\tau$  converges to  $\rho$ , not only in the weak topology as  $\tau \rightarrow 0$ , but also in the topology of convergence w.r.t. bounded measurable functions on  $(0, T) \times \mathfrak{G}$ .

Since we have the bounds  $|\nabla \cdot \phi| \leq \|\phi\|_{L^\infty}$  and  $|\phi \cdot \nabla V| \leq \|\phi\|_{L^\infty} \|\nabla V\|_{L^\infty}$  on space-time, we may pass to the the limit in (62) as  $\rho^\tau \rightarrow \rho$  in the topology of convergence on bounded measurable functions.  $\square$

## 7. GRADIENT FLOWS IN WASSERSTEIN SPACES OVER METRIC GRAPHS

In this section we consider a combination  $\mathcal{F} := \text{Ent} + \mathcal{V}$  of an entropy functional as given in (47) and a potential energy functional as defined in (63) below.

**Assumptions 7.1.** Throughout this section, we make the following assumptions:

- (i) The potential function  $V : \mathfrak{G} \rightarrow \mathbb{R}$  is Lipschitz continuous.
- (ii) The initial measure  $\rho_0 \in \mathcal{P}(\mathfrak{G})$  satisfies  $\mathcal{F}(\rho_0) < +\infty$ .

Below *convexity* of a functional defined on a space of probability measures is always understood with respect to convex combinations of measures (and not along geodesics in some Wasserstein space).

**Proposition 7.2.** *Let  $X$  be a Polish metric space.*

- (i) *Let  $\nu$  be a finite positive measure on  $X$ . If  $f : \mathbb{R}^+ \rightarrow \mathbb{R}$  is a convex and lower semicontinuous function, then the internal energy functional*

$$\mathcal{F}_{\text{int}}(\mu) := \int_X f(\rho(x)) d\nu(x) + \mu^{\text{sing}}(X) \sup_{t>0} \frac{f(t)}{t} \quad \text{for } \mu = \rho \cdot \nu + \mu^{\text{sing}}$$

*is convex and lower semicontinuous with respect to the topology of weak convergence on  $\mathcal{P}(X)$ .*

*If  $f$  is strictly convex such that  $\lim_{t \rightarrow \infty} f(t)/t = +\infty$ , then  $\mathcal{F}_{\text{int}}$  is strictly convex as well.*

- (ii) *Let  $V : X \rightarrow \mathbb{R}$  be a bounded function.  $\mathcal{V}$  is (lower semi-)continuous, precisely, when the potential energy functional*

$$\mathcal{V}(\mu) := \int_X V d\mu \quad (63)$$

*is (lower semi-)continuous with respect to the topology of weak convergence on  $\mathcal{P}(X)$ .*

*Proof.* See Proposition 7.7 and Proposition 7.1 in [San15] (the results are stated in a Euclidean setting; however the proofs carry over to the general setting above without any modification).  $\square$

**Definition 7.3.** Let  $V$  be a Lipschitz function on  $\mathfrak{G}$ . Define a functional  $\mathcal{I}_V$  on  $\mathcal{P}(\mathfrak{G})$  by

$$\mathcal{I}_V(\mu) := \begin{cases} \int_{\mathfrak{E}} \left| \frac{\nabla \rho}{\rho} + \nabla V \right|^2 d\mu & \text{if } \mu = \rho \cdot \lambda \text{ for } \rho \in W^{1,1}(\mathfrak{E}), \\ +\infty & \text{otherwise.} \end{cases}$$

For the case  $V \equiv 0$ , this functional is the usual Fisher information.

Below we collect some basic facts about  $\mathcal{I}_V$  (see e.g. Lemma 2.2 in [GST09], where  $\mathcal{I}_V$  is expressed in terms of a relative Fisher information).

**Lemma 7.4.** *Let  $V$  be a Lipschitz function on  $\mathfrak{G}$ . For a probability measure  $\mu = \rho \cdot \lambda \in \mathcal{P}(\mathfrak{G})$ , the functional  $\mathcal{I}_V$  satisfies the following properties:*

- (i)  $\mathcal{I}_V(\mu) < \infty$  iff  $\sqrt{\rho} \in W^{1,2}(\mathfrak{E})$ .
- (ii) For every sequence  $(\mu_n)_{n \in \mathbb{N}}$  of probability measures  $\mu_n = \rho_n \cdot \lambda \in \mathcal{P}(\mathfrak{G})$  such that  $\sup_n \mathcal{I}_V(\mu_n) < \infty$ , there exists  $\mu = \rho \cdot \lambda$  such that (up to a subsequence):
  - (a)  $\mu_n$  converges weakly in  $\mathcal{P}(\mathfrak{G})$  to  $\mu$ ,
  - (b)  $\rho_n$  converges strongly in  $L^1(\mathfrak{E})$  to  $\rho$ ,
  - (c)  $\rho_n$  converges strongly in  $L^\infty(\overline{\mathfrak{E}})$  to  $\rho$ ,
  - (d) the weak derivatives  $\nabla \rho_n$  converge weakly in  $L^1(\mathfrak{E})$  to  $\nabla \rho$ ,
  - (e)  $\sqrt{\rho_n}$  converges strongly in  $L^2(\mathfrak{E})$  to  $\sqrt{\rho}$ ,
  - (f) the weak derivatives  $\nabla \sqrt{\rho_n}$  converge weakly in  $L^2(\mathfrak{E})$  to  $\nabla \sqrt{\rho}$ ,
  - (g)  $\liminf_{n \rightarrow \infty} \mathcal{I}_V(\mu_n) \geq \mathcal{I}_V(\mu)$ .
- (iii) If the sequence  $(\mu_n)_{n \in \mathbb{N}}$  above satisfies  $\limsup_{n \rightarrow \infty} \mathcal{I}_V(\mu_n) \leq \mathcal{I}_V(\mu)$  as well, then (up to a subsequence):
  - (a) the weak derivatives  $\nabla \rho_n$  converge strongly in  $L^1(\mathfrak{E})$  to  $\nabla \rho$ ,
  - (b) the weak derivatives  $\nabla \sqrt{\rho_n}$  converge strongly in  $L^2(\mathfrak{E})$  to  $\nabla \sqrt{\rho}$ .

**7.1. The Entropy-Fisher dissipation equality.** The next result represents a chain rule for the derivative of the functional  $\mathcal{I}_V$  along an absolutely continuous curve.

**Proposition 7.5.** *Let  $(\mu_t)_{t \in [0, T]}$  be a 2-absolutely continuous curve in  $(\mathcal{P}(\mathfrak{G}), W_2)$  with  $\mu_t = \rho_t \cdot \lambda$  such that  $\int_0^T \mathcal{I}_V(\mu_t) dt < +\infty$  and let  $J_t = U_t \cdot \lambda$  be an optimal family of momentum vectorfields such that  $(\mu_t, J_t)_{t \in [0, T]}$  solves the continuity equation in the weak sense. Then,  $t \mapsto \mathcal{F}(\mu_t)$  is absolutely continuous and we have*

$$\frac{d}{dt} \mathcal{F}(\mu_t) = \int_{\mathfrak{E}} \langle \nabla \log \rho_t + \nabla V, U_t \rangle dx \quad \text{for a.e. } t \in [0, T]. \quad (64)$$

In particular, the functional  $\sqrt{\mathcal{I}_V}$  is a strong upper gradient for  $\mathcal{F}$ , i.e. for every 2-absolutely continuous curve  $(\mu_t)_{t \in [0, T]}$  in  $(\mathcal{P}(\mathfrak{G}), W_2)$ , the inequality

$$|\mathcal{F}(\mu_t) - \mathcal{F}(\mu_s)| \leq \int_s^t \sqrt{\mathcal{I}_V(\mu_r)} |\dot{\mu}_r| dr \quad \forall s, t \in [0, T] : s \leq t \quad (65)$$

holds.

*Proof.* Theorem 4.7 implies the existence of a vectorfield  $(v_t)_{t \in [0, T]}$  such that  $\|v_t\|_{L^2(\mu_t)} = |\dot{\mu}_t|$  for a.e.  $t$ .

At any time  $t \in [0, T]$ , we introduce the regularised measure  $\mu_t^\varepsilon = \rho_t^\varepsilon \cdot \lambda$  of  $\mu_t$  on  $\mathfrak{G}_{\text{ext}}$  by means of (24). Moreover, we write  $J_t^\varepsilon = v_t^\varepsilon \cdot \mu_t^\varepsilon$  for a vectorfield  $v_t^\varepsilon(x) \in L^2(\mu_t^\varepsilon)$  as done in Section 4.1.

Using a family  $(\eta^\varepsilon)_{\varepsilon > 0}$  of even and smooth approximation kernels with compact supports  $\text{supp } \eta^\varepsilon[-\varepsilon, \varepsilon]$ , we additionally employ a regularisation of the curves in time,

given by

$$\rho_t^{\varepsilon, \delta, \gamma} := \int_0^T \eta^\delta(t-s) \rho_s^{\varepsilon, \gamma} ds \quad \text{with} \quad \rho_t^{\varepsilon, \gamma} := \frac{1}{1+\gamma} \left( \rho_t^\varepsilon + \frac{\gamma}{\lambda(\mathfrak{G})} \right)$$

for constants  $\delta > 0$  and  $\gamma > 0$ . Note that

$$|\log \rho_t^{\varepsilon, \delta, \gamma}| \leq C_\gamma (1 + \rho_t^{\varepsilon, \delta, \gamma}) \quad \forall t \in [0, T] \quad (66)$$

for some constant  $C_\gamma \geq 1$  depending only on  $\gamma$ . This bound, in turn, yields the estimate

$$\begin{aligned} \left| \frac{d}{dt} (\rho_t^{\varepsilon, \delta, \gamma} \log \rho_t^{\varepsilon, \delta, \gamma} + V \rho_t^{\varepsilon, \delta, \gamma}) \right| &= \left| \log \rho_t^{\varepsilon, \delta, \gamma} + 1 + V \right| \cdot \left| \frac{d}{dt} \rho_t^{\varepsilon, \delta, \gamma} \right| \\ &\leq C_\gamma (2 + \|V\|_\infty + \sup_{x,t} \rho_t^{\varepsilon, \delta, \gamma}) \sup_t \left| \frac{d}{dt} \eta^\delta(t) \right| \int_0^T \rho_s^\varepsilon ds. \end{aligned}$$

Since the right-hand side belongs to  $L^1(\mathfrak{G}_{\text{ext}})$ , we may invoke the dominated convergence theorem to take the time derivative inside the integral of the expression

$$\frac{d}{dt} \mathcal{F}(\rho_t^{\varepsilon, \delta, \gamma}) = \frac{d}{dt} \int_{\mathfrak{G}_{\text{ext}}} \rho_t^{\varepsilon, \delta, \gamma} (\log \rho_t^{\varepsilon, \delta, \gamma} + V) dx,$$

which shows that the mapping  $t \mapsto \int_{\mathfrak{G}_{\text{ext}}} \rho_t^{\varepsilon, \delta, \gamma} (\log \rho_t^{\varepsilon, \delta, \gamma} + V) dx$  is continuously differentiable. In particular, integrating the resulting expression over the time interval  $(s, t)$ , we arrive at

$$\begin{aligned} \mathcal{F}(\rho_t^{\varepsilon, \delta, \gamma}) - \mathcal{F}(\rho_s^{\varepsilon, \delta, \gamma}) &= \int_s^t \int_{\mathfrak{G}_{\text{ext}}} (\log \rho_r^{\varepsilon, \delta, \gamma} + V) \frac{d}{dr} \rho_r^{\varepsilon, \delta, \gamma} dx dr \\ &= - \int_s^t \int_{\mathfrak{G}_{\text{ext}}} (\log \rho_r^{\varepsilon, \delta, \gamma} + V) \left( \int_0^T \frac{d}{dh} \eta^\delta(h-r) \rho_h^{\varepsilon, \gamma} dh \right) dx dr \\ &= \int_s^t \int_{\mathfrak{G}_{\text{ext}}} (\log \rho_r^{\varepsilon, \delta, \gamma} + V) \left( \int_0^T \eta^\delta(h-r) \frac{d}{dh} \rho_h^{\varepsilon, \gamma} dh \right) dx dr \\ &= \frac{1}{1+\gamma} \int_s^t \int_0^T \eta^\delta(h-r) \frac{d}{dh} \left( \int_{\mathfrak{G}} \psi(r, x) d\mu_h^\varepsilon \right) dh dr, \end{aligned} \quad (67)$$

where we used the identity  $\frac{d}{dr} \eta^\delta(h-r) = -\frac{d}{dh} \eta^\delta(h-r)$ , together with integration by parts with respect to the time variable  $h$  and  $\psi := \log \rho_r^{\varepsilon, \delta, \gamma} + V$ . Note that for every time  $r \in [0, T]$ , the function  $\psi(r, \cdot)$  is absolutely continuous on  $\mathfrak{G}_{\text{ext}}$ . Indeed,  $\mu_r \ll \lambda$  and so the regularised density  $\rho_r^{\varepsilon, \delta, \gamma}$  is absolutely continuous on  $\mathfrak{G}_{\text{ext}}$  by the regularising effect stated in Proposition 4.15.ii. Since  $\rho_r^{\varepsilon, \delta, \gamma}$  is bounded away from zero by a constant  $c > 0$  and  $\log$  is Lipschitz continuous on  $(c, +\infty)$ , we infer that  $\psi(r, \cdot)$  is absolutely continuous as well (see e.g. Lemma 5.3.2 in [Bog07]).

Therefore, we may invoke the continuity equation in form of (26), in order to express  $\frac{d}{dh} \int_{\mathfrak{G}} \psi^\varepsilon d\mu_h$  in terms of the momentum field  $J_h^\varepsilon = \alpha^\varepsilon v_h^\varepsilon \cdot \mu_h^\varepsilon$ . Hence, we may write (67) as

$$\begin{aligned} \mathcal{F}(\rho_t^{\varepsilon, \delta, \gamma}) - \mathcal{F}(\rho_s^{\varepsilon, \delta, \gamma}) &= \frac{1}{1+\gamma} \int_s^t \int_0^T \eta^\delta(h-r) \frac{d}{dh} \left( \int_{\mathfrak{G}} \psi^\varepsilon d\mu_h \right) dh dr \\ &= - \frac{1}{1+\gamma} \int_s^t \int_0^T \eta^\delta(h-r) \int_{\mathfrak{E}_{\text{ext}}} \nabla \psi dJ_h^\varepsilon dh dr. \end{aligned} \quad (68)$$

In the next part of the proof, we will pass to the limits  $\varepsilon, \delta, \gamma \searrow 0$  in this equation. We start with the right-hand side of (68):

By weak continuity of  $(\mu_t)_{t \in [0, T]}$ , the regularised curve  $t \mapsto \rho_t^\varepsilon(x)$  is continuous for every  $x \in \mathfrak{G}_{\text{ext}}$ . Therefore,  $\rho_t^{\varepsilon, \delta, \gamma}$  converges to  $\rho_t^{\varepsilon, \gamma}$ , uniformly in  $t \in [0, T]$  as  $\delta \searrow 0$ .

In addition,  $|J_h^\varepsilon(x)|$  (as a density function) is uniformly bounded in  $(h, x)$  by the term  $\|\nabla \eta^\varepsilon\|_\infty \|v_t\|_{L^2(\mu_h)}$  and we have the estimate

$$\left| \frac{\nabla \rho_r^{\varepsilon, \delta, \gamma}}{\rho_r^{\varepsilon, \delta, \gamma}} + \nabla V \right| \leq \frac{C}{\gamma} \|\nabla \eta^\varepsilon\|_\infty$$

for some constant  $C > 0$ . This means that we may invoke dominated convergence to pass to the limit in the right-hand side of (68) as  $\delta \searrow 0$ ; thus, yielding the expression

$$\lim_{\delta \searrow 0} \int_s^t \int_0^T \eta^\delta(h-r) \int_{\mathfrak{E}_{\text{ext}}} \nabla \psi \, dJ_h^\varepsilon \, dh \, dr = \int_s^t \int_{\mathfrak{E}_{\text{ext}}} \nabla \psi \, dJ_r^\varepsilon \, dr$$

Identifying the signed measure  $J_h^\varepsilon$  with its density, we may estimate the right-hand side of the equality by means of Young's inequality as

$$\frac{|\nabla \psi \cdot J_r^\varepsilon|}{1+\gamma} = \frac{|(\nabla \rho_r^{\varepsilon, \gamma} + \rho_r^{\varepsilon, \gamma} \nabla V) \cdot J_r^\varepsilon|}{(1+\gamma)\rho_r^{\varepsilon, \gamma}} \leq \frac{|\nabla \rho_r^{\varepsilon, \gamma}|^2}{(1+\gamma)\rho_r^{\varepsilon, \gamma}} + |\nabla V|^2 (\rho_r^\varepsilon + \gamma/\lambda(\mathfrak{G})) + \frac{|J_h^\varepsilon|^2}{\rho_r^\varepsilon + \gamma/\lambda(\mathfrak{G})}. \quad (69)$$

Since

$$\frac{|\nabla \rho_r^{\varepsilon, \gamma}|^2}{(1+\gamma)\rho_r^{\varepsilon, \gamma}} = \frac{1}{(1+\gamma)^2} \frac{|\nabla \rho_r^\varepsilon|^2}{\rho_r^\varepsilon + \gamma/\lambda(\mathfrak{G})},$$

the three terms in the right-hand side of (69) are either uniformly bounded or monotonically increasing as  $\gamma \searrow 0$ . In particular,

$$|\nabla \psi \cdot J_r^\varepsilon| \leq \frac{|\nabla \rho_r^\varepsilon|^2}{\rho_r^\varepsilon} + |\nabla V|^2 \rho_r^\varepsilon + C + \frac{|J_r^\varepsilon|^2}{\rho_r^\varepsilon} \quad (70)$$

for some constant  $C > 0$ .

Recalling the identity (33) and invoking Jensen's inequality for the convex function  $(a, b) \mapsto a^2/b$ , we obtain the estimate

$$\frac{|\nabla \rho_r^\varepsilon|^2}{\rho_r^\varepsilon} \leq C_\varepsilon \left( \frac{|\nabla \rho_r|}{\rho_r} \right)^\varepsilon. \quad (71)$$

for some constant  $C_\varepsilon \searrow 1$  as  $\varepsilon \searrow 0$ .

For the right-hand side of (65) to be finite (otherwise there is nothing to show), we may assume  $\mathcal{I}_V(\mu_r)$  to be finite for a.e.  $r \in (s, t)$ . In particular, by Lemma 7.4.i, the density function  $\sqrt{\rho_r}$  belongs to  $W^{1,2}(\mathfrak{E})$  for a.e.  $r$ . Fix any such  $r \in (s, t)$ .

Hence, we may invoke Proposition 4.15.v to show that the right-hand side of (71) converges to  $\frac{|\nabla \rho_r|^2}{\rho_r}$  in  $L^1(\mathfrak{G}_{\text{ext}})$  as  $\varepsilon \rightarrow 0$ .

The same proposition implies that  $\rho_r^\varepsilon \rightarrow \rho_r$  in  $L^1(\mathfrak{G}_{\text{ext}})$  as  $\varepsilon \rightarrow 0$ . Taking the kinetic energy bound (25) into account as well, we infer that the right-hand side of (70) converges not only in  $L^1(\mathfrak{G}_{\text{ext}})$  for a.e.  $r \in (s, t)$  but also in  $L^1((s, t) \times \mathfrak{G})$  as  $\varepsilon \rightarrow 0$ .

Consequently,  $\nabla \psi \cdot J_r^\varepsilon$  converges as well, due to (a variant) of the dominated convergence theorem and we may pass to the limits  $\varepsilon, \delta, \gamma \searrow 0$  on the right-hand side of (68).

It remains to pass to the limits on the left-hand side in (68). To this aim, we note that for fixed  $\varepsilon > 0$ , the regularised density  $\rho_r^\varepsilon$  is bounded and  $\rho_r^{\varepsilon, \delta, \gamma}$  converges to  $\rho_r^\varepsilon$  as

$\delta, \gamma \searrow 0$ , both uniformly for all  $r \in [0, T]$ . Thus,

$$\lim_{\varepsilon \rightarrow 0} \left( \mathcal{F}(\rho_t^\varepsilon) - \mathcal{F}(\rho_s^\varepsilon) \right) = \int_s^t \langle \nabla \log \rho_r + \nabla V, U_t \rangle dr. \quad (72)$$

In order to remove the spatial regularisation on the left-hand side of this inequality, we note first note that the modulus of each side of this equation is bounded by  $\int_0^T \sqrt{\mathcal{I}_V(\mu_r)} |\dot{\mu}_r| dr < +\infty$  for all times  $s, t \in [0, T]$  and all  $\varepsilon > 0$ .

Fix any time  $s \in [0, T]$  such that  $\rho_s \in W^{1,1}(\mathfrak{G})$ . Then  $\rho_s^\varepsilon$  converges uniformly to  $\rho_s$  and so  $\text{Ent}(\rho_s^\varepsilon) \rightarrow \text{Ent}(\rho_s) < +\infty$  as well.

Together with the uniform bound for (72), this means that  $\text{Ent}(\rho_t) < +\infty$  for all  $t \in [0, T]$ .

Jensen's inequality implies for the convex integrand  $f(x) := x \log x$  the estimate  $f(\rho_t^\varepsilon) \leq (f(\rho_t))^\varepsilon$  with a right-hand side converging to  $\rho_t \log \rho_t$  in  $L^1(\mathfrak{G}_{\text{ext}})$  as  $\varepsilon \rightarrow 0$ . As a result, we may again appeal to the dominated convergence theorem to obtain  $\text{Ent}(\rho_s^\varepsilon) \rightarrow \text{Ent}(\rho_s)$  for all times  $t \in [0, T]$ .

Since may pass to the limit in  $\mathcal{V}(\rho_r^\varepsilon)$  as well, for we know from Proposition 4.15.iv that  $\rho_r^\varepsilon \rightarrow \rho_r$  for every time  $r \in [0, T]$  as  $\varepsilon \searrow 0$ , we conclude that

$$\mathcal{F}(\rho_t^\varepsilon) - \mathcal{F}(\rho_s^\varepsilon) = \int_s^t \langle \nabla \log \rho_r + \nabla V, U_t \rangle dr \quad \forall s, t \in [0, T] : s \leq t. \quad (73)$$

From this equation we easily infer that  $t \mapsto \text{Ent}(\mu_t)$  is absolutely continuous and (64) holds. In addition, Hölder's inequality implies the estimate in (65) as well.  $\square$

**Corollary 7.6.** *Let  $(\mu_t)_{t \in [0, T]}$  be a 2-absolutely continuous curve in  $(\mathcal{P}(\mathfrak{G}), W_2)$  with  $\mathcal{F}(\mu_0) < \infty$ . Then  $(\mu_t)_{t \in [0, T]}$  is a weak solution for the Fokker-Planck equation  $\frac{d}{dt} \mu_t = \Delta \mu_t + \nabla \cdot (\mu_t \nabla V)$  in the sense of Definition 4.2, precisely, when the Entropy-Fisher dissipation equality*

$$\mathcal{F}(\mu_t) + \frac{1}{2} \int_s^t |\dot{\mu}_r|^2 dr + \frac{1}{2} \int_s^t \mathcal{I}_V(\mu_r) dr = \mathcal{F}(\mu_s) \quad \forall s, t \in [0, T] : s \leq t \quad (74)$$

holds.

*Proof.* Note that the right-hand side of (64) may be estimated by means of Hölder's and Young's inequality as

$$\int_{\mathbb{E}} \langle \nabla \log \rho_t + \nabla V, U_t \rangle dx \leq \frac{1}{2} \int_{\mathbb{E}} |\nabla \log \rho_t + \nabla V|^2 + |U_t|^2 dx$$

with equality if and only if  $U_t = -\nabla \log \rho_t - \nabla V$  for a.e.  $t \in [0, T]$ . Thus, the claim follows by integrating both sides of (64) over the time interval  $(s, t)$ .  $\square$

*Remark 7.7.* In Theorem 8.1 of [AGS14] it was shown that the Entropy-Fisher dissipation equality (74), together with uniform  $L^\infty$ -bounds on the probability densities of  $(\rho_t)_{t \geq 0}$ , implies that the curve  $(\rho_t)_{t \geq 0}$  is actually the unique gradient flow starting from  $\rho_0$  with respect to Cheeger's energy in  $L^2(\mathfrak{G})$ . To this end, we recall one possible definition of Cheeger's energy  $\text{Ch}_* : L^2(\mathfrak{G}) \rightarrow [0, +\infty]$ , given by the relaxation functional

$$\text{Ch}_*(f) := \frac{1}{2} \inf \left\{ \liminf_{n \rightarrow \infty} \int_{\mathfrak{G}} |\nabla f_n| dx \right\},$$

where the infimum is taken over all sequences  $(f_n)_{n \in \mathbb{N}}$  of Lipschitz functions  $f_n : \mathfrak{G} \rightarrow \mathbb{R}$ , converging to  $f$  with respect to  $\|\cdot\|_{L^2}$ .

Now, under the assumptions above, the curve of probability densities  $(\rho_t)_{t \geq 0}$  satisfies the energy dissipation equality

$$\text{Ch}_*(\rho_t) + \int_s^t |\dot{\rho}_r|^2 dr + \frac{1}{2} \int_s^t |\partial \text{Ch}_*|^2(\rho_r) dr = \text{Ch}_*(\rho_s) \quad \forall s, t \in \mathbb{R}_0^+ : s \leq t,$$

where we emphasise that the underlying space for the metric derivative  $|\dot{\rho}_r|$  and the metric slope  $|\partial \text{Ch}_*|$  is actually  $L^2(\mathfrak{G})$  instead of  $(\mathcal{P}(\mathfrak{G}), W_2)$ .

In particular, since  $L^2(\mathfrak{G})$  is a Hilbert space, it is also possible to characterise this gradient flow by the notion of subdifferentials; see Section 4.2 in [AGS14] for details.

**7.2. The energy-dissipation equality for the lower semicontinuous envelope of the metric slope.** The goal of this subsection is to identify the Fisher information  $\mathcal{I}_V$  with the *lower semicontinuous envelope*  $|\partial^- \mathcal{F}|$  along any solution of (74). Recall that the lower semicontinuous envelope of  $|\partial \mathcal{F}|$  is given by

$$|\partial^- \mathcal{F}|(\mu) := \inf \left\{ \liminf_{n \rightarrow \infty} |\partial \mathcal{F}|(\mu_n) : \mu_n \rightharpoonup \mu, \sup_n \{W_2(\mu_n, \mu), \mathcal{F}(\mu_n)\} < +\infty \right\}.$$

Moreover, recall from Proposition 7.2 that the functional  $\mathcal{F}$  is (sequentially) lower semicontinuous on  $\mathcal{P}(\mathfrak{G}, W_2)$ . Due to our assumption on the potential  $V$ , the functional  $\mathcal{V}$  and, therefore, also  $\mathcal{F}$  is bounded from below. Therefore, we may invoke Theorem 2.3.3 in [AGS08] to obtain the following result.

**Proposition 7.8.** *For every initial value  $\mu_0 \in \mathcal{P}(\mathfrak{G})$  with  $\mathcal{F}(\mu_0) < \infty$ , there exists a 2-absolutely continuous curve  $(\mu_t)_{t \in [0, T]}$  in  $(\mathcal{P}(\mathfrak{G}), W_2)$  satisfying the energy dissipation equality for  $|\partial^- \mathcal{F}|$ , i.e.*

$$\mathcal{F}(\mu_t) + \frac{1}{2} \int_s^t |\dot{\mu}_r|^2 dr + \frac{1}{2} \int_s^t |\partial^- \mathcal{F}|^2(\mu_r) dr = \mathcal{F}(\mu_s) \quad \forall s, t \in [0, T] : s \leq t. \quad (75)$$

In order to identify the curves solving (74) and (75), the following result is vital.

**Proposition 7.9.** *For any probability measure  $\mu = \rho \cdot \lambda \in \mathcal{P}(\mathfrak{G})$  with finite slope  $|\partial \text{Ent}|(\mu) < +\infty$ , the density  $\rho$  belongs to  $W^{1,1}(\mathfrak{G})$  such that  $\nabla \rho / \rho \in L^2(\mu)$  and the bound*

$$\mathcal{I}_V(\mu) \leq |\partial \mathcal{F}|^2(\mu)$$

is satisfied.

In particular, both the metric slope  $|\partial \mathcal{F}|$  and its lower semicontinuous envelope  $|\partial^- \mathcal{F}|$  are strong upper gradients for  $\mathcal{F}$  in the sense of (65).

For the proof of this statement, we need the following result which is an adaptation of Lemma 10.4.4 in [AGS08] to the metric graph setting.

**Lemma 7.10.** *Let  $\mu = \rho \cdot \lambda$  be a finite measure concentrated on a metric edge  $e$  in  $\mathfrak{E}$ , satisfying  $\mathcal{F}(\mu) := \text{Ent}(\mu) + \mathcal{V}(\mu) < +\infty$ , together with  $\mathbf{r} \in L^2(\mu)$  and  $\bar{t} > 0$  such that*

- (i)  $\mathbf{r} - \text{Id}$  is a  $C^\infty$ -function on the interval  $[0, m_e]$  identified with the edge  $e$ ;
- (ii) the mapping  $\mathbf{r}_t := (1-t)\text{Id} + t\mathbf{r}$  takes values in  $[0, m_e]$  for all  $t \leq \bar{t}$ ;
- (iii)  $\mathcal{F}((\mathbf{r}_{\bar{t}})_\# \mu) < +\infty$ .

Then the derivative of the functional  $\mathcal{F}$  at  $\mu$  in direction of  $\mathbf{r}$  is given by the identity

$$\lim_{t \searrow 0} \frac{\mathcal{F}((\mathbf{r}_t)_\# \mu) - \mathcal{F}(\mu)}{t} = \int_0^{m_e} (\mathbf{r} - \text{Id}) \nabla V - \nabla(\mathbf{r} - \text{Id}) d\mu. \quad (76)$$

*Proof.* We follow the proof of Lemma 10.4.4 in [AGS08] adapted to the functional  $\mathcal{F} = \text{Ent} + \mathcal{V}$ :

Note that  $\mathbf{r}$  is bounded on  $[0, m_e]$ ; therefore, the mapping  $\mathbf{r}_t$  is actually injective for every  $t$  small enough. Without loss of generalisation, we may choose  $\bar{t} > 0$  accordingly so that  $|\nabla \mathbf{r}_t| > 0$  for every  $t \leq \bar{t}$ . In particular, we may employ a change of variables argument (see e.g. Lemma 5.5.3 in [AGS08]) to express the density of the pushforward  $(\mathbf{r}_t)_\# \mu$  by means of

$$(\mathbf{r}_t)_\# \mu(A) = \int_{A \cap \text{ran } \mathbf{r}_t} \frac{\rho \circ \mathbf{r}_t^{-1}}{|\nabla \mathbf{r}_t \circ \mathbf{r}_t^{-1}|} dx$$

for every Borel set  $A$  and  $t \leq \bar{t}$ . Hence, using this representation for the density of the pushforward, together with a change of variables under with respect to  $\mathbf{r}_t$ , we may write

$$\begin{aligned} \mathcal{F}((\mathbf{r}_t)_\# \mu) - \mathcal{F}(\mu) &= \int_e \log\left(\frac{\rho}{|\nabla \mathbf{r}_t|}\right) - \log(\rho) d\mu + \int_e V \circ \mathbf{r}_t - V d\mu \\ &= - \int_e \log(\nabla \mathbf{r}_t) d\mu + \int_e V \circ \mathbf{r}_t - V d\mu. \end{aligned}$$

Note that the functions

$$\frac{d}{dt} \log(\nabla \mathbf{r}_t) = \frac{\nabla(\mathbf{r} - \text{Id})}{\mathbf{r}_t} \quad \text{and} \quad \frac{d}{dt} V(\mathbf{r}_t) = (\mathbf{r} - V) \nabla V$$

are uniformly integrable in  $L^1(\mu)$  with respect to  $t \in [0, \bar{t}]$ . Thus, we may pass to the limit of  $\frac{1}{t}(\mathcal{F}((\mathbf{r}_t)_\# \mu) - \mathcal{F}(\mu))$  as  $t \searrow 0$  to arrive at (76).  $\square$

*Proof of Proposition 7.9.* In the first part of the proof, we assume that the measure  $\mu$  is concentrated on a single metric edge  $e$  in  $\mathfrak{E}$ . Fix a function  $\mathbf{t} := \mathbf{r} - \text{Id} \in C_c^\infty(0, m_e)$ . Then there exists a constant  $\bar{t} > 0$  such that the assumptions of Lemma 7.10 are satisfied. In addition, we have

$$W_2^2(\mu, (\mathbf{r}_t)_\# \mu) \leq \int_0^{m_e} |t(\mathbf{r} - \text{Id})|^2 d\mu = t^2 \|\mathbf{t}\|_{L^2(\mu)}^2.$$

This estimate, together with (76), implies

$$\int_0^{m_e} \mathbf{t} \nabla V - \nabla \mathbf{t} d\mu \leq |\partial J|(\mu) \|\mathbf{t}\|_{L^2(\mu)}.$$

By linearity, this inequality generalises to probability measures  $\mu$  with support in  $\mathfrak{G}$  and functions  $\mathbf{t} \in C_c^\infty(\mathfrak{E})$  viz.

$$\int_{\mathfrak{E}} \mathbf{t} \nabla V - \nabla \mathbf{t} d\mu \leq |\partial J|(\mu) \|\mathbf{t}\|_{L^2(\mu)}.$$

The integral on the left-hand side of this inequality defines a bounded linear functional; by means of the Hahn-Banach theorem, we may extend this linear functional to  $L^2(\mu)$ . Moreover, we may invoke the Riesz representation theorem to find  $w \in L^2(\mu)$  such that  $\|w\|_{L^2(\mu)} \leq |\partial J|(\mu)$  and

$$\int_{\mathfrak{E}} \mathbf{t} \nabla V - \nabla \mathbf{t} d\mu = \int_{\mathfrak{E}} w \cdot \mathbf{t} d\mu \quad \forall \mathbf{t} \in C_c^\infty(\mathfrak{E}).$$

Recalling that  $\nabla V$  is  $\lambda$ -a.e. bounded, we infer that the weak derivative  $\nabla \rho$  exists and belongs to  $L^2(\mathfrak{E})$ . In particular,  $\rho \in W^{1,1}(\mathfrak{G})$  and  $\sqrt{\mathcal{I}_V(\mu)} = \|\nabla \rho / \rho + \nabla V\|_{L^2(\mu)} \leq |\partial J|(\mu)$ .



Now, the last two claims now follow from (65) and the definition of the lower semi-continuous envelope  $|\partial^- \mathcal{F}|$ .  $\square$

**Corollary 7.11.** *Let  $(\mu_t)_{t \in [0, T]}$  be a 2-absolutely continuous curve in  $(\mathcal{P}(\mathfrak{G}), W_2)$  with  $\mathcal{F}(\mu_0) < +\infty$ . If  $(\mu_t)_{t \in [0, T]}$  satisfies the energy-dissipation equality (75), then it is also a weak solution for the Fokker-Planck equation  $\frac{d}{dt}\mu_t = \Delta\mu_t + \nabla \cdot (\mu_t \nabla V)$  in the sense of Definition 4.2.*

*Proof.* Both (75) and Proposition 7.9 yield

$$\mathcal{F}(\mu_t) + \frac{1}{2} \int_s^t |\dot{\mu}_r|^2 dr + \frac{1}{2} \int_s^t \mathcal{I}_V(\mu_r) dr \leq \mathcal{F}(\mu_s) \quad \forall s, t \in [0, T] : s \leq t.$$

Since the opposite inequality holds as a consequence of (65) and Young's inequality, we infer that the curve  $(\mu_t)_{t \in [0, T]}$  satisfies the entropy-Fisher equality (74) as well. Now the claim follows by Corollary 7.6.  $\square$

**7.3. The energy-dissipation equality for the metric slope.** This subsection is mainly based on the following central result based on semi-group methods.

**Proposition 7.12.** *For  $c \in L^\infty(\mathfrak{G})$  with  $c \geq C_0$  for some constant  $C_0 > 0$  and  $f \in L^\infty(\mathfrak{G})$ , the initial value problem*

$$\begin{aligned} \frac{d}{dt}u_t &= \nabla \cdot (c \nabla u_t) - f \cdot u_t, \\ u_0 &= \bar{u} \in L^1(\mathfrak{G}) \quad \text{and} \quad 0 \neq \bar{u} \geq 0, \end{aligned} \tag{77}$$

*together with standard node conditions is well-posed in  $L^1(\mathfrak{G})$  for all times  $t \geq 0$ . The unique solution  $(u_t)_{t \geq 0}$  belongs to the class  $C^\infty(\mathbb{R}^+, L^1(\mathfrak{G})) \cap C(\mathbb{R}^+, C^\infty(\mathfrak{G}))$  and satisfies  $u_t > 0$  for every time  $t > 0$ .*

*Proof.* The first part of the statement is taken from section 6.5 in [Mug14]. Strict positivity of  $u_t$  for all times  $t > 0$  follows from the fact that the underlying positive contraction semi-group is irreducible, which in turn is deduced from connectedness of the metric graph  $\mathfrak{G}$ ; see Theorem 2.10 in [Ouh09] and the proof of Proposition 6.77 in [Mug14].  $\square$

Assume that the potential  $V$  belongs to  $W^{2, \infty}(\mathfrak{G})$ , so that we may choose

$$c \equiv 1 \quad \text{and} \quad f = \frac{1}{4}(\nabla V)^2 - \frac{1}{2}\Delta V$$

in (77). Let  $(u_t)_{t \geq 0}$  be the corresponding solution to (77) with the initial value  $u_0 = e^{V/2}\bar{u}$  for some probability density  $\bar{u}$  on  $\mathfrak{G}$ . Then one may verify that  $(\rho_t)_{t \geq 0}$  with  $\rho_t = e^{-V/2}u_t$  is the unique weak solution to the Fokker-Planck equation  $\frac{d}{dt}\rho_t = \Delta\rho_t + \nabla \cdot (\rho_t \nabla V)$  with initial value  $\rho_0 = \bar{u}$ .

The regularity of the solution  $(\rho_t)_{t \geq 0}$  allows us to directly compute the energy production of  $\mathcal{F}$  along the corresponding curve of probability measures  $\mu_t = \rho_t \cdot \lambda$  viz.

$$\begin{aligned} \frac{d}{dt}\mathcal{F}(\mu_t) &= \frac{d}{dt} \left( \int_{\mathfrak{G}} \rho_t \log \rho_t dx + \int_{\mathfrak{G}} V d\rho_t \right) = \int_{\mathfrak{G}} (\log \rho_t + V) \frac{d}{dt}\rho_t dx \\ &= - \int_{\mathfrak{E}} \nabla (\log \rho_t + V) \cdot (\nabla \rho_t + \rho_t \nabla V) dx = -\mathcal{I}_V(\mu_t). \end{aligned}$$

In particular, we may integrate both sides of this equality with respect to  $t$  and employ the identity  $|\dot{\mu}_t| = \|v_t\|_{L^2(\mu_t)}$  a.e. in time for the vectorfield  $v_t = \nabla \rho_t / \rho_t + \nabla V$ . Thus, using Young's inequality, we arrive at

$$\mathcal{F}(\mu_s) - \mathcal{F}(\mu_t) = \int_s^t \mathcal{I}_V(\mu_r) dr = \int_s^t |\dot{\mu}_r|^2 dr \quad \forall s, t \in \mathbb{R}_0^+ : s \leq t. \quad (78)$$

Note that, in contrast to the previous results, the semi-group approach illustrated above requires the initial condition to be a density, not merely a measure. Nevertheless, the solution obtained in Proposition 6.10 (for arbitrary initial condition in  $\mathcal{P}(\mathfrak{G})$ ) immediately regularises to probability measures  $\mu_t$  which are absolutely continuous with respect to  $\lambda$  for all times  $t > 0$ . Hence, we may identify this solution with the one obtained in Corollary 7.6 via  $\rho_t = e^{-V/2} u_t$  for positive times  $t > 0$ , due to uniqueness of the latter.

In order to identify the functional  $\mathcal{I}_V$  with the squared metric slope  $|\partial\mathcal{F}|^2$ , we recall Theorem 7.5 from [AGS14], taking the following form in our case of the compact metric space  $(\mathfrak{G}, d)$  with finite volume  $\lambda(\mathfrak{G}) < \infty$ .

**Lemma 7.13.** *Let  $\mu = \rho \cdot \lambda \in \mathcal{P}(\mathfrak{G})$  with a Lipschitz continuous density  $\rho > 0$ . Then*

$$|\partial\mathcal{F}|^2(\mu) \leq \int_{\mathfrak{E}} \left| \frac{\nabla \rho}{\rho} + \nabla V \right|^2 d\mu. \quad (79)$$

Recalling from Proposition 7.12 that  $u_t$  and, therefore, also  $\rho_t = e^{-V/2} u_t$  is strictly positive for every time  $t > 0$ , we may infer that (79) holds along  $(\mu_t)_{t>0}$ . Combining this inequality with Proposition 7.9, we obtain the identity  $|\partial\mathcal{F}|^2(\rho_t) = \mathcal{I}_V(\rho_t)$  for every  $t > 0$ . In view of (74), the following result is now a direct consequence.

**Proposition 7.14.** *Assume that the potential  $V$  belongs to  $W^{2,\infty}(\mathfrak{G})$ . Let  $(\mu_t)_{t \in [0, T]}$  be a 2-absolutely continuous curve in  $(\mathcal{P}(\mathfrak{G}), W_2)$  with  $\mathcal{F}(\mu_0) < \infty$ . Then  $(\mu_t)_{t \in [0, T]}$  satisfies the entropy-Fisher equality (74), precisely, when the energy dissipation equality for the metric slope  $|\partial\mathcal{F}|$  holds, i.e.*

$$\mathcal{F}(\mu_t) + \frac{1}{2} \int_s^t |\dot{\mu}_r|^2 dr + \frac{1}{2} \int_s^t |\partial\mathcal{F}|^2(\mu_r) dr = \mathcal{F}(\mu_s) \quad \forall s, t \in [0, T] : s \leq t.$$

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# A VARIATIONAL STRUCTURE FOR NON-REVERSIBLE MARKOV CHAINS

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## 1. INTRODUCTION

Many classical applications of Markov chain theory – amongst them the celebrated Metropolis-Hastings algorithm [MRR<sup>+</sup>53], [Has70] – are based on reversible Markov chains, i.e. chains that satisfy so-called detailed balance conditions.

However, in more recent works, applications of Markov chains that violate those detailed-balance conditions (then called non-reversible Markov chains) are studied with the goal to exploit their favourable behaviour in terms of convergence to equilibrium, when compared to their reversible counterparts. Indeed, amongst numerous results, non-reversible Markov chains perform better with respect to the notions of asymptotic variance [Bie16], [CH13], [SSG10], large deviations [RBS15], [RBS16] and spectral gap [RBS16] [CLP99], [DHN00], [LP17].

The aim of this article is twofold: First, we briefly investigate how a non-reversible perturbation of a reversible continuous-time Markov chain affects convergence to equilibrium in terms of relative entropy. In particular, we give a numerical example showing that such a perturbation may decrease the rate of convergence, in contrast to the results above.

The main part is devoted to convergence to equilibrium in terms of a metric  $\mathcal{W}$  on the space of discrete probability measures  $\mathcal{P}(X)$  over the finite state space  $X$  of an irreducible continuous-time Markov chain. In the setting of reversible chains, such a distance was introduced independently in the works [Maa11], [Mie13], and [CHLZ12] as a discrete counterpart to the  $L^2$ -Wasserstein distance. In particular,  $\mathcal{W}$  gives rise to discrete counterparts for two important applications of the  $L^2$ -Wasserstein distance: heat flows in Euclidean space corresponding to metric gradient flows for entropy functionals on  $\mathcal{P}(\mathbb{R}^d)$  [JKO98] as well as a synthetic notion of lower Ricci curvature bounds for metric measure spaces  $X$  based on geodesic convexity of entropy functionals on  $\mathcal{P}(X)$  [S<sup>+</sup>06], [LV09]; see also [EM12].

In this article, we generalise the notion of the metric  $\mathcal{W}$  to irreducible continuous-time Markov chains which need not satisfy the detailed-balance conditions. To some extent, our approach can be seen as a discrete counterpart to [Ket16] where the notion of synthetic lower Ricci curvature bounds is extended to non-symmetric diffusion operators on metric measure spaces arising from Riemannian manifolds.

We characterise a local contraction estimate with respect to  $\mathcal{W}$  for the evolution of non-reversible Markov chains in terms of convexity of a one-parameter family of energy functionals  $\tau \mapsto \phi_\tau$  on the space of geodesics in  $(\mathcal{P}(X), \mathcal{W})$ . Each of those functionals consists of an entropy part plus a path-dependent term  $V_\tau$ . In the case of a reversible Markov chain,  $V_\tau$  depends only on the end-points of the geodesic segment between times  $t = 0$  and  $t = \tau$  and may be expressed in terms of a discrete potential energy functional on  $\mathcal{P}(X)$ .

In both the settings of synthetic lower Ricci curvature bounds as well as reversible Markov chains, contraction estimates and convexity of an entropy functional along geodesics are linked to a notion of gradient flows in metric spaces via the so-called evolution variational inequality. In the non-reversible context, we provide a similar characterisation in terms of a generalised inequality which already appeared in [Ket16] for non-symmetric diffusions.

Similar to its classical counterpart, the generalised evolution variational inequality is a valuable tool, in order to derive functional inequalities: We provide generalised notions for HWI, logarithmic Sobolev, Talagrand, and Poincaré inequalities, based on explicit path dependence of geodesics between the evaluation points and the equilibrium of the Markov chain.

**Open problem.** It remains unclear whether  $(\mathcal{P}(X), \mathcal{W})$  forms a uniquely geodesic space, i.e. whether every constant-speed geodesic in  $(\mathcal{P}(X), \mathcal{W})$  is uniquely defined by its end-points. A positive result in this direction has direct consequences on several results in this article which are currently limited to local versions; amongst them the contraction estimate in Theorem 3.8 as well the Talagrand and Poincaré inequalities in Section 7.

**Organisation of the article.** The first part of this article consists of Section 2 and is devoted to a brief numerical example illustrating the effect of a non-reversible perturbation of a reversible continuous-time Markov chain on convergence to equilibrium in terms of relative entropy.

In Section 3 we introduce the metric  $\mathcal{W}$  defined on a space of discrete probability measures on the state space of the corresponding non-reversible Markov chain. The first main result gives a characterisation of a local contraction estimate with respect to  $\mathcal{W}$  in terms of convexity of a family of energy functionals on the space of geodesics in  $(\mathcal{P}(X), \mathcal{W})$  as well a generalised evolution variational inequality.

Section 4 covers lower bounds for the convexity parameter which appears in the main result of the previous section.

In Section 5 we not only show that  $(\mathcal{P}(X), \mathcal{W})$  is a complete metric space but also that any two points in  $(\mathcal{P}(X), \mathcal{W})$  may be joined by a constant-speed geodesic.

In Section 6 we derive bounds with respect to the  $L^1$ - and  $L^2$ -Wasserstein distances corresponding to the graph metric induced by the Markov chain.

Several functional inequalities are derived in Section 7 by means of the generalised evolution variational inequality which appeared in Section 3. In particular, we obtain variants for the HWI, logarithmic Sobolev, Talagrand, and Poincaré inequalities.

Finally, Appendix 8 is devoted to the logarithmic mean and all its fundamental properties which are used throughout this article.

**Notation.** Throughout this article, we will consider irreducible continuous-time Markov chains on a finite state space  $[N] = \{1, \dots, N\}$ . We will assume that corresponding infinitesimal generators, usually denoted by the letters  $A$  and  $Q$ , are row stochastic, i.e.  $A\mathbb{1} = 0$  and  $Q\mathbb{1} = 0$  for  $\mathbb{1} := \{1, \dots, N\}^\top$ .

A steady state for the infinitesimal generator  $A$  will be denoted by the row vector  $w$ . Irreducibility of the Markov chain implies that  $w$  is nowhere vanishing.

Throughout the text we will denote by  $\rho$  the density of a discrete probability measure  $u$  on  $[N]$  with respect to  $w$ , expressed in coordinates by  $\rho_i = u_i/w_i$ .

2. NON-REVERSIBLE PERTURBATIONS OF CONTINUOUS-TIME MARKOV CHAINS

In this section we are going to study time-continuous Markov chains with infinitesimal generators of the form

$$A = Q + \text{diag}(w)^{-1}\Gamma, \tag{1}$$

where  $Q$  is the generator of an irreducible and reversible Markov chain with stationary distribution  $w$  and a suitable anti-symmetric matrix  $\Gamma \in \mathbb{R}^{N \times N}$  satisfying  $\Gamma \mathbb{1} = 0$ . As direct consequence of this structure,  $w$  is a stationary distribution of  $A$  as well, however  $A$  need not be reversible.

It is easy to see that a decomposition of the form (1) always exists, provided that the infinitesimal generator  $A$  is irreducible. Indeed, in case of a finite state space,  $A$  is then positive recurrent as well. In general, both irreducibility and positive recurrence of the Markov chain imply that there exists a unique and ergodic stationary distribution  $w$  for  $A$  (see e.g. Theorem 12.25 in [Kal06]). This ensures that  $\text{diag}(w)$  is regular and  $Q$  and  $\Gamma$  are obtained via the symmetric and anti-symmetric part of the matrix  $\text{diag}(w)A$  respectively:

$$Q = \text{diag}(w)^{-1} \text{Sym}(\text{diag}(w)A) \quad \text{and} \quad \Gamma = \text{Alt}(\text{diag}(w)A).$$

As part of those considerations, it is clear that  $\Gamma$  vanishes, precisely, when the infinitesimal generator  $A$  satisfies the detailed balance condition, i.e.  $\text{diag}(w)A$  is symmetric.

A natural question is whether the non-reversible perturbation  $\Gamma$  influences the (exponential) convergence behaviour of a solution to the Kolmogorv equation  $\dot{u}(t) = A^\top u(t)$  towards the steady state  $w$ .

As a warm-up, it is easy to see that perturbed generators of the form  $A = Q + \text{diag}(w)^{-1}\Gamma$  show the same  $\ell_2$ -convergence behaviour as an unperturbed  $Q$ . Indeed, for a solution  $u(t)$  as above, we have

$$\frac{d}{dt} \frac{1}{2} \sum_i |\rho_i(t) - 1|^2 w_i = \sum_{i,j} \rho_i(t) Q_{ij} w_i \rho_j + \sum_{i,j} \rho_i(t) \Gamma_{ij} \rho_j(t) = \sum_{i,j} \rho_i^t Q_{ij} w_i \rho_j. \tag{2}$$

Next, we investigate the same question for convergence with respect to the log-entropy relative to the stationary distribution  $w$  for  $Q$ , defined by

$$\text{Ent}(u) := \sum_i u_i \log(\rho_i) \quad \text{with} \quad \rho_i = \frac{u_i}{w_i}.$$

To this aim, we have to compute the entropy production for this entropy functional, i.e. we consider a solution to the Kolmogorv equation  $\dot{u}(t) = A^\top u(t)$  and write the derivative of  $\text{Ent}$  along  $u(t)$  in the following way:

$$\begin{aligned} \frac{d}{dt} \text{Ent}(u(t)) &= \sum_i (\log \rho_i(t) + 1) \dot{u}_i(t) = \sum_{i,j} \log \rho_i(t) Q_{ji} u_j(t) + \sum_{i,j} \log \rho_i(t) \Gamma_{ji} \rho_j(t) \\ &= \frac{1}{2} \sum_{i,j} (\log \rho_i(t) - \log \rho_j(t))^2 Q_{ij} w_i \theta_{\log}(\rho_{ij}(t), \rho_j(t)) + \sum_{i,j} \log \rho_i(t) \Gamma_{ji} \rho_j(t), \end{aligned}$$

where  $\rho_i(t) = u_i(t)/w_i$  and  $\theta_{\log}$  denotes the logarithmic mean, defined for positive  $a \neq b$  by

$$\theta_{\log}(a, b) := \frac{a - b}{\log a - \log b} = \int_0^1 a^r b^{1-r} dr;$$

see Appendix 8 for properties of this mean. We identify the first term in the second line of this computation as the entropy production for the reversible part  $Q$  of the infinitesimal generator  $A$ .

In order to analyse the second term above more carefully, we write

$$\begin{aligned} T_0(u) &:= \sum_{i,j} \log \rho_i \Gamma_{ji} \rho_j = \frac{1}{2} \sum_{i,j} (\log \rho_i - \log \rho_j) \Gamma_{ji} (\rho_i + \rho_j) \\ &= \sum_{\substack{i,j \\ i < j}} (\log \rho_i - \log \rho_j) \Gamma_{ji} (\rho_i + \rho_j). \end{aligned}$$

Note that this term usually does not vanish, in contrast to the entropy production for solutions of a Fokker-Plank equations, where a *divergence-free condition* is enough to ensure that the corresponding term vanishes (cf. [AAS15], [ACJ08]).

The following simple example allows us to get a glimpse of how a non-reversible perturbation may influence convergence with respect to log-entropy.

**Example 2.1.** We consider an infinitesimal generator of form  $A = Q + \text{diag}(w)^{-1} \Gamma$  with

$$Q = \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}, \quad \Gamma = \frac{1}{4} \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{pmatrix}, \quad w = \frac{1}{3}(1, 1, 1),$$

in order to find optimal  $\lambda_Q > 0$  and  $\lambda_A > 0$  such that

$$\text{Ent}(u) \leq -\frac{1}{2\lambda_Q} \sum_{i,j} \log \rho_j Q_{ij} u_i \quad \forall u \in \mathcal{P}_3 \quad (3)$$

and

$$\text{Ent}(u) \leq -\frac{1}{2\lambda_A} \sum_{i,j} \log \rho_j Q_{ij} u_i + \sum_{i,j} \log \rho_i \Gamma_{ij} \rho_j \quad \forall u \in \mathcal{P}_3, \quad (4)$$

respectively.

Due to the particularly simple structure of (3), a numerical analysis of this inequality is rather straightforward: Indeed, for computation of the optimal values we employ the `fmincon` function for numerical minimisation under constraints in MATLAB. As a result, we obtain

$$\begin{aligned} \lambda_Q &\approx 2.94 \quad \text{attained at} \quad u_Q \approx \frac{1}{4}(2, 1, 1), \\ \lambda_A &\approx 2.83 \quad \text{attained at} \quad u_A \approx \frac{1}{100}(61, 14, 25). \end{aligned} \quad (5)$$

We deduce that the perturbed infinitesimal generator  $A$  behaves worse with respect to convergence in log-entropy when compared to the unperturbed  $Q$ .



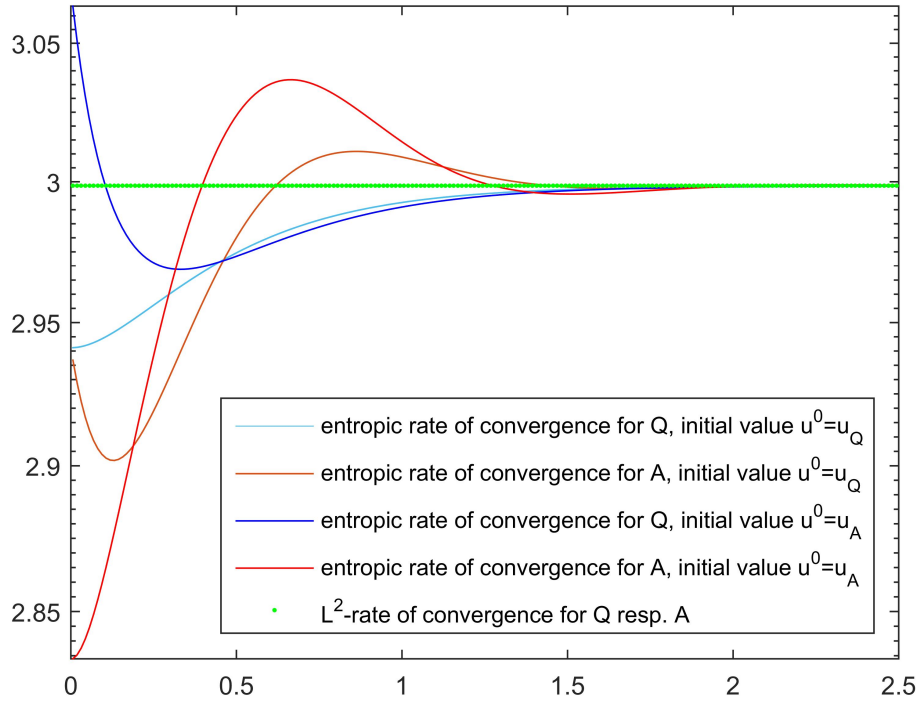


FIGURE 1. Rates of convergence along flows  $(u^t)_{t>0}$  as given for the entropy by  $-\frac{1}{2}(\frac{d}{dt} \text{Ent}(u^t))/\text{Ent}(u^t)$  and for the variance by  $-\frac{1}{2}(\frac{d}{dt} \text{var}_w(u^t))/\text{var}_w(u^t)$ , respectively. The initial values  $u^0$  for the flows along  $Q$  and  $A$  are given by the respective values  $u_Q$  and  $u_A$  as defined in (5).

### 3. THE MODIFIED ONSAGER OPERATOR FOR NON-REVERSIBLE MARKOV CHAINS

In this section, we investigate exponential convergence of a solution to the Kolmogorov equation  $\dot{u}(t) = A^\top u(t)$  towards the steady state  $w$  with respect to the distance  $\mathcal{W}$ . To this aim, we will extend the framework of Ricci curvature from reversible Markov chains to non-reversible ones, which allows us to obtain rates for exponential convergence in terms of  $\mathcal{W}$ .

**Notation.** Throughout the following sections,  $A$  denotes the infinitesimal generator of an irreducible continuous-time Markov chain on a finite state space  $[N]$ . Moreover, we assume that  $A$  satisfies the following condition

$$\forall i, j \in [N] : A_{ij} > 0 \Rightarrow A_{ji} > 0. \quad (6)$$

Note that (6) implies that the infinitesimal generator can be written in form of a (usually non-unique) decomposition  $A = Q \circ B$ , where  $Q$  denotes a reversible, irreducible continuous-time Markov chain with unique nowhere-vanishing stationary distribution  $w$ ,  $B$  is a perturbation matrix with strictly positive elements, and  $Q \circ B$  is the *Schur product* of the matrices  $Q$  and  $B$  given by elementwise multiplication  $(Q \circ B)_{ij} := Q_{ij}B_{ij}$ .

Indeed, starting with an infinitesimal generator of form (1), we see that

$$B_{ij} = 1 + \frac{1}{w_i} \frac{\Gamma_{ij}}{Q_{ij}} \quad \forall i, j \in [N] : Q_{ij} \neq 0.$$

Moreover, for a discrete probability measure  $u$  on  $[N]$ ,  $\rho$  denotes the corresponding density function, given by  $\rho_i := u_i/w_i$ .

**Definition 3.1.** We define the *Onsager operator* with respect to a generator  $A = Q \circ B$  as the symmetric matrix

$$\check{\mathbb{K}}(u) := \frac{1}{2} \sum_{i,j} \check{K}_{ij}(u) (e_i - e_j) \otimes (e_i - e_j),$$

where the coefficients  $\check{K}_{ij}(u)$  are given by the logarithmic mean

$$\check{K}_{ij}(u) := \frac{A_{ij}u_i - A_{ji}u_j}{\log(A_{ij}u_i) - \log(A_{ji}u_j)} = Q_{ij}w_i \frac{B_{ij}\rho_i - B_{ji}\rho_j}{\log \rho_i - \log \rho_j + \log B_{ij} - \log B_{ji}}. \quad (7)$$

Here we made use of the detailed balance condition  $Q_{ij}w_i = Q_{ji}w_j$  to establish the second equality in (7). As a result, the Onsager operator  $\check{\mathbb{K}}$  does not depend on the particular decomposition of  $A$  in terms of  $Q$  and  $B$ .

For a matrix  $L \in \mathbb{R}^{N \times N}$  we introduce the notation

$$\check{\mathbb{K}}(u)[L] := \frac{1}{2} \sum_{i,j} \check{K}_{ij}(u) (L_{ij} - L_{ji}) (e_i - e_j).$$

*Remark 3.2.* For a vector  $\xi \in \mathbb{R}^N$ , the expression  $\check{\mathbb{K}}(u)[L]$  is related to  $\check{\mathbb{K}}(u)$  by the identity

$$\xi^\top \check{\mathbb{K}}(u) \eta = \xi^\top \check{\mathbb{K}}(u)[L] \quad (8)$$

with a matrix  $L_{ij} = \frac{1}{2}(\eta_i - \eta_j)$ .

Conversely, for every matrix  $L \in \mathbb{R}^{N \times N}$ , the vector  $\check{\mathbb{K}}(u)[L]$  belongs to  $\text{span}\{\mathbb{1}\}^\perp$ . Hence, one may choose

$$\xi = \check{\mathbb{K}}^{-1}(u) \check{\mathbb{K}}(u)[L] \quad (9)$$

such that (8) holds. Note that the vector  $\xi$  in general depends on the point  $u$ .

In addition, we introduce the following functionals:

First, we recall the log-entropy relative to the stationary distribution  $w$  for  $Q$ , defined by

$$\text{Ent}(u) := \sum_i u_i \log(u_i/w_i).$$

Consider a pair  $(g^t, \zeta^t)_{t \in [0,1]}$  of piecewise smooth curves of discrete probability measures  $g^t$  and vectorfields  $\zeta^t$  in  $\mathbb{R}^N$ , satisfying the *continuity equation*

$$\frac{d}{dt}g^t = \check{\mathbb{K}}(g^t)\zeta^t \tag{c\epsilon}$$

for all times  $t \in [0, 1]$ . Then we define

$$V_\tau(g) := \int_0^\tau (\zeta^r)^\top \check{\mathbb{K}}(g^r)[L] dr \quad \text{with } L_{ij} = \log B_{ij} \quad \forall \tau \in [0, 1].$$

*Remark 3.3.* In case, we have  $L_{ij} = v_i - v_j$  for some vector  $v \in \mathbb{R}^N$ , the functional  $V_1$  depends only on the end-points of the curve  $g$ . Indeed,

$$V_\tau(g) = \int_0^\tau (\zeta^r)^\top \check{\mathbb{K}}(g^r)v dr = \int_0^\tau (\dot{g}^r)^\top v dr = (g^\tau - g^0)^\top v.$$

**Lemma 3.4.** *For every nowhere-vanishing probability measure  $u$ , the Onsager operator  $\check{K}(u)$  is positive definite on  $\text{span}\{\mathbb{1}\}^\perp$ .*

*Proof.* Given  $\zeta \in \text{span}\{\mathbb{1}\}^\perp$ , we can find indices  $i_1, j_K$  such that  $\zeta_{i_1} - \zeta_{j_K}$  does not vanish. Additionally, the irreducibility of  $A$  implies that there exist  $(i_k, j_k)$  such that  $A_{i_k, j_k} > 0$  for all  $1 \leq k \leq K$  and  $j_k = i_{k+1}$  for all  $1 \leq k < K$ . Note that we also have  $A_{j_k, i_k} > 0$ , due to our assumption in (6). We infer that  $\check{K}_{i_k, j_k} > 0$  for all  $1 \leq k \leq K$ . As  $\zeta_{i_k} - \zeta_{j_k} \neq 0$  for at least one  $k$ , we conclude that  $\zeta^\top \check{\mathbb{K}}(u)\zeta > 0$ .  $\square$

**Notation.** Let us denote by  $\mathcal{P}_N$  the (discrete) probability measures on  $[N]$ . Then  $\text{int } \mathcal{P}_N$  is precisely the subset of nowhere-vanishing probability measures on  $[N]$ .

Now the preceding lemma tells us that  $\check{K}$  is invertible on  $\text{int } \mathcal{P}_N$ . Since  $\check{K}$  is symmetric, we obtain the following result.

**Corollary 3.5.** *The Onsager operator  $\check{\mathbb{K}}(u)$  is symmetric and invertible for all  $u \in \text{int } \mathcal{P}_N$ . In particular,  $\mathbb{G} = \check{\mathbb{K}}^{-1}$  defines a Riemannian metric on the embedded submanifold  $\text{int } \mathcal{P}_N \subseteq \mathbb{R}^N$ .*

As a consequence,  $\text{int } \mathcal{P}_N$  is endowed with a Riemannian distance  $\mathcal{W}$  which in terms of the Onsager operator may be expressed as

$$\mathcal{W}^2(u, v) := \inf \int_0^1 (\zeta^t)^\top \check{\mathbb{K}}(g^t)\zeta^t dt \tag{10}$$

where the infimum is taken over all pairs  $(g^t, \zeta^t)_{t \in [0,1]}$  of piecewise smooth curves, satisfying the continuity equation (c\epsilon) such that  $g$  joins  $u$  to  $v$ .

*Remark 3.6.* Note that  $V_\tau$  depends on the parametrisation of the curve. In particular, we have the following transformation rule as a consequence of the change of variables formula: For every constant-speed geodesic  $g : [0, 1] \rightarrow \text{int } \mathcal{P}_N$  with corresponding reparametrised constant-speed geodesic segments  $g^{g^s \rightarrow g^t} : [0, 1] \rightarrow \text{int } \mathcal{P}_N$  connecting  $g^s$  to  $g^t$  for  $s, t \in [0, 1]$ , we have

$$V_1(g^{g^s \rightarrow g^t}) = V_t(g) - V_s(g) \quad \forall s, t \in [0, 1]. \tag{11}$$

In particular, this transformation rule implies for a change of orientation  $V_1(g^{\gamma^0 \rightarrow \gamma^1}) = -V_1(g^{\gamma^1 \rightarrow \gamma^0})$ .

**Lemma 3.7.** *Let  $(g^t, \zeta^t)_{t \in [0,1]}$  be a pair of curves, satisfying  $(\mathbf{c}\epsilon)$  with initial conditions  $g^0 = u$  and  $\zeta^0 = \xi$ . Then we have the identity*

$$\begin{aligned} \frac{d}{d\tau} \Big|_{\tau=0} (\text{Ent}(g^\tau) + V_\tau(g)) = \\ \frac{1}{2} \sum_{i,j} (\xi_i - \xi_j) \check{K}_{ij}(u) (\log \rho_i - \log \rho_j + \log B_{ij} - \log B_{ji}) = - \sum_{i,j} \xi_i A_{ji} u_j. \end{aligned} \quad (12)$$

In perspective of the *Kolmogorov forward equation*

$$\frac{d}{dt} u^t = A^\top u \quad \text{in } \text{int } \mathcal{P}_N, \quad (13)$$

Lemma 3.7 states that (13) is actually equivalent to the variational equation

$$\frac{d}{dt} u^t = -\text{grad}_{\mathbb{G}} \text{Ent}(u^t) - \check{\mathbb{K}}(u^t)[L] \quad \text{with } L_{ij} = \log B_{ij} \quad \text{in } \text{int } \mathcal{P}_N, \quad (14)$$

where  $\text{grad}_{\mathbb{G}} \text{Ent}(u^t) = \check{\mathbb{K}}(u^t) \nabla \text{Ent}(u^t)$  denotes the gradient of  $\text{Ent}$  with respect to the Riemannian metric  $\mathbb{G} = \check{\mathbb{K}}^{-1}$ .

In order to verify (14), take geodesics pairs  $(g^\tau, \zeta^\tau)_{\tau \in [0,1]}$  with initial values  $g_0 = u^t$  and  $\zeta^0 = \xi$ , such that equation (12) becomes

$$\xi^\top \check{\mathbb{K}}(u^t) \nabla \text{Ent}(u^t) + \xi^\top \check{\mathbb{K}}(u^t)[L] = -(A\xi)^\top u^t. \quad (15)$$

Since this equality holds for all initial velocity vectors  $\xi \in \mathbb{R}^N$ , we infer the equivalence of (13) and (14).

*Proof of Lemma 3.7.* The first equality in (12) follows directly from the chain rule applied to  $\tau \mapsto \text{Ent}(g^\tau) + V_\tau(g)$ , together with application of the continuity equation  $(\mathbf{c}\epsilon)$ .

For the second equality in (12), with the definition of the Onsager operator at hand, we arrive at

$$\sum_{i,j} (\xi_i - \xi_j) \check{K}_{ij}(u) (\log \rho_i - \log \rho_j + B_{ij} - B_{ji}) = \frac{1}{2} \sum_{i,j} (\xi_i - \xi_j) (A_{ij} u_i - A_{ji} u_j).$$

To conclude, we use the fact that  $\sum_i A_{ji} = 0$ . □

For point (iv) in the theorem below, we recall that the *upper right-hand Dini derivative* of a real-valued function  $f$  is defined as

$$\frac{d^+}{dt} f := \limsup_{h \searrow 0} \frac{f(t+h) - f(t)}{h}.$$

We present the main result of this section.

**Theorem 3.8.** *For a constant  $\lambda \in \mathbb{R}$  the following statements are equivalent:*

(i) *In the sense of positive semidefinite matrices,*

$$M(u) \geq \lambda \check{\mathbb{K}}(u) \quad \forall u \in \text{int } \mathcal{P}_N, \quad (16)$$

where the matrix  $M(u)$  is given by

$$M(u) = D_u \chi(u) \check{\mathbb{K}}(u) - \frac{1}{2} D_u \check{\mathbb{K}}(u) (\chi(u)) \quad (17)$$

$$= -A^\top \check{\mathbb{K}}(u) + \frac{1}{2} D_u \check{\mathbb{K}}(u) (A^\top u), \quad (18)$$

where  $\chi$  is a vectorfield given by

$$\chi(u) = \check{\mathbb{K}}(u) \nabla_u \text{Ent}(u) + \check{\mathbb{K}}(u) [L] = -A^\top u \quad \text{with } L_{ij} = \log B_{ij}.$$

(ii) For every smooth constant-speed geodesic pair  $(g^t, \zeta^t)_{t \in [0,1]}$  satisfying  $(\mathbf{c}\epsilon)$  in  $\text{int } \mathcal{P}_N$ ,

$$\frac{d^2}{dt^2} (\text{Ent}(g^t) + V_t(g)) \geq \lambda (\zeta^t)^\top \check{\mathbb{K}}(g^t) \zeta^t. \quad (19)$$

(iii) Along every constant-speed geodesic  $(g^t)_{t \in [0,1]}$  in  $\text{int } \mathcal{P}_N$ , the function  $t \mapsto \text{Ent}(g^t) + V_t(g)$  is  $\lambda$ -convex.

(iv) Every solution  $(u^t)_{t \geq 0}$  of the Kolmogorov forward equation

$$\frac{d}{dt} u_i^t = \sum_j A_{ji} u_j^t \quad \text{in } \text{int } \mathcal{P}_N \quad (20)$$

satisfies the modified evolution variational inequality

$$\frac{1}{2} \frac{d^+}{dt} \mathcal{W}^2(u^t, v) + \frac{\lambda}{2} \mathcal{W}^2(u^t, v) \leq \text{Ent}(v) - \text{Ent}(u^t) + V_1(g) \quad \forall t > 0, \quad (\text{EVI}_{\lambda, \infty})$$

for all  $v \in \text{int } \mathcal{P}_N$  and every constant-speed geodesic  $(g^t)_{t \in [0,1]}$  joining  $u^t$  to  $v$  in  $\text{int } \mathcal{P}_N$ .

(v) For every point  $z \in \text{int } \mathcal{P}_n$  there exists a geodesic ball  $B$  centred at  $z$  such that every two solutions  $(u^t)_{t \in [0, \varepsilon]}, (v^t)_{t \in [0, \varepsilon]} \subset B$  of the Kolmogorov forward equation (20) satisfies the local contraction property

$$\mathcal{W}(u^t, v^t) \leq e^{-\lambda t} \mathcal{W}(u^0, v^0) \quad \forall t \in [0, \varepsilon]. \quad (21)$$

*Remark 3.9.* Note that the expression  $-A^\top \check{\mathbb{K}}(u)$  appearing in the definition of  $M(u)$  need not be symmetric, contrary to  $D_u \check{\mathbb{K}}(u) (\chi(u))$  which is symmetric by definition of the modified Onsager operator  $\check{K}$ . Nevertheless, one may replace this expression with its symmetric part, that is  $-\text{Sym}(A^\top \check{\mathbb{K}}(u))$ , with no loss of generality.

In case, the infinitesimal generator  $A$  is reversible, say  $B_{ij} = 1$ , the functional  $V_\tau$  vanishes for all  $\tau$ . Then the expression  $M(u)$  corresponds to the so-called *contravariant representation of the Hessian* of the functional  $\text{Ent}(u)$  with respect to the Riemannian metric  $\mathbb{G} = \check{\mathbb{K}}^{-1}$ .

*Proof of Theorem 3.8. (i  $\Leftrightarrow$  ii).* By introducing the shorthand notation  $Y_{ij}(u) := \frac{1}{2} (\log \rho_i - \log \rho_j) + \log B_{ij}$ , we may express the vector field in (17) as  $\chi(u) = \check{\mathbb{K}}(u) [Y(u)]$ .

We start by computing the second derivative of  $r \mapsto \text{Ent}(g^r) + V_r(g)$  along a constant-speed geodesic pair  $(g^t, \zeta^t)_{t \in [0,1]}$  satisfying  $(\mathbf{c}\epsilon)$  in  $\text{int } \mathcal{P}_N$  viz.

$$\begin{aligned} & \frac{d^2}{dr^2} (\text{Ent}(g^r) + V_r(g)) = \frac{d}{dr} (D_u \text{Ent}(g^r) \check{\mathbb{K}}(g^r) \zeta^r + \check{\mathbb{K}}(g^r) [L]) \\ &= \frac{d}{dr} ((\zeta^r)^\top \check{\mathbb{K}}(g^r) [Y(g^r)]) = \frac{d}{dr} ((\zeta^r)^\top \chi(g^r)) = (\dot{\zeta}^r)^\top \chi(g^r) + (\zeta^r)^\top D_u \chi(g^r) \check{\mathbb{K}}(g^r) \zeta^r. \end{aligned}$$

By their very definition in terms of Riemannian geometry, constant-speed geodesics satisfy  $\frac{d}{dr}\langle \dot{g}^r, \dot{g}^r \rangle_{\mathbb{G}} = 0$ , which expands into the geodesic equation

$$\dot{\zeta}^r + \frac{1}{2} \frac{d}{du} \Big|_{u=g^r} (\zeta^r)^\top \check{\mathbb{K}}(u) \zeta^r = 0. \quad (22)$$

Hence, using (22), we infer that

$$\frac{d^2}{dr^2} \left( \text{Ent}(g^r) + V_r(g) \right) = -\frac{1}{2} (\zeta^r)^\top D_u \check{\mathbb{K}}(g^r) (\chi(g^r)) \zeta^r + (\zeta^r)^\top D_u \chi(g^r) \check{\mathbb{K}}(g^r) \zeta^r.$$

Evaluating this equation at time  $r = 0$  for a geodesic  $g^t$  starting from  $g^0 = u$ , establishes the expression for  $M(u)$  as in line (17). Finally, the expression in (18) follows from the simple identity  $\chi(u) = -A^\top u$ .

(*ii*  $\Rightarrow$  *iii*). This is a standard argument of convex analysis (see e.g. Proposition 16.2 in [Vil08]).

(*iii*  $\Rightarrow$  *iv*). Let  $(g^\tau, \zeta^\tau)_{\tau \in [0,1]}$  be a smooth constant-speed geodesic pair joining  $u^t$  to  $v$  in  $\text{int } \mathcal{P}_N$ , satisfying (c $\epsilon$ ). Then by the *first variational formula of Riemannian geometry*, we have

$$\frac{1}{2} \frac{d^+}{dt} \mathcal{W}^2(u^t, v) = -\langle \dot{g}^0, \dot{u}^t \rangle_{\mathbb{G}} = -\sum_{i,j} \xi_i A_{ji} u_j(t).$$

Together with (12), we arrive at

$$\frac{1}{2} \frac{d^+}{dt} \mathcal{W}^2(u^t, v) \leq \frac{d}{d\tau} \Big|_{\tau=0} (\text{Ent}(g^\tau) + V_\tau(g)). \quad (23)$$

To conclude, we note that  $\lambda$ -convexity of  $t \mapsto \text{Ent}(g^t) + V_t(g)$  in differential form reads as

$$\frac{d}{d\tau} \Big|_{\tau=0} (\text{Ent}(g^\tau) + V_\tau(g)) \leq \text{Ent}(v) - \text{Ent}(u^t) + V_1(g) - \frac{\lambda}{2} \mathcal{W}^2(u^t, v),$$

which, together with (23), implies (EVI $_{\lambda, \infty}$ ).

(*iv*  $\Rightarrow$  *v*). Adding up (EVI $_{\lambda, \infty}$ ), once for a curve  $u_1$  at time  $t > 0$  with  $v = u_2^s$ , and once for a curve  $u_2$  at time  $s > 0$  with  $v = u_1^t$ , we arrive at the inequality

$$\frac{1}{2} \frac{d^+}{dt} \mathcal{W}^2(u_1^t, u_2^s) + \frac{1}{2} \frac{d^+}{ds} \mathcal{W}^2(u_1^t, u_2^s) + \lambda \mathcal{W}^2(u_1^t, u_2^s) \leq V_1(g^{u_1^t \rightarrow u_2^s}) + V_1(g^{u_2^s \rightarrow u_1^t}). \quad (24)$$

We may choose the initial conditions  $u_1^0$  and  $u_2^0$  close enough and  $\varepsilon > 0$  small enough such that for all  $t \leq \varepsilon$ , both curves  $u_1^t$  and  $u_2^t$  belong to some geodesic ball  $B$ . We may choose the radius of this geodesic ball  $B$  small enough such that any two points in  $B$  are connected by a unique geodesic. Thus,  $g^{u_1^t \rightarrow u_2^s}$  and  $g^{u_2^s \rightarrow u_1^t}$  describe the same curve up to parametrisation. In particular, the right-hand side of this inequality cancels out, due to reparametrisation property (11) of the functional  $V_1$ . Moreover, setting  $s = t$ , we may invoke Lemma 4.3.4 in [AGS08] to estimate the time derivative of  $\frac{1}{2} \mathcal{W}^2(u_1^t, u_2^t)$  in terms of the two upper-right Dini derivatives appearing on the left-hand side of (24). Therefore, we arrive at

$$\frac{d}{dt} \mathcal{W}^2(u_1^t, u_2^t) \leq -2\lambda \mathcal{W}^2(u_1^t, u_2^t) \quad \text{a.e. } t \in [0, \varepsilon],$$

which in turn yields the contraction property via an application of *Grönwall's inequality* (see e.g. Theorem 2.1.1 in [Qin17]).

( $v \Rightarrow ii$ ). First we notice that the contraction property (21) implies the differential inequality

$$\frac{d^+}{dt} \mathcal{W}^2(u^t, v^t) \Big|_{t=0} \leq -2\lambda \mathcal{W}^2(u^0, v^0). \tag{25}$$

Indeed, as equality holds in (21) for  $t = 0$ , we may pass to the upper right-hand Dini derivative on both sides of the contraction estimate as  $t \searrow 0$  to arrive at (25).

Now we show that (25) actually implies (19). To this aim, we invoke the first variational formula of Riemannian geometry for the geodesic  $g^\tau = \exp_{u^0}(\varepsilon\tau y)$  joining points  $u^0$  to  $v^0 = \exp_{u^0}(\varepsilon y)$  for some non-vanishing vector  $y$  in the tangent space at  $u^0$ . Hence, we compute

$$\begin{aligned} \frac{d^+}{dt} \mathcal{W}^2(u^t, v^t) \Big|_{t=0} &= \frac{1}{2} (\langle \dot{g}^0, \dot{u}^0 \rangle_{\mathbb{G}} - \langle \dot{g}^1, \dot{v}^0 \rangle_{\mathbb{G}}) = -\frac{1}{2} \frac{d}{d\tau} \Big|_{\tau=0}^1 (\text{Ent}(g^\tau) + V_\tau(g)) \\ &= -\frac{\varepsilon}{2} \frac{d}{d\tau} \Big|_{\tau=0}^\varepsilon (\text{Ent}(\tilde{g}^\tau) + V_\tau(\tilde{g})) = -\frac{\varepsilon}{2} \int_0^\varepsilon \frac{d^2}{d\tau^2} (\text{Ent}(\tilde{g}^\tau) + V_\tau(\tilde{g})) d\tau, \end{aligned}$$

where we used transformation rule (11) in form of  $V_\tau(g) = V_{\varepsilon\tau}(\tilde{g})$  for the rescaled geodesic  $\tilde{g}^\tau := \exp_{u^0}(\tau y)$ . Combining this equation with (25) and using that  $\mathcal{W}(u^0, v^0) = \varepsilon|y|_{\mathbb{G}}$ , we arrive at

$$\lambda|y|_{\mathbb{G}}^2 = \frac{\lambda}{\varepsilon^2} \mathcal{W}^2(u^0, v^0) \leq \frac{1}{\varepsilon} \int_0^\varepsilon \frac{d^2}{d\tau^2} (\text{Ent}(\tilde{g}^\tau) + V_\tau(\tilde{g})) d\tau. \tag{26}$$

Passing to the limit in (26) as  $\varepsilon \searrow 0$ , we conclude that

$$\lambda|y|_{\mathbb{G}}^2 \leq \frac{d^2}{d\tau^2} \Big|_{\tau=0} (\text{Ent}(\tilde{g}^\tau) + V_\tau(\tilde{g})).$$

□

**Example 3.10.** Let  $A$  be the infinitesimal generator of a Markov chain which satisfies one of the equivalent  $\lambda$ -convexity conditions in Theorem 3.8 for some  $\lambda \in \mathbb{R}$ . Then for  $\kappa > 0$ , the *lazy Markov chain* with infinitesimal generator  $A_\kappa := \kappa A$  is  $(\kappa\lambda)$ -convex.

Indeed, this follows directly from (16), together with the 2-homogeneity of  $M(u)$  and the 1-homogeneity of  $\mathbb{K}(u)$ , both in the variable  $\kappa$  for the underlying infinitesimal generator  $A_\kappa$ .

**Example 3.11.** Let  $(A^m)_{m \leq \bar{m}}$  be a finite family of infinitesimal generators  $A^m = Q^m \circ B^m$ , each of an irreducible Markov chain on  $[N^m]$ , satisfying (6) with stationary distribution  $w^m$  for  $Q^m$ . Let  $(\kappa_m)_{m \leq M}$  be positive weights. Consider the *product chain* on  $\prod_m [N^m]$  with an infinitesimal generator given for multi-indices  $\mathbf{i} = (i_1, \dots, i_{\bar{m}})$  and  $\mathbf{j} = (j_1, \dots, j_{\bar{m}})$  by

$$A_{\mathbf{i}, \mathbf{j}} = \begin{cases} \kappa_m A_{i_m j_m}^m & \text{if } i_k = j_k \text{ for precisely one } k = m, \\ -\sum_m \kappa_m A_{i_m i_m}^m & \text{if } i_k = j_k \text{ for all } k \in \{1, \dots, \bar{m}\}, \\ 0 & \text{otherwise.} \end{cases}$$

Note that the product chain corresponding to  $A$  is again irreducible. Likewise, we define

$$Q_{\mathbf{i}, \mathbf{j}} = \begin{cases} \kappa_m Q_{i_m j_m}^m & \text{if } i_k = j_k \text{ for precisely one } k = m, \\ -\sum_m \kappa_m Q_{i_m i_m}^m & \text{if } i_k = j_k \text{ for all } k \in \{1, \dots, \bar{m}\}, \\ 0 & \text{otherwise.} \end{cases}$$

Note that the product chain corresponding to  $Q$  is both irreducible and reversible with unique stationary distribution  $w = w^1 \otimes \dots \otimes w^m$ .

The following result clarifies how the product chain inherits  $\lambda$ -convexity from the infinitesimal generators  $(A^m)_{m \leq \bar{m}}$ .

**Proposition 3.12.** *Let  $(A^m)_{m \leq \bar{m}}$  be a finite family of infinitesimal generators as in Example 3.11, together with corresponding Onsager operators  $(\check{\mathbb{K}}^m)_{i \leq \bar{m}}$ . Assume for each  $m \in \{1, \dots, \bar{m}\}$ , there exists  $\lambda_m \in \mathbb{R}$  such that  $A^m$  satisfies the  $\lambda_m$ -convexity condition*

$$M^m(u^m) \geq \lambda_m \check{\mathbb{K}}^m(u^m) \quad \forall u^m \in \mathcal{P}_{N^m} \quad (27)$$

of Theorem 3.8. Then the infinitesimal generator of the product chain is  $\lambda$ -convex for  $\lambda := \min_m \{\lambda_m\}$  in the sense of Theorem 3.8.

*Proof.* We express the the corresponding terms for the product chain by

$$M(u) = \frac{1}{2} D_u \check{\mathbb{K}}(u) (A^\top u) - A^\top \check{\mathbb{K}}(u)$$

with

$$\begin{aligned} \frac{1}{2} D_u \check{\mathbb{K}}(u) (A^\top u) &= \frac{1}{4} \sum_{i,j,l} \left( \partial_1 \theta_{\log}(A_{ij} u_i, A_{ji} u_j) A_{ij} A_{li} \right. \\ &\quad \left. + \partial_2 \theta_{\log}(A_{ij} u_i, A_{ji} u_j) A_{ji} A_{lj} \right) u_l (e_i - e_j) \otimes (e_i - e_j) \end{aligned} \quad (28)$$

and

$$A^\top \check{\mathbb{K}}(u) = \frac{1}{2} \sum_{i,j,l} \theta_{\log}(A_{ij} u_i, A_{ji} u_j) (A_{li} - A_{lj}) e_l \otimes (e_i - e_j). \quad (29)$$

Due to the special structure of the infinitesimal generator of the product chain, we note that, in order for a term inside the sum of either (28) or (29) not to vanish,  $i_m \neq j_m$  is required for at least one subindex  $m \in \{1, \dots, \bar{m}\}$ . As a result, using the notation  $\delta_{i \neq j} := 1 - \delta_{ij}$ , we may write

$$\frac{1}{2} D_u \check{\mathbb{K}}(u) (A^\top u) = \sum_{\substack{m,n \\ m \neq n}} \sum_{\substack{i_m, j_m \\ i_m \neq j_m}} \sum_{\substack{i_n, l_n \\ i_n \neq l_n}} \Xi_{i_n i_n l_n}^{i_m j_m} + \sum_m \sum_{\substack{i_m, j_m \\ i_m \neq j_m}} \sum_{l_m} \Xi_{i_m j_m l_m}^{i_m j_m} \quad (30)$$

with

$$\begin{aligned} \Xi_{i_n, j_n, l_n}^{i_m j_m} &= \frac{1}{4} \left( \partial_1 \theta_{\log}(A_{i_m j_m}^m u_{i_m}, A_{j_m i_m}^m u_{j_m}) A_{i_m j_m}^m A_{l_n i_n}^n \delta_{l_n \neq i_n} \right. \\ &\quad \left. + \partial_2 \theta_{\log}(A_{i_m j_m}^m u_{i_m}, A_{j_m i_m}^m u_{j_m}) A_{j_m i_m}^m A_{l_n j_n}^n \delta_{l_n \neq j_n} \right) u_{l_n} (e_{i_m} - e_{j_m}) \otimes (e_{i_m} - e_{j_m}) \end{aligned}$$

and

$$A^\top \check{\mathbb{K}}(u) = \sum_{\substack{m,n \\ m \neq n}} \sum_{\substack{i_m, j_m \\ i_m \neq j_m}} \sum_{\substack{i_n, l_n \\ i_n \neq l_n}} \Pi_{i_n i_n l_n}^{i_m j_m} + \sum_m \sum_{\substack{i_m, j_m \\ i_m \neq j_m}} \sum_{l_m} \Pi_{i_m j_m l_m}^{i_m j_m} \quad (31)$$

with

$$\Pi_{i_n, j_n, l_n}^{i_m j_m} = \frac{1}{2} \theta_{\log}(A_{i_m j_m}^m u_{i_m}, A_{j_m i_m}^m u_{j_m}) (A_{l_n i_n}^n \delta_{l_n \neq i_n} - A_{l_n j_n}^n \delta_{l_n \neq j_n}) e_{l_n} \otimes (e_{i_m} - e_{j_m}).$$



Due to (63) and (64), the expression  $\Xi_{i_n, j_n, l_n}^{i_m, j_m}$  is always non-negative for any  $i_m \neq j_m$  or any  $i_n = j_n \neq l_n$ . In addition,  $\Pi_{i_n, j_n, l_n}^{i_m, j_m}$  vanishes when  $i_n = j_n$ . Therefore, we may ignore the respective sums with  $m \neq n$  in (30) and (31), which yields

$$\begin{aligned} M(u) &\geq \sum_m \sum_{\substack{i_m, j_m \\ i_m \neq j_m}} \sum_{l_m} (\Xi_{i_m, j_m, l_m}^{i_m, j_m} - \Pi_{i_m, j_m, l_m}^{i_m, j_m}) = \sum_m \sum_{i_m, j_m} M_{i_m, j_m}^m(u^m) e_{i_m} \otimes e_{j_m} \\ &\geq \sum_m \lambda_m \sum_{i_m, j_m} \check{\mathbb{K}}_{i_m, j_m}^m(u^m) e_{i_m} \otimes e_{j_m} \\ &\geq \min_m \{\lambda_m\} \sum_m \sum_{i_m, j_m} \check{\mathbb{K}}_{i_m, j_m}^m(u^m) e_{i_m} \otimes e_{j_m} = \min_m \{\lambda_m\} \check{\mathbb{K}}(u), \end{aligned}$$

where we used (27) to pass from the first to the second line. This means that the infinitesimal generator  $A$  of the product chain is  $\lambda$ -convex for  $\lambda := \min_m \{\lambda_m\}$  in the sense of Theorem 3.8.  $\square$

#### 4. LOWER CONVEXITY BOUNDS IN TERMS OF THE INFINITESIMAL GENERATOR

Lower bounds for the convexity parameter  $\lambda$  of Theorem 3.8 in terms of the infinitesimal generator  $A$  are provided by the following technical result.

**Proposition 4.1.** *Assume an infinitesimal generator  $A$  is given such that  $A_{ij} > 0$  for all off-diagonal entries  $i \neq j$ . Then the convexity parameter  $\lambda$  of Theorem 3.8 always belongs to  $\mathbb{R}$ , satisfying the lower bound*

$$\lambda \geq -\frac{1}{2} \max_{i, j} \left\{ \bar{\mu}_{ij} + \sum_{n \notin \{i, j\}} \tilde{\mu}_{ij}^n \right\}, \quad (32)$$

where the constants  $\bar{\mu}_{ij}$  and  $\tilde{\mu}_{ijl}$  are given by

$$\bar{\mu}_{ij} := \max\{A_{ii}, A_{jj}\} - A_{ij} - A_{ji} - \min\{A_{ij}, A_{ji}\},$$

and

$$\tilde{\mu}_{ij}^n := \min\{A_{ij}A_{ni}, A_{ji}A_{nj}\} \tilde{g}(\beta_{ijn}^{\max} / \beta_{ijn}^{\min})$$

respectively, with  $\tilde{g}(\beta_{ij}^n)$  expressed in terms of the function  $\tilde{g}$  as in (72) and constants

$$\begin{aligned} \beta_{ijn}^{\max} &:= \max\left\{0, (A_{ni} - A_{ji})A_{nj}, (A_{ni} - A_{ji})\frac{A_{jn}}{A_{ji}}, (A_{nj} - A_{ij})A_{ni}, (A_{nj} - A_{ij})\frac{A_{in}}{A_{ij}}\right\}, \\ \beta_{ijn}^{\min} &:= \min\{A_{ij}A_{ni}, A_{ji}A_{nj}\}. \end{aligned} \quad (33)$$

For the proof, we will make use of the following simple observation.

**Lemma 4.2.** *The positive semidefiniteness condition*

$$M(u) \geq \lambda \check{\mathbb{K}}(u) \quad \forall u \in \text{int } \mathcal{P}_N \quad (34)$$

of Theorem 16.i holds for some constant  $\lambda \in \mathbb{R}$ , provided that for every  $u \in \text{int } \mathcal{P}_N$ , the matrices  $M(u)$  and  $\check{\mathbb{K}}(u)$  satisfy the elementwise relation

$$\text{Sym } M_{ij}(u) \leq -\lambda \check{\mathbb{K}}_{ij}(u) \quad \forall i, j \in [N] : i \neq j. \quad (35)$$

In the the vein of Remark 3.9, one may replace the matrix  $M(u)$  in (35) by its symmetric part  $\text{Sym } M(u)$ .

*Proof.* As all off-diagonal elements of  $\check{\mathbb{K}}(u)$  are nonpositive, (35) implies that the off-diagonal elements of the matrix

$$N(u) := \text{Sym } M(u) - \lambda \check{\mathbb{K}}(u)$$

are nonpositive as well. Moreover, we recall that  $\check{\mathbb{K}}(u)\mathbb{1} = 0$ ; likewise  $\text{Sym } M(u)\mathbb{1} = 0$ , due to  $D_u \check{\mathbb{K}}(u)\mathbb{1} = 0$  and  $\check{\mathbb{K}}(u)A\mathbb{1} = 0$ . This implies that the diagonal elements of the matrix  $N(u)$  have to satisfy

$$N_{ii}(u) = - \sum_{j \neq i} N_{ij}(u) = \sum_{j \neq i} |N_{ij}(u)|;$$

in other words, the symmetric matrix  $N(u)$  is *weakly diagonally dominant*, a notion which is well-known to imply positive semidefiniteness of  $N(u) = M(u) - \lambda \check{\mathbb{K}}(u)$ .  $\square$

*Proof of Proposition 4.1.* In order to apply Lemma 4.2, we have to establish (16) for some appropriate constant  $\lambda \in \mathbb{R}$ . To this aim, we notice that each element  $\check{K}_{ij}(u)$  depends only on  $u_i$  and  $u_j$ , whereas  $\text{Sym } M_{ij}(u)$  may depend on all elements of  $u$ . We will make use of this observation by writing  $\text{Sym } M(u)$  in the form

$$\text{Sym } M_{ij}(u) = \frac{1}{2} \overline{M}_{ij}(u_i, u_j) + \frac{1}{2} \sum_{n \notin \{i, j\}} \widetilde{M}_{ij}^n(u_i, u_j, u_n), \quad (36)$$

which highlights the dependencies of  $\text{Sym } M(u)$  on the specific elements of  $u$  in detail.

In order to find suitable matrices  $\overline{M}$  and  $\widetilde{M}^n$ , we examine the following expressions involved in the definition of  $\text{Sym } M(u)$ . We start with

$$\begin{aligned} -2 \text{Sym}(A^\top \check{\mathbb{K}})_{ij}(u) &= - \sum_{k, l} \check{K}_{kl}(u) \frac{1}{2} \left( (A_{ki} - A_{li})(\delta_{jk} - \delta_{jl}) + (A_{kj} - A_{lj})(\delta_{ik} - \delta_{il}) \right) \\ &= \frac{1}{2} \sum_k \left( \check{K}_{kj}(u)(A_{ki} - A_{ji}) + \check{K}_{ki}(u)(A_{kj} - A_{ij}) \right) \\ &\quad + \frac{1}{2} \sum_l \left( \check{K}_{jl}(u)(A_{li} - A_{ji}) + \check{K}_{il}(u)(A_{lj} - A_{ij}) \right) \\ &= \check{K}_{ij}(u)(A_{ii} + A_{jj} - A_{ij} - A_{ji}) + \sum_{n \notin \{i, j\}} \left( \check{K}_{nj}(u)(A_{ni} - A_{ji}) + \check{K}_{ni}(u)(A_{nj} - A_{ij}) \right), \end{aligned} \quad (37)$$

where we used that  $\check{K}_{ij}(u) = \check{K}_{ji}(u)$ .

In a similar spirit, we write

$$\begin{aligned} D_u \check{K}_{ij}(u)(A^\top u) &= -\partial_1 \theta_{\log}(A_{ij}u_i, A_{ji}u_j) A_{ij}(A^\top u)_i - \partial_2 \theta_{\log}(A_{ij}u_i, A_{ji}u_j) A_{ji}(A^\top u)_j \\ &= -\partial_1 \theta_{\log}(A_{ij}u_i, A_{ji}u_j) A_{ij}(A_{ii}u_i + A_{ji}u_j) - \partial_2 \theta_{\log}(A_{ij}u_i, A_{ji}u_j) A_{ji}(A_{ij}u_i + A_{jj}u_j) \\ &\quad - \sum_{n \notin \{i, j\}} (\partial_1 \theta_{\log}(A_{ij}u_i, A_{ji}u_j) A_{ij} A_{ni} u_n + \partial_2 \theta_{\log}(A_{ij}u_i, A_{ji}u_j) A_{ji} A_{nj} u_n) \end{aligned} \quad (38)$$

Now we collect all terms in (37) and (38), which only depend on  $u^i$  and  $u^j$  into  $\overline{M}_{ij}$ , whereas the terms which depend on  $u^n$  as well are collected in  $\widetilde{M}_{ij}^n$ :

$$\begin{aligned} \overline{M}_{ij}(u_i, u_j) &:= \check{K}_{ij}(u)(A_{ii} + A_{jj} - A_{ij} - A_{ji}) \\ &- \partial_1 \theta_{\log}(A_{ij}u_i, A_{ji}u_j)A_{ij}(A_{ii}u_i + A_{jj}u_j) - \partial_2 \theta_{\log}(A_{ij}u_i, A_{ji}u_j)A_{ji}(A_{ij}u_i + A_{jj}u_j), \\ \widetilde{M}_{ij}^n(u_i, u_j, u_n) &:= \check{K}_{nj}(u)(A_{ni} - A_{ji}) + \check{K}_{ni}(u)(A_{nj} - A_{ij}) \\ &- \partial_1 \theta_{\log}(A_{ij}u_i, A_{ji}u_j)A_{ij}A_{ni}u_n - \partial_2 \theta_{\log}(A_{ij}u_i, A_{ji}u_j)A_{ji}A_{nj}u_n. \end{aligned}$$

We control the terms involving derivatives in  $\overline{M}_{ij}$  by means of (65) and (66) in the forms of

$$-\partial_1 \theta_{\log}(A_{ij}u_i, A_{ji}u_j)A_{ij}u_i - \partial_2 \theta_{\log}(A_{ij}u_i, A_{ji}u_j)A_{ji}u_j = -\theta_{\log}(A_{ij}u_i, A_{ji}u_j)$$

and

$$-\partial_1 \theta_{\log}(A_{ij}u_i, A_{ji}u_j)A_{ji}u_j - \partial_2 \theta_{\log}(A_{ij}u_i, A_{ji}u_j)A_{ij}u_i \leq -\theta_{\log}(A_{ij}u_i, A_{ji}u_j)$$

respectively. Hence, we may estimate  $\overline{M}_{ij}$  as

$$\begin{aligned} \overline{M}_{ij}(u_i, u_j) &\leq \check{K}_{ij}(u)(A_{ii} + A_{jj} - A_{ij} - A_{ji} - \min\{A_{ii}, A_{jj}\} - \min\{A_{ij}, A_{ji}\}) \\ &= \check{K}_{ij}(u)(\max\{A_{ii}, A_{jj}\} - A_{ij} - A_{ji} - \min\{A_{ij}, A_{ji}\}). \end{aligned} \quad (39)$$

For an estimate of  $\widetilde{M}_{ij}^n$ , we first note that monotonicity of  $(a, b) \mapsto \theta_{\log}(a, b)$  implies

$$\begin{aligned} \check{K}_{nj}(u) &\leq \max\left\{A_{nj}, \frac{A_{jn}}{A_{ji}}\right\} \theta_{\log}(u_n, A_{ji}u_j) \\ \check{K}_{ni}(u) &\leq \max\left\{A_{ni}, \frac{A_{in}}{A_{ij}}\right\} \theta_{\log}(u_n, A_{ij}u_i). \end{aligned}$$

With those two inequalities at hand, we appeal to (71) to arrive at

$$\begin{aligned} \widetilde{M}_{ij}^n(u_i, u_j, u_n) &\leq \min\{A_{ij}A_{ni}, A_{ji}A_{nj}\} \beta_{ij}^n (\check{K}_{nj}(u) + \check{K}_{ni}(u)) \\ &\quad - \min\{A_{ij}A_{ni}, A_{ji}A_{nj}\} (\partial_1 \theta_{\log}(A_{ij}u_i, A_{ji}u_j) + \partial_2 \theta_{\log}(A_{ij}u_i, A_{ji}u_j)) u_n \\ &\leq \min\{A_{ij}A_{ni}, A_{ji}A_{nj}\} \tilde{g}(\beta_{ij}^n) \check{K}_{ij}(u), \end{aligned}$$

where we used a constant  $\beta_{ij}^n$  as given in (33).  $\square$

In the following, we consider an additive perturbation of the infinitesimal generator as described in Example 4.7 of [Mie13].

**Example 4.3.** For a fixed probability measure  $w \in \mathcal{P}_N$  and  $\kappa > 0$ , we define

$$Q = \kappa(\mathbb{1} \otimes w - \text{Id}).$$

It is immediate to check that  $Q$  is the infinitesimal generator of a reversible and irreducible Markov chain with unique steady state  $w$ . Consider a perturbation matrix  $B \in \mathbb{R}^{N \times N}$  such that  $B\mathbb{1} = 0$  and  $\sup_i |B_{ii}| < \varepsilon$ . Provided that  $\varepsilon > 0$  is chosen small enough,  $A = Q + B$  is again the infinitesimal generator of some irreducible Markov chain.

In order to apply Proposition 4.1, we note that

$$\overline{\mu}_{ij} = -\kappa - 2\kappa \min\{w_i, w_j\} + \mathcal{O}(\varepsilon),$$

whereas all  $\tilde{\mu}_{ij}^n$  belong to  $\mathcal{O}(\varepsilon)$  as  $\varepsilon \searrow 0$ . Therefore, the convexity parameter  $\lambda$  for the perturbed infinitesimal generator  $A$  is bounded by

$$\lambda \geq \frac{\kappa}{2} + \kappa \min_i \{w_i\} + \mathcal{O}(\varepsilon).$$

## 5. THE COMPLETE GEODESIC SPACE $(\mathcal{P}_N, \mathcal{W})$

According to Corollary 3.5, we may define a Riemannian metric  $\mathbb{G}(u)$  at every point  $u \in \text{int } \mathcal{P}_N$  by inverting the Onsager operator  $\check{\mathbb{K}}(u)$  on the tangent space (identified with)  $\text{span}\{\mathbb{1}\}^\perp$ . However, even in the case of a reversible Markov generator  $A$ , this construction fails on the boundary  $\partial\mathcal{P}_N := \mathcal{P}_N \setminus \text{int } \mathcal{P}_N$  as the Onsager operator  $\check{\mathbb{K}}$  may not be regular anymore.

Nevertheless, the following result shows the Riemannian distance function  $\mathcal{W}$  defined by (10) defines a metric on  $\mathcal{P}_N$

**Theorem 5.1.**  *$\mathcal{P}_N$  together with the distance function  $\mathcal{W}$  as defined in (10) forms a complete geodesic space, whose topology agrees with the standard Euclidean topology on  $\mathcal{P}_N$ .*

For the proof of this result we require two lemmas.

**Lemma 5.2** (characterisation of  $\mathcal{W}$ ). *The distance function  $\mathcal{W}$  as defined in (10) is given by the convex minimisation problem*

$$\mathcal{W}^2(u, v) = \inf \int_0^1 \sum_{\substack{i,j \\ A_{ij} > 0}} (V_{ij}^t)^2 / \check{K}_{ij}(g^t) dt, \quad (40)$$

where the infimum is taken over the convex set of all pairs  $(g^t, V^t)_{t \in [0,1]}$  of continuous curves  $g : [0, 1] \rightarrow \mathbb{R}^N$  and locally integrable  $V : [0, 1] \rightarrow \mathbb{R}^{N \times N}$  such that

$$\frac{d}{dt} g^t = \sum_{i,j} V_{ij}^t (e_i - e_j) \quad (\mathbf{CE}^*)$$

in the sense of distributions.

*Remark 5.3.* We note that the integrand of the functional

$$(g, V) \mapsto \mathcal{A}(g, V) := \int_0^1 \sum_{\substack{i,j \\ A_{ij} > 0}} (V_{ij}^t)^2 / \check{K}_{ij}(g^t) dt \quad (41)$$

is a lower semicontinuous and convex function. Indeed, this follows from a representation of the integrand as a composition of the mapping  $(x, y) \mapsto x^2/y$ , which is convex on the open half-plane  $\mathbb{R} \times \mathbb{R}^+$ , and the logarithmic mean  $\theta_{\log}$  which is concave on  $\mathbb{R}_0^+ \times \mathbb{R}_0^+$ . Semicontinuity of the integrand in both arguments follows along the same lines.

As a consequence,  $\mathcal{A}$  is semicontinuous convex as well.

*Proof of Lemma 5.2.* In order to show (40), we first note that the inequality  $\mathcal{W}^2(u, v) \geq$  (RHS) follows from writing

$$V_{ij}^t = (\zeta_i^t - \zeta_j^t) \check{K}_{ij}(g^t),$$

which shows that the minimisation problem in (40) corresponds to the one in (10) over a larger set of admissible pairs of curves.

The converse inequality  $\mathcal{W}^2(u, v) \leq (RHS)$  will be subsequently shown by a standard mollification argument. To this aim, we consider a non-negative mollifier  $\eta_\varepsilon$  on the real line with  $\text{supp } \eta_\varepsilon \subseteq [-\varepsilon, \varepsilon]$  and  $\|\eta_\varepsilon\|_1 = 1$  for  $\varepsilon > 0$  and set

$$(\tilde{g}^t, \tilde{V}^t) := \begin{cases} (g^0, 0) & \text{if } t \in [-\varepsilon, \varepsilon), \\ (g^{(t-\varepsilon)/(1-2\varepsilon)}, \frac{1}{1-2\varepsilon} V^{(t-\varepsilon)/(1-2\varepsilon)}) & \text{if } t \in [\varepsilon, 1-\varepsilon), \\ (g^1, 0) & \text{if } t \in [1-\varepsilon, 1+\varepsilon) \end{cases}$$

for an admissible pair  $(g^t, V^t)_{t \in [0,1]}$ . Apparently, the pair  $(\tilde{g}^t, \tilde{V}^t)$  is admissible as well.

Denoting by  $*$  the convolution with respect to time  $t$  and extending the underlying curves with zero outside of their domain  $[0, 1]$ , we note that the mollified pair  $(\tilde{g} * \eta_\varepsilon, \tilde{V} * \eta_\varepsilon)$  is admissible as well. Hence, Jensen's inequality with respect to the convex integrand, followed by Young's inequality for convolutions, implies

$$\begin{aligned} \int_0^1 (\tilde{V}_{ij} * \eta_\varepsilon(t))^2 / \check{K}_{ij}(\tilde{g} * \eta_\varepsilon(t)) dt &\leq \int_0^1 ((\tilde{V}_{ij})^2 / \check{K}_{ij}(\tilde{g})) * \eta_\varepsilon(t) dt \\ &\leq \int_{-\varepsilon}^{1+\varepsilon} (\tilde{V}_{ij}^t)^2 / \check{K}_{ij}(\tilde{g}^t) dt = \frac{1}{1-2\varepsilon} \int_0^1 (V_{ij}^t)^2 / \check{K}_{ij}(g^t) dt. \end{aligned}$$

In order for the right-hand side of (40) to be finite,  $V_{ij}^t$  needs to vanish for a.e. times  $t \in [0, 1]$  whenever  $\check{K}_{ij}(g^t) = 0$ . This means that the smooth function  $\tilde{V}_{ij} * \eta_\varepsilon$  may vanish only when  $\check{K}_{ij}(\tilde{g} * \eta_\varepsilon)$  vanishes. Hence, there exists a measurable function  $\psi_\varepsilon : [0, 1] \rightarrow \mathbb{R}^{N \times N}$  such that

$$\tilde{V}_{ij} * \eta_\varepsilon(t) = \psi_\varepsilon^t \check{K}_{ij}(\tilde{g} * \eta_\varepsilon(t))$$

for all times  $t \in [0, 1]$ .

Thus, it is enough to consider an admissible pair  $(\tilde{g} * \eta_\varepsilon, \zeta_\varepsilon)$  for the continuity equation (cε) by means of

$$\sum_{i,j} \tilde{V}_{ij} * \eta_\varepsilon(t) (e_i - e_j) = \frac{d}{dt} \tilde{g} * \eta_\varepsilon(t) = \check{\mathbb{K}}(\tilde{g} * \eta_\varepsilon(t)) \zeta_\varepsilon^t.$$

Since

$$(\zeta_\varepsilon^t)^\top \check{\mathbb{K}}(\tilde{g} * \eta_\varepsilon(t)) \zeta_\varepsilon^t \leq \sum_{\substack{i,j \\ A_{ij} > 0}} (\tilde{V}_{ij} * \eta_\varepsilon(t))^2 / \check{K}_{ij}(\tilde{g} * \eta_\varepsilon(t)),$$

we conclude

$$\begin{aligned} \int_0^1 (\zeta_\varepsilon^t)^\top \check{\mathbb{K}}(\tilde{g} * \eta_\varepsilon(t)) \zeta_\varepsilon^t dt &\leq \int_0^1 \sum_{\substack{i,j \\ A_{ij} > 0}} (\tilde{V}_{ij} * \eta_\varepsilon(t))^2 / \check{K}_{ij}(\tilde{g} * \eta_\varepsilon(t)) dt \\ &\leq \frac{1}{1-2\varepsilon} \int_0^1 \sum_{\substack{i,j \\ A_{ij} > 0}} (V_{ij}^t)^2 / \check{K}_{ij}(g^t) dt. \end{aligned}$$

for arbitrarily small  $\varepsilon > 0$ . □

**Lemma 5.4.** *A lower bound for the  $\mathcal{W}$ -distance is provided by the standard Euclidean distance  $|\cdot|_2$  viz.*

$$|u - v|_2 \leq \sqrt{\|\check{\mathbb{K}}(\mathbb{1})\|} \mathcal{W}(u, v) \quad \forall u, v \in \mathcal{P}_N, \tag{42}$$

where  $\|\check{\mathbb{K}}(\mathbb{1})\|$  denotes the operator norm of  $\check{\mathbb{K}}$  at  $\mathbb{1} = (1, \dots, 1)$  with respect to  $|\cdot|_2$  on  $\mathbb{R}^N$ .

*Proof.* It suffices to consider the case when  $\mathcal{W}(u, v)$  remains finite. Then, for every  $\varepsilon$  we may find a pair of curves  $(g^t, \zeta^t)_{t \in [0,1]}$  connecting  $u$  to  $v$ , admissible according to the definition of the  $\mathcal{W}$ -distance, such that

$$\int_0^1 (\zeta^t)^\top \check{\mathbb{K}}(g^t) \zeta^t dt \leq \mathcal{W}^2(u, v) + \varepsilon. \quad (43)$$

Now  $(\mathbf{c}\epsilon)$  and the Cauchy-Schwarz inequality applied to the positive-semidefinite bilinearform  $(\xi, \zeta) \mapsto \xi^\top \check{\mathbb{K}} \zeta$  imply for an arbitrary  $z \in \mathbb{R}^N$  that

$$\sum_i z_i (u_i - v_i) = \int_0^1 z^\top \dot{g}^r dr = \int_0^1 z^\top \check{\mathbb{K}}(g^r) \zeta^r dr \quad (44a)$$

$$\leq \left( \int_0^1 z^\top \check{\mathbb{K}}(g^r) z dr \right)^{1/2} \left( \int_0^1 (\zeta^r)^\top \check{\mathbb{K}}(g^r) \zeta^r dr \right)^{1/2}. \quad (44b)$$

The first factor in the second line may be estimated by

$$z^\top \check{\mathbb{K}}(g^r) z \leq z^\top \check{\mathbb{K}}(\mathbb{1}) z \leq |z|_2^2 \|\check{\mathbb{K}}(\mathbb{1})\|,$$

whereas the second factor is bounded by (43). Since  $\varepsilon > 0$  is arbitrary, we arrive at

$$\sum_i z_i (u_i - v_i) \leq |z|_2 \sqrt{\|\check{\mathbb{K}}(\mathbb{1})\|} \mathcal{W}(u, v).$$

Setting  $z = u - v$  in this inequality, we conclude.  $\square$

*Proof of Theorem 5.1. We show that  $(\mathcal{P}_N, \mathcal{W})$  is a metric space.* In order to check that the distance function  $\mathcal{W}$  remains finite on all of  $\mathcal{P}_N$ , it is enough to find an inward-pointing curve segment  $(g^t, V^t)_{t \in [0,1]}$  for every initial point  $g^0 = u \in \partial \mathcal{P}_N$  such that (41) remains bounded along this segment. With no loss of generality, we will assume that  $u$  vanishes precisely at the first  $k$  coordinates. Hence, we may consider the curve

$$g_i^t = \begin{cases} t^2/N & \text{if } 1 \leq i \leq k \\ 1/N & \text{if } k < i < N \\ (k+1 - kt^2)/N & \text{if } i = N \end{cases} \quad (45)$$

Note that, according to  $(\mathbf{c}\epsilon^*)$ , all corresponding  $V_{ij}^t$  belong to  $\mathcal{O}(t)$  as  $t \searrow 0$ . Thus, the estimate

$$N \check{K}_{ij}(g^t) \geq \theta_{\log}(A_{ij}t^2, A_{ji}t^2) = t^2 \theta_{\log}(A_{ij}, A_{ji}) \quad \forall i, j \in [N],$$

implies that  $(V_{ij}^t)^2 / \check{K}_{ij}(g^t)$  remains bounded as  $t \searrow 0$ . As a result,  $\mathcal{A}(g, V)$ , defined in (41), is finite as well.

The triangle inequality follows from the fact that the reparametrised curve of two geodesics, linked together at one common endpoint, is still admissible for the minimisation problem in (10).

Finally, the lower bound in terms of the  $\ell^p$ -distance provided in Lemma 5.4 shows that  $\mathcal{W}(u, v)$  vanishes, precisely, when  $u = v$ .

**We show that the topology induced by  $\mathcal{W}$  agrees with the Euclidean subspace topology on  $\mathcal{P}_N$ .** Clearly, the topology induced by  $\mathcal{W}$ , restricted to the interior of  $\mathcal{P}_N$ , agrees with the standard Euclidean topology on  $\text{int } \mathcal{P}_N$ , due

to standard results of Riemannian geometry. Hence, it remains to show that a sequence  $(u^n)_{n \in \mathbb{N}}$  in  $\mathcal{P}_N$  is converging to a limit point  $u$  on the boundary of  $\mathcal{P}_N$  with respect to the Euclidean subspace topology, precisely, when  $\mathcal{W}(u^n, u) \rightarrow 0$  as  $n \rightarrow \infty$ .

The claim that convergence in Euclidean topology follows from  $\mathcal{W}$ -convergence is a direct consequence of Lemma 5.4. For the converse implication, it poses no restriction to assume that  $(u^n)_{n \in \mathbb{N}}$  belongs to the interior of  $\mathcal{P}_N$ . Following a construction similar to (45), we may construct an inward-pointing curve  $(\tilde{g}^t)_{t \in [0,1]}$  with initial point  $\tilde{g}^0 = u$ , reparametrised to constant-speed in such a way that  $\mathcal{W}^2(u, \tilde{g}^t) \leq t\mathcal{A}(\tilde{g}, V) < \infty$ . In particular, for every  $\varepsilon > 0$  exists a time  $t_0$  such that  $\mathcal{W}(u, \tilde{g}^{t_0}) < \varepsilon/2$ . In addition, the aforestated equivalence of the Euclidean and the  $\mathcal{W}$ -induced topology in the interior of  $\mathcal{P}_N$  implies the existence of  $n_0 \in \mathbb{N}$  such that  $\mathcal{W}(u^n, \tilde{g}^{t_0}) < \varepsilon/2$  for all  $n \geq n_0$ . Therefore, we conclude

$$\mathcal{W}(u^n, u) \leq \mathcal{W}(u^n, \tilde{g}^{t_0}) + \mathcal{W}(u, \tilde{g}^{t_0}) < \varepsilon \quad \forall n \geq n_0.$$

**We show that the metric space  $(\mathcal{P}_N, \mathcal{W})$  is complete.** By the considerations above, this follows directly from the compactness of  $\mathcal{P}$  with respect to the Euclidean subspace topology.

**We show that  $(\mathcal{P}_N, \mathcal{W})$  is a geodesic space,** i.e. that for any two points  $u, v \in \mathcal{P}_N$  the infimum in the right-hand side of (40) is attained by a geodesic pair  $(g^t, V^t)_{t \in [0,1]}$  joining  $u$  to  $v$ . To this aim, we appeal to the *direct method in the calculus of variations*:

Let  $(g_n, V_n)_{n \in \mathbb{N}}$  be a sequence of admissible pairs as considered in Lemma 5.2, minimising the functional  $\mathcal{A}$  in (41). Since  $\mathcal{A}$  only takes nonnegative values, we may assume that  $\mathcal{A}(g_n, V_n)$  is uniformly bounded for all  $n \in \mathbb{N}$ .

*Extraction of a weakly-\* converging subsequence.* In order to obtain a subsequence of  $(V_n)_{n \in \mathbb{N}}$ , weakly-\* converging in the dual of  $C[0, 1]$ , we invoke the Banach-Alaoglu theorem. To this end, we show that the sequence of signed Borel measures corresponding to the densities  $(V_n)_{ij}$  is uniformly bounded in the total variation norm by means of the estimate

$$\left( \int_B |(V_n^t)_{ij}| dt \right)^2 \leq \mathcal{L}^1(B) \int_0^1 (V_{ij}^t)^2 dt \tag{46a}$$

$$\leq \mathcal{L}^1(B) \max_{i,j} \{A_{ij}\} \int_0^1 \sum_{\substack{i,j \\ A_{ij} > 0}} (V_n^t)_{ij}^2 / \check{K}_{ij}(g_n^t) dt \tag{46b}$$

$$\leq \mathcal{L}^1(B) \max_{i,j} \{A_{ij}\} \sup_{n \in \mathbb{N}} \mathcal{A}(g_n, V_n) \tag{46c}$$

for all Borel subsets  $B \subseteq [0, 1]$ , where we used the monotonicity of the logarithmic mean in the form of the upper bound  $\check{K}_{ij}(g_n^t) \leq \max_{i,j} \{A_{ij}\}$ . As a result of this uniform total variational bound, we may extract a subsequence  $((V_{n_k})_{ij})_{k \in \mathbb{N}}$ , converging weakly-\* to a signed measure on  $[0, 1]$ . Moreover, (46a) implies that this measure is absolutely continuous with respect to the Lebesgue measure on  $[0, 1]$ , thus represented by a density which will be denoted by  $V_{ij}$ .

For  $(g_n)_{n \in \mathbb{N}}$  we can even extract a subsequence, converging pointwise to a limit function. Indeed, in integrated form,  $(\mathbf{c}\epsilon^*)$  reads as

$$g_{n_k}^t - g_{n_k}^0 = \int_0^t \sum_{i,j} (V_{n_k}^r)_{ij} (e_i - e_j) dr \quad \forall t \in [0, 1]. \quad (47)$$

Observing that the right-hand side of this equation converges as  $k \rightarrow \infty$  (see Proposition 5.1.10 in [AGS08]) and the initial point  $g_{n_k}^0$  is the same for all  $k \in \mathbb{N}$ , we obtain a pointwise limit curve  $(g^t)_{t \in [0,1]}$ . In addition, the dominated convergence theorem yields that  $(g_{n_k})_{k \in \mathbb{N}}$  converges weakly- $*$  to  $g$  as  $k \rightarrow \infty$ .

Now we may use the weak- $*$  convergence of both  $((V_{n_k})_{ij})_{k \in \mathbb{N}}$  and  $(g_{n_k})_{k \in \mathbb{N}}$  to infer that the limit pair  $(g, V)$  satisfies  $(\mathbf{c}\epsilon^*)$  in the sense of distributions as well. Passing to the limit in (47) as  $k \rightarrow \infty$ , we obtain the continuity of the limit curve  $(g^t)_{t \in [0,1]}$ . Hence, the pair  $(g, V)$  is admissible for the minimisation problem in Lemma 5.2.

*Lower semicontinuity of the action functional  $\mathcal{A}$ .* We recall that the integrand (41) is jointly convex and lowersemicontinuous as stated in Remark 5.3. By means of Theorem 5.19 in [FL07], this implies that the integral functional  $\mathcal{A}$  is jointly (sequently) lower semicontinuous with respect to weak- $*$  convergence in the sense of measures. As a result, we may pass to the limit

$$\mathcal{W}^2(u, v) = \liminf_{n \rightarrow \infty} \mathcal{A}(g_n, V_n) \geq \mathcal{A}(g, V), \quad (48)$$

which means that the pair  $(g^t, V^t)_{t \in [0,1]}$  corresponds to a length minimising geodesic joining  $u$  to  $v$ .  $\square$

## 6. BOUNDS FOR $\mathcal{W}$ IN TERMS OF WASSERSTEIN DISTANCES

In order to consider a Wasserstein distance on  $\mathcal{P}_N$ , we need to endow  $[N]$  with some metric. Suitable candidates are:

- (i) the graph metric on the graph induced by the infinitesimal generator  $A$ , i.e. the vertex set  $[N]$  together with edges  $\{(i, j) : A_{ij} > 0\}$ ;
- (ii)  $\mathcal{W}$  restricted to Dirac measures, i.e.  $\mathcal{W}(\delta_i, \delta_j)$  for the distance between vertices  $i$  and  $j$  in  $[N]$ .

**Notation.** The  $L^p$ -Wasserstein distance with respect to the former metric will be denoted by  $W_p^{\text{gra}}$ , whereas the  $L^p$ -Wasserstein distance with respect to the latter will be denoted by  $W_p^{\mathcal{W}}$ .

**Proposition 6.1.**  *$\mathcal{W}$  is bounded by Wasserstein distances in terms of*

$$\sqrt{2} \left( \max_i \{ \sqrt{|A_{ii}|} \} \right)^{-1} W_1^{\text{gra}}(u, v) \leq \mathcal{W}(u, v) \leq W_2^{\mathcal{W}}(u, v) \quad \forall u, v \in \mathcal{P}_N. \quad (49)$$

*Proof.* We show the lower bound in terms of  $W_1^{\text{gra}}$ -distance. In contrast to the second part of the proof, we will make use of the dual characterisation of the  $L^1$ -Wasserstein distance via the *Kantorovich-Rubinstein theorem* (cf. e.g. Theorem 8.10.45 in vol. 2 of [Bog07]):

$$W_1^{\text{gra}}(u, v) = \sup \left\{ \sum_i z_i (u_i - v_i) \right\}, \quad (50)$$

where the supremum is taken over all  $z \in \mathbb{R}^N$  with Lipschitz constant  $C_z < 1$  with respect to the graph metric induced by the infinitesimal generator  $A$ .



Appealing to Theorem 5.1, for every pair of points  $u, v \in \mathcal{P}_N$ , we may find a constant-speed geodesic pair  $(g^t, \zeta^t)_{t \in [0,1]}$  joining  $u$  to  $v$ , minimising (10). Then, for  $z \in \mathbb{R}^N$ , a computation in the vein of (44) shows

$$\sum_i z_i(u_i - v_i) \leq \left( \int_0^1 z^\top \check{\mathbb{K}}(g^r) z \, dr \right)^{1/2} \mathcal{W}(u, v). \tag{51}$$

In order to estimate the first factor on the right-hand side of this inequality, we use the fact that the graph metric between  $i \neq j$  equals to 1 whenever  $A_{ij} > 0$ ; therefore,

$$z^\top \check{\mathbb{K}}(g^r) z \, dr = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} (z_i - z_j)^2 \check{K}_{ij}(g^r) \leq C_z^2 \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \check{K}_{ij}(g^r).$$

To estimate the sum on the right-hand side of this equation, we shall make use of an upper bound of the logarithmic mean in terms of the arithmetic mean as stated in (61). Thus,

$$\sum_{i \neq j} \check{K}_{ij}(g^r) \leq \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} A_{ij} u_i + A_{ji} u_j = \sum_{\substack{i,j \\ i \neq j}} A_{ij} u_i \leq \max_i \left\{ \sum_{j \neq i} A_{ij} \right\} = \max_i \{ |A_{ii}| \}.$$

Taking those estimates for (51) into account, we arrive at

$$\sum_i z_i(u_i - v_i) \leq \frac{C_z}{\sqrt{2}} \max_i \{ \sqrt{|A_{ii}|} \} \mathcal{W}(u, v).$$

Appealing to the Kantorovich-Rubinstein theorem (50), we conclude the first part of the proof.

**We show the upper bound in terms of  $W_2^{\mathcal{W}}$ -distance.** For every pair of Dirac measures  $\delta_i, \delta_j \in \mathcal{P}_N$ , Theorem 5.1 allows us to find a constant-speed geodesic pair  $(g^{i \rightarrow j}, V^{i \rightarrow j})$  joining  $u$  to  $v$ , minimising (40). Consider an optimal plan  $q \in \mathcal{P}_{N \times N}$  between probability measures  $u$  and  $v$  in  $\mathcal{P}_N$ . Now the crucial observation is constituted by the fact that convex combinations of  $(g^{i \rightarrow j}, V^{i \rightarrow j})$ , weighted according to  $q$  in form of

$$g = \sum_{i,j} q_{ij} g^{i \rightarrow j} \quad \text{and} \quad V = \sum_{i,j} q_{ij} V^{i \rightarrow j}$$

still satisfy (cε\*); thus the pair  $(g, V)$  is admissible for the minimisation problem in (40) and, invoking convexity of the functional  $\mathcal{A}$  as noted in Remark 5.3, we infer

$$\mathcal{W}(u, v)^2 \leq \mathcal{A}(g, V) \leq \sum_{i,j} q_{ij} \mathcal{A}(g^{i \rightarrow j}, V^{i \rightarrow j}) = \sum_{i,j} q_{ij} \mathcal{W}^2(\delta_i, \delta_j) = W_2^{\mathcal{W}}(u, v)^2.$$

□

## 7. FUNCTIONAL INEQUALITIES

The first goal of this chapter is to prove a variant of the *HWI*-inequality which has been established in [EM12] for reversible Markov chains. The crucial difference between the argument in [EM12] and the one presented below consists of the fact that we use the *first variational formula of Riemannian geometry* to estimate  $\frac{d^+}{dt} \mathcal{W}(u^t, v)$  instead of a *Benamou-Brenier*-like argument.

The rôle of the *discrete Fisher information* in the following inequality will be taken over by  $|Y|_{\mathbb{G}}$  with a vectorfield  $Y$  on  $\mathcal{P}_N$  which, in addition to the logarithmic entropy, also takes the functional  $V_\tau$  into account:

$$Y(u) := \text{grad}_{\mathbb{G}} \text{Ent}(u) + \check{\mathbb{K}}(u)[L] \quad (52)$$

This definition is motivated by the fact that the vectorfield  $Y$  describes the evolution of the Markov chain with an infinitesimal generator  $A$  as stated in (14).

**Lemma 7.1.** *Let  $(u^t)_{t \geq 0}$  be a solution of the Kolmogorov forward equation  $\dot{u}^t = A^\top u^t$ . Denote by  $g_\varepsilon$  the constant-speed geodesic starting from  $u^t$  in direction of  $\varepsilon \dot{u}^t$ , i.e.  $g_\varepsilon^r := \exp_{u^t}(r\varepsilon \dot{u}^t)$ . Then we have the relation*

$$\frac{d}{dt} \text{Ent}(u^t) + \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} V_1(g_\varepsilon) = -|Y|_{\mathbb{G}}^2(u^t) \quad \forall t > 0. \quad (53)$$

*Proof.* The left-hand side of (53) takes the form

$$\frac{d}{dt} \text{Ent}(u^t) + \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} V_1(g_\varepsilon) = (\dot{u}^t)^\top \nabla \text{Ent}(u^t) + \lim_{\varepsilon \rightarrow 0} \int_0^1 \left( \mathbb{G}(g_\varepsilon^r) \frac{\dot{g}_\varepsilon^r}{\varepsilon} \right)^\top \check{\mathbb{K}}(g_\varepsilon^r)[L] dr.$$

By means of Markov chain theory, we can assume that  $g^r$  takes values in the interior of  $\mathcal{P}_N$  for all  $t \in (0, 1)$ . Passing to the limit in the integral term on the right-hand side of the equation above, we see that both  $\check{\mathbb{K}}(g_\varepsilon^r) \rightarrow \check{\mathbb{K}}(u^t)$  and  $\mathbb{G}(g_\varepsilon^r) \rightarrow \mathbb{G}(u^t)$  as  $\varepsilon \rightarrow 0$ . In addition, we have  $g_\varepsilon^r/\varepsilon \rightarrow \dot{u}^t$ , due to the particular definition of the geodesic  $g_\varepsilon$ . Therefore, appealing to the variational equation (14), we arrive at

$$\begin{aligned} & \frac{d}{dt} \text{Ent}(u^t) + \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} V_1(g_\varepsilon) \\ &= (\dot{u}^t)^\top \left( \mathbb{G}(u^t) \text{grad}_{\mathbb{G}} \text{Ent}(u^t) + \mathbb{G}(u^t) \check{\mathbb{K}}(u^t)[L] \right) = -|Y|_{\mathbb{G}}^2(u^t). \end{aligned}$$

□

**Proposition 7.2.** *Let  $A = Q \circ B$  be an infinitesimal generator with stationary distribution  $w$  for  $Q$  and  $\lambda \in \mathbb{R}$  a convexity parameter as defined in Theorem 3.8. Then we have the following discrete HWI-inequality:*

$$\text{Ent}(u) + V_1(g^{u \rightarrow w}) \leq \mathcal{W}(u, w) |Y|_{\mathbb{G}}(u) - \frac{\lambda}{2} \mathcal{W}^2(u, w) \quad \forall u \in \text{int } \mathcal{P}_N. \quad (\text{HWI}_\lambda)$$

*Proof.* Let  $(u^t)_{t \geq 0}$  be the solution of the Kolmogorov forward equation  $\dot{u}^t = A^\top u^t$  with initial condition  $u^0 = u$ . As a result, choosing  $v = w$  in  $(\text{EVI}_{\lambda, \infty})$  at time  $t = 0$ , we obtain the inequality

$$\text{Ent}(u) + V_1(g^{u \rightarrow w}) \leq -\frac{1}{2} \frac{d^+}{dt} \Big|_{t=0} \mathcal{W}^2(u^t, w) - \frac{\lambda}{2} \mathcal{W}^2(u, w). \quad (54)$$

Now the *first variational formula of Riemannian geometry*, followed by an application of the *Cauchy-Schwarz inequality*, implies the estimate

$$-\frac{1}{2} \frac{d^+}{dt} \mathcal{W}^2(u^t, w) = \langle \dot{g}^0, \dot{u}^t \rangle_{\mathbb{G}} \leq |\dot{g}^0|_{\mathbb{G}} |\dot{u}^t|_{\mathbb{G}}, \quad (55)$$

where  $(g^r)_{r \in [0, 1]}$  denotes a constant-speed geodesic joining  $u^t$  to  $w$ . As  $\exp_{u^t}(\dot{g}^0) = g^1 = w$ , we have  $|\dot{g}^0|_{\mathbb{G}} = \mathcal{W}(u^t, w)$ . Hence, (54), together with (55) at time  $t = 0$ , implies  $(\text{HWI}_\lambda)$ . □

**Corollary 7.3.** *Let  $A = Q \circ B$  be an infinitesimal generator with stationary distribution  $w$  for  $Q$  and  $\lambda > 0$  be a positive convexity parameter as defined in Theorem 3.8. Then we have the following discrete modified logarithmic Sobolev inequality:*

$$\text{Ent}(u) + V_1(g^{u \rightarrow w}) \leq \frac{1}{2\lambda} |Y|_{\mathbb{G}}^2(u) \quad \forall u \in \text{int } \mathcal{P}_N. \quad (\text{MLSI}_\lambda)$$

*Proof.* We estimate the product term  $\mathcal{W}(u, w)|Y|_{\mathbb{G}}(u)$  in  $(\text{HWI}_\lambda)$  via Young’s inequality  $ab \leq a^2/2 + b^2/2$  with  $a = \sqrt{\lambda}\mathcal{W}(u, w)$  and  $b = |Y|_{\mathbb{G}}(u)/\sqrt{\lambda}$  as

$$\mathcal{W}(u, w)|Y|_{\mathbb{G}}(u) \leq \frac{\lambda}{2} \mathcal{W}^2(u, w) + \frac{1}{2\lambda} |Y|_{\mathbb{G}}^2(u).$$

As a result, this estimate, together with  $(\text{HWI}_\lambda)$ , implies  $(\text{MLSI}_\lambda)$  as desired.  $\square$

For the following result, we consider a stationary distribution  $\pi$  for the non-reversible generator  $A$  has, not necessarily agreeing with  $w$  for the reversible generator  $Q$ . As already pointed out in Section 2, imposing a decomposition of form (1) forces both stationary distributions of  $A$  and  $B$  to coincide.

As usual, the entropy functional  $\text{Ent}$  is defined relative to  $w$ .

**Proposition 7.4.** *Let  $A$  be an irreducible infinitesimal generator with stationary distribution  $\pi$ . Provided that  $(\text{EVI}_{\lambda, \infty})$  holds for some convexity parameter  $\lambda \in \mathbb{R}$ , we have the following discrete modified Talagrand inequality:*

$$\frac{\lambda}{2} \mathcal{W}^2(v, \pi) \leq \text{Ent}(v) - \text{Ent}(\pi) + V_1(g^{\pi \rightarrow v}) \quad \forall v \in B_{\text{inj}}(\pi), \quad (\text{T}_\lambda^{\mathcal{W}})$$

where  $B_{\text{inj}}(\pi) \subseteq \mathcal{P}_N$  denotes a geodesic ball of injectivity radius centred at  $\pi$ .

In particular, whenever  $\pi = w$ , the  $\mathcal{W}$ -distance is bounded via

$$\frac{\lambda}{2} \mathcal{W}^2(v, w) \leq \text{Ent}(v) + V_1(g^{w \rightarrow v}) \quad \forall v \in B_{\text{inj}}(w). \quad (56)$$

A proof following the approach of Otto and Villani in [OV00] for the statement above is impeded by the fact that the functional  $V_1$  may also take negative values. Instead, we will take a more direct approach, choosing  $(\text{EVI}_{\lambda, \infty})$  as starting point.

*Proof of Proposition 7.4.* The central idea is to infer  $(\text{T}_\lambda^{\mathcal{W}})$  by passing to the limit in  $(\text{EVI}_{\lambda, \infty})$  as  $t \rightarrow \infty$ . To this aim, we need to show that  $\lim_{t \rightarrow \infty} \text{Ent } u^t + V_1(g^{u^t \rightarrow v}) = \text{Ent}(\pi) + V_1(g^{\pi \rightarrow v})$  and the upper-right Dini derivative of  $\mathcal{W}^2(u^t, v)$  vanishes in the limit. Indeed, the former claim follows directly from continuity of the entropy functional  $\text{Ent}$  with respect to Euclidean topology and the equivalence of both topologies as shown in Theorem 5.1.

In the same spirit, noting that the geodesic  $g^{z \rightarrow v}$  depends smoothly on  $v, z \in B_{\text{inj}}(\pi)$ , we infer that  $\lim_{t \rightarrow \infty} V_1(g^{u^t \rightarrow v}) = V_1(g^{\pi \rightarrow v})$ .

For the latter claim we invoke the *first variational formula of Riemannian geometry* in the form of

$$\frac{1}{2} \frac{d^+}{dt} \mathcal{W}^2(v, u^t) = -\langle \dot{g}^0, \dot{u}^t \rangle_{\mathbb{G}}, \quad (57)$$

where  $(g^r)_{r \in [0,1]}$  denotes a constant speed-geodesic joining  $u^t$  to  $v$ . Note that  $u^t$  converges to  $\pi$  with respect to  $\mathcal{W}$  as well. Hence,  $|\dot{g}^0|_{\mathbb{G}} = \mathcal{W}(v, u^t)$  remains bounded as  $t \rightarrow \infty$ . Moreover, this implies that there exist  $T > 0$  and a geodesic ball  $B_{\mathcal{W}}(\pi) \subseteq \text{int } \mathcal{P}_N$  such that  $(u^t)_{t \geq T}$  stays inside  $B_{\mathcal{W}}(\pi)$ . In particular, the metric tensor  $\mathbb{G}$  remains bounded along  $u^t$  for all times  $t \geq T$ .

In addition, passing to the limit in the Kolmogorov forward equation (13) shows that  $\dot{u}^t$  vanishes with respect to the Euclidean topology as  $t \rightarrow \infty$ . Thus, we may estimate (57) via *Cauchy-Schwarz inequality* as

$$\frac{1}{2} \left| \frac{d^+}{dt} \mathcal{W}^2(v, u^t) \right| \leq |\dot{g}^0|_{\mathbb{G}} |\dot{u}^t|_{\mathbb{G}} \leq \mathcal{W}(v, u^t) \|\mathbb{G}(u^t)\| \cdot |\dot{u}^t|, \quad (58)$$

which clearly vanishes in the limit as  $t \rightarrow \infty$ .

Finally, (56) follows from the fact that the entropy functional  $\text{Ent}$  vanishes at  $w$ .  $\square$

**Proposition 7.5.** *Let  $A = Q \circ B$  be an infinitesimal generator with stationary distribution  $w$  for both  $A$  and  $Q$ . Assume there is a positive  $\lambda > 0$  such that  $(\text{MLSI}_\lambda)$  holds for all  $u$  inside a neighbourhood of  $w$ . Then we have the following discrete Poincaré inequality:*

$$\frac{5}{3} \sum_i \frac{\varphi_i^2}{w_i} - \frac{1}{3} \sum_{i,j} A_{ij} w_i \left( \frac{\varphi_i}{w_i} - \frac{\varphi_j}{w_j} \right) (\zeta_i - \zeta_j) \leq \frac{1}{\lambda} |A^\top \varphi|_{\mathbb{G}(w)}^2 \quad \forall \varphi \in \mathbb{R}^N : \varphi \perp \mathbb{1}, \quad (\text{P}_\lambda)$$

where  $\zeta = \mathbb{G}(w)\varphi$  and the terms on the left-hand side satisfy the bound

$$\sum_i \frac{\varphi_i^2}{w_i} \leq \frac{1}{2} \sum_{i,j} A_{ij} w_i \left( \frac{\varphi_i}{w_i} - \frac{\varphi_j}{w_j} \right) (\zeta_i - \zeta_j), \quad (59)$$

with equality achieved in (59) when the infinitesimal generator  $A$  is reversible.

In particular,  $(\text{P}_\lambda)$  together with (59) implies the weaker inequality

$$\sum_i \frac{\varphi_i^2}{w_i} \leq \frac{1}{\lambda} |A^\top \varphi|_{\mathbb{G}(w)}^2 \quad \forall \varphi \in \mathbb{R}^N : \varphi \perp \mathbb{1}. \quad (\text{P}_\lambda^\dagger)$$

Either of the inequalities above holds when  $A$  satisfies one of the conditions for  $\lambda$ -convexity stated in Theorem 3.8.

*Proof.* We follow a standard linearisation procedure of  $(\text{MLSI}_\lambda)$ . To this aim, consider  $u^\varepsilon := \exp_w(\varepsilon\varphi) \in \text{int } \mathcal{P}_n$  for any  $\varphi \perp \mathbb{1}$  and sufficiently small  $\varepsilon > 0$ . We have to show:

- (i)  $\lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon^2} \text{Ent}(u^\varepsilon) = D^2 \text{Ent}(w)(\varphi, \varphi) = \frac{1}{2} \sum_i \frac{\varphi_i^2}{w_i}$ ,
- (ii)  $\lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon^2} V_1(g^{u^\varepsilon \rightarrow w}) = \zeta^\top D\check{\mathbb{K}}(w)[L]\varphi = \frac{1}{3} \sum_i \frac{\varphi_i^2}{w_i} - \frac{1}{6} \sum_{i,j} A_{ij} w_i \left( \frac{\varphi_i}{w_i} - \frac{\varphi_j}{w_j} \right) (\zeta_i - \zeta_j)$ ,
- (iii)  $\lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon^2} |Y|_{\mathbb{G}}^2(u^\varepsilon) = |A^\top \varphi|_{\mathbb{G}(w)}^2$ .

The first equality in (i) follows from the fact that  $\text{Ent}(w) = 0$  as well as  $D \text{Ent}(w)\varphi = \sum_i \varphi = 0$ . Now the second equality boils down to a direct computation of  $D^2 \text{Ent}(w)(\varphi, \varphi)$ .

Regarding (ii), we first note that reversibility of  $Q$  implies

$$\begin{aligned} \check{\mathbb{K}}(w)[L] &= \frac{1}{2} \sum_{\substack{i,j \\ B_{ij} \neq B_{ji}}} \frac{A_{ij} w_i - A_{ji} w_j}{\log(Q_{ij} B_{ij} w_i) - \log(Q_{ji} B_{ji} w_j)} (\log B_{ij} - \log B_{ji})(e_i - e_j) \\ &= \frac{1}{2} \sum_{\substack{i,j \\ B_{ij} \neq B_{ji}}} (A_{ij} w_i - A_{ji} w_j)(e_i - e_j) = \frac{1}{2} \sum_{i,j} (A_{ij} w_i - A_{ji} w_j)(e_i - e_j) = 0. \end{aligned}$$

Hence, using that both  $u \mapsto \check{\mathbb{K}}(u)$  and the exponential map are smooth in a neighbourhood of  $w$ , we have

$$\lim_{\varepsilon \rightarrow 0} \check{\mathbb{K}}(g_r^{w \rightarrow u^\varepsilon})[L]/\varepsilon = \lim_{\varepsilon \rightarrow 0} \check{\mathbb{K}}(\exp_w(r\varepsilon\varphi))[L]/\varepsilon = rD\check{\mathbb{K}}(w)[L]\varphi.$$

A direct computation shows

$$\begin{aligned} D\check{\mathbb{K}}(w)[L]\varphi &= \frac{1}{2} \sum_{\substack{i,j \\ B_{ij} \neq B_{ji}}} (A_{ij}\varphi_i - A_{ji}\varphi_j - (Q_{ij}\varphi_i - Q_{ji}\varphi_j)\theta_{\log}(B_{ij}, B_{ji}))(e_i - e_j) \\ &= \frac{1}{2} \sum_{i,j} A_{ij}w_i \left( \frac{\varphi_i}{w_i} - \frac{\varphi_j}{w_j} \right) (e_i - e_j) - \frac{1}{2} \sum_{i,j} \check{K}_{ij}(w) \left( \frac{\varphi_i}{w_i} - \frac{\varphi_j}{w_j} \right) (e_i - e_j), \end{aligned}$$

where we used (70), the reversibility of  $Q$  and the identity  $Q_{ij}w_i\theta_{\log}(B_{ij}, B_{ji}) = \check{K}_{ij}(w)$ ; in particular, we have

$$\zeta^\top D\check{\mathbb{K}}(w)[L]\varphi = \frac{1}{2} \sum_{i,j} A_{ij}w_i \left( \frac{\varphi_i}{w_i} - \frac{\varphi_j}{w_j} \right) (\zeta_i - \zeta_j) - \sum_i \frac{\varphi_i^2}{w_i}.$$

Now the remaining first equality in (ii) follows from a change of orientation in form of  $V_1(g^{u^\varepsilon \rightarrow w}) = -V_1(g^{w \rightarrow u^\varepsilon})$  as legitimised by (11), together with an application of the dominated convergence theorem, viz.

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon^2} V_1(g^{u^\varepsilon \rightarrow w}) &= - \lim_{\varepsilon \rightarrow 0} \int_0^1 (\mathbb{G}(g_r^{w \rightarrow u^\varepsilon}) \dot{g}_r^{w \rightarrow u^\varepsilon} / \varepsilon)^\top \check{\mathbb{K}}(g_r^{w \rightarrow u^\varepsilon})[L]/\varepsilon dr \\ &= - \int_0^1 r^2 \zeta^\top D\check{\mathbb{K}}(w)[L]\varphi dr = \frac{1}{3} \sum_i \frac{\varphi_i^2}{w_i} - \frac{1}{6} \sum_{i,j} A_{ij}w_i \left( \frac{\varphi_i}{w_i} - \frac{\varphi_j}{w_j} \right) (\zeta_i - \zeta_j). \end{aligned}$$

For the proof of (59), we note that the right-hand of this inequality may be written as

$$\frac{1}{2} \sum_{i,j} A_{ij}w_i \left( \frac{\varphi_i}{w_i} - \frac{\varphi_j}{w_j} \right) (\zeta_i - \zeta_j) = \langle \phi, S\zeta \rangle$$

for a density given by  $\phi_i := \varphi_i/w_i$  and a symmetric matrix given by

$$S =: \frac{1}{2} \sum_{i,j} \frac{A_{ij}w_i + A_{ji}w_j}{2} (e_i - e_j) \otimes (e_i - e_j).$$

Note that by comparison of the logarithmic and the arithmetic mean as in (61), we have that  $\check{\mathbb{K}}(w) \leq S$  in the sense of positive semidefinite matrices. By symmetry of all involved matrices, this also means that we have  $\check{\mathbb{K}}(w)\mathbb{G}(w)\text{diag}(w) \leq S\mathbb{G}(w)\text{diag}(w)$ ; in particular,

$$\phi^\top \check{\mathbb{K}}(w)\mathbb{G}(w)\text{diag}(w)\phi \leq \phi^\top S\mathbb{G}(w)\text{diag}(w)\phi,$$

which translates into inequality (59) as to be shown.

In order to check the equality in (iii), we compute

$$\begin{aligned} Y(u^\varepsilon) &= \check{\mathbb{K}}(u^\varepsilon)D\text{Ent}(u^\varepsilon) + \check{\mathbb{K}}(u^\varepsilon)[L] \\ &= \frac{1}{2} \sum_{i,j} \check{K}_{ij}(u^\varepsilon) \left( \log \frac{u_i^\varepsilon}{w_i} - \log \frac{u_j^\varepsilon}{w_j} + \log B_{ij} - \log B_{ji} \right) (e_i - e_j) = -A^\top u^\varepsilon. \end{aligned}$$

Since  $w$  as a stationary distribution for  $A$  satisfies  $A^\top w = 0$ , we may use the identity in (15) to obtain

$$\lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon} Y(u^\varepsilon) = -A^\top \varphi.$$

Finally, Corollary 7.3 shows that  $(P_\lambda)$  is already implied by any of the  $\lambda$ -convexity conditions in Theorem 3.8.  $\square$

**Proposition 7.6.** *Let  $A = Q \circ B$  be an infinitesimal generator with stationary distribution  $w$  for both  $A$  and  $Q$ . If there is a positive  $\lambda > 0$  such that  $(T_\lambda^W)$  holds for all  $u$  inside a neighbourhood of  $w$ , then also the following discrete Poincaré inequality:*

$$\sum_i \phi_i^2 w_i \leq \frac{1}{\lambda} \phi^\top \check{K}(w) \phi \quad \forall \phi \in \mathbb{R}^N : \phi \perp w. \quad (P_\lambda^*)$$

The inequality above holds when  $A$  satisfies one of the conditions for  $\lambda$ -convexity stated in Theorem 3.8.

*Proof.* Denote by  $\phi$  the density corresponding to  $\varphi$ , i.e.  $\phi_i := \varphi_i/w_i$  for some  $\varphi \perp \mathbb{1}$ . Let  $u^\varepsilon := \exp_w(\varepsilon \phi) \in \text{int } \mathcal{P}_n$  for  $\varepsilon > 0$ , sufficiently small such that  $u^\varepsilon$  belongs to a ball of injectivity radius centred at  $w$ .

We write

$$\sum_i \phi_i^2 w_i = \sum_i \varphi_i \phi_i = \sum_i \varphi_i \frac{u_i^\varepsilon - w_i}{\varepsilon} + \chi^\varepsilon$$

with an error term  $\chi^\varepsilon \in \mathcal{O}(\varepsilon^2)$ . Following the notation of Lemma 5.2, consider a geodesic pair  $(g^t, V^t)_{t \in [0,1]}$  joining  $u^\varepsilon$  to  $w$ . Using  $(\mathbf{C}\mathbf{E}^*)$ , we may write the difference quotient in the equation above as

$$\begin{aligned} \sum_i \varphi_i \frac{u_i^\varepsilon - w_i}{\varepsilon} &= \frac{1}{\varepsilon} \sum_i \int_0^1 \varphi_i g_i^r dr = \frac{1}{\varepsilon} \sum_{i,j} \int_0^1 V_{ij}^r (\varphi_i - \varphi_j) dr \\ &\leq \frac{1}{\varepsilon} \left( \sum_{i,j} \int_0^1 \frac{(V_{ij}^r)^2}{\check{K}_{ij}(g^r)} dr \right)^{1/2} \left( \sum_{i,j} \int_0^1 (\varphi_i - \varphi_j)^2 \check{K}_{ij}(g^r) dr \right)^{1/2} \\ &= \frac{1}{\varepsilon} \mathcal{W}(u^\varepsilon, w) \left( \sum_{i,j} (\varphi_i - \varphi_j)^2 \int_0^1 \check{K}_{ij}(g^r) dr \right)^{1/2}, \end{aligned}$$

where we used Hölder's inequality for the estimate in the second line and the fact that  $(g^t, V^t)_{t \in [0,1]}$  is length-minimising in the last line. In total, taking into account  $(T_\lambda^W)$ , we arrive at the estimate

$$\sum_i \phi_i^2 w_i \leq \frac{1}{\varepsilon} \left( \frac{2}{\lambda} \text{Ent}(u^\varepsilon) + V_1(g^{w \rightarrow u^\varepsilon}) \right)^{1/2} \left( \sum_{i,j} (\varphi_i - \varphi_j)^2 \int_0^1 \check{K}_{ij}(g^r) dr \right)^{1/2} + \chi^\varepsilon. \quad (60)$$

We already know from (i) and (ii) in the proof of Proposition 7.5 as well as (59) that

$$\begin{aligned} &\lim_{\varepsilon \rightarrow 0} \frac{1}{\varepsilon^2} ((\text{Ent}(u^\varepsilon) + V_1(g^{w \rightarrow u^\varepsilon})) \\ &= \frac{5}{6} \sum_i \phi_i^2 w_i - \frac{1}{6} \sum_{i,j} A_{ij} w_i (\phi_i - \phi_j) (\zeta_i - \zeta_j) \leq \frac{1}{2} \sum_i \phi_i^2 w_i, \end{aligned}$$

where  $\zeta = \mathbb{G}(w)\varphi$ . Hence, it remains to show

$$\lim_{\varepsilon \rightarrow 0} \int_0^1 \check{K}_{ij}(g^r(\varepsilon)) dr = \check{K}_{ij}(w) \quad \forall i, j \in [N],$$

in order to conclude. Indeed, this claim follows readily from Lemma 5.4 which – by equivalence of norms in  $\mathbb{R}^N$  – implies the bound

$$\sum_i |g_i^r - w_i| \leq C\mathcal{W}(g^r, w) \leq C\mathcal{W}(u^\varepsilon, w) \quad \forall r \in [0, 1]$$

for some constant  $C > 0$ . This estimate yields  $g^r \rightarrow w$  uniformly in  $r \in [0, 1]$  as  $\varepsilon \rightarrow 0$ , which in turn implies the claim.

Finally, Proposition 7.4 shows that  $(P_\lambda^*)$  is already implied by any of the  $\lambda$ -convexity conditions in Theorem 3.8.  $\square$

## 8. APPENDIX: PROPERTIES OF THE LOGARITHMIC MEAN

In this appendix we collect some properties of the logarithmic mean, used throughout the text. Most of the proofs may be found in Appendix A of [Mie13]; except for the proofs of (67) and (71) to be found in [Mie13] (see Proposition 4.5) and [EM12] (see Lemma 2.2), respectively.

**Definition 8.1.** The logarithmic mean  $\theta_{\log} : \mathbb{R}_0^+ \times \mathbb{R}_0^+ \rightarrow \mathbb{R}_0^+$  is defined by

$$\theta_{\log}(a, b) := \int_0^1 a^r b^{1-r} dr.$$

**Facts 8.2.** The logarithmic mean  $\theta_{\log}$  satisfies the following properties:

(i) Representation formula:

$$\theta_{\log}(a, b) = \frac{a - b}{\log a - \log b} \quad \forall a, b > 0 : a \neq b.$$

(ii) Bounds by geometric and arithmetic means:

$$\frac{2ab}{a+b} \leq \sqrt{ab} \leq \theta_{\log}(a, b) \leq \frac{a+b}{2}. \quad (61)$$

(iii) 1-homogeneity:

$$\theta_{\log}(\alpha a, \alpha b) = \alpha \theta_{\log}(a, b) \quad \forall \alpha > 0. \quad (62)$$

(iv) Non-vanishing behaviour in the interior:

$$\theta_{\log}(a, b) > 0 \quad \text{and} \quad \partial_1 \theta_{\log}(a, b) > 0 \quad \forall a, b > 0. \quad (63)$$

(v) Vanishing behaviour on the boundary:

$$\theta_{\log}(a, 0) = \theta_{\log}(0, a) = 0 \quad \text{and} \quad \partial_1 \theta_{\log}(a, 0) = 0 \quad \forall a > 0. \quad (64)$$

(vi) Identities and bounds for the derivatives of  $\theta_{\log}$ :

$$a \partial_1 \theta_{\log}(a, b) + b \partial_2 \theta_{\log}(a, b) = \theta_{\log}(a, b), \quad (65)$$

$$b \partial_1 \theta_{\log}(a, b) + a \partial_2 \theta_{\log}(a, b) \geq \theta_{\log}(a, b), \quad (66)$$

$$s \partial_1 \theta_{\log}(a, b) + t \partial_2 \theta_{\log}(a, b) \geq \theta_{\log}(s, t), \quad (67)$$

$$\partial_1 \theta_{\log}(a, b) + \partial_2 \theta_{\log}(a, b) = \frac{\theta_{\log}^2(a, b)}{ab} \geq 1, \quad (68)$$

$$a \partial_2 \theta_{\log}(a, b) = \max_{r>0} \{ \theta_{\log}(r, a) - r \partial_1 \theta_{\log}(a, b) \}, \quad (69)$$

$$\partial_1 \theta_{\log}(a, b) = \frac{1 - \theta_{\log}(a, b)/a}{\log a - \log b}, \quad (70)$$

(vii) For all  $\beta \geq 0$ , we have the estimate

$$\beta (\theta_{\log}(r, a) + \theta_{\log}(a, b)) - s (\partial_1 \theta_{\log}(r, b) + \partial_2 \theta_{\log}(r, b)) \leq \tilde{g}(\beta) \theta_{\log}(r, b) \quad \forall r, a, b > 0, \quad (71)$$

where

$$\tilde{g} := \begin{cases} 2\beta & \text{if } 0 \leq \beta \leq 1/2, \\ 4\beta \ell(1/(4\beta)) & \text{if } 1/2 \leq \beta, \end{cases} \quad (72)$$

with a decreasing convex function  $\ell(t) := \max_{r>0} \{ \theta_{\log}(1, r) - rt \}$ .



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