Bulletin of Mathematical Sciences
Vol. 10, No. 2 (2020) 2050011 (26 pages)

DOI: 10.1142/S1664360720500113

Optimal transport with discrete long-range mean-field interactions

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Received 17 December 2019
Revised 24 February 2020
Accepted 9 March 2020
Published 12 May 2020

Communicated by Neil Trudinger

We study an optimal transport problem where, at some intermediate time, the mass is either accelerated by an external force field or self-interacting. We obtain the regularity of the velocity potential, intermediate density, and optimal transport map, under the conditions on the interaction potential that are related to the so-called Ma–Trudinger–Wang condition from optimal transport [X.-N. Ma, N. S. Trudinger and X.-J. Wang, Regularity of potential functions of the optimal transportation problems, *Arch. Ration. Mech. Anal.* **177** (2005) 151–183.].

Keywords: Optimal transport; reconstruction problem; time-discrete.

Mathematics Subject Classification: 35J96, 37J50

1. Introduction

1.1. *Motivations*

The optimal transport problem goes back to a cost-minimization problem in civil engineering proposed by Monge [1], later generalized to a class of optimization problems by Kantorovich [2, 3], with an elegant economic interpretation. Later, through

[‡]Corresponding author. This work was partially supported by the Australian Research Council DP170100929 and DP200101084.

the contributions of Brenier [4], Benamou and Brenier [5], Frisch and co-workers [6–8], Loeper [9], and Lee and McCann [10], the connection between optimal transport and classical mechanics has also appeared very naturally. Indeed, a natural approach in Hamiltonian mechanics is to look for critical points of the action of a Lagrangian in order to find the evolution equation of the system. In some cases where the Lagrangian has some form of coercivity [as in the natural action $\int_{[0,T]\times\mathbb{R}^d} \rho(t,x)|v|^2(t,x)dtdx$, cf. [5]], critical points of the action can be obtained by minimization, which has a natural formulation as an optimal transport problem. The continuous time formulation of the problem in terms of curves on a space of probability measures is extensively addressed in the book by Ambrosio *et al.* [11], and also in the books by Villani [12, 13].

One of the main differences between the *economic* point of view and the *mechanical* point of view is the addition of the time variable. The original transport problem starts with a cost function $c(x, y)$ that depends only on the starting and arrival points. The action minimizing problem looks for curves or vector fields (depending on whether one uses the Lagrangian or Eulerian point of view). We shall speak either of the *point-to-point* or *time-continuous* problem to distinguish between these two situations.

Although in both cases the existence of optimizers rests now on a well-established theory, the question of their regularity is relatively well understood for the point-to-point problems, while it is still largely unexplored in the time-continuous case (see references below). In the point-to-point problem, by regularity we mean the smoothness of the optimal map sending one distribution of mass to the other; in the time-continuous case, such a map usually exists too, but is more difficult to characterize. The main reason for that difference is that the regularity of the point-to-point problem relies on the study of an associated Monge–Ampère equation, which is not always accessible in the time-continuous case.

1.2. *An example*: *The reconstruction problem in cosmology*

As an illustrative example, we go back to a previous work by Loeper [9], where he studies the motion of self-gravitating matter, classically described by the Euler–Poisson system, for an application in cosmology, known as the *reconstruction problem*, a problem that has received a lot of attention in cosmology (see [6–8] and the references therein). Let us recall the model here: a continuous distribution of matter with density ρ moves along a velocity field v, and is accelerated by a gravitational field, with itself being given as the gradient of a potential p, linked to ρ through the Poisson equation. The system is thus the following:

$$\begin{cases} \partial_t\rho + \nabla\cdot(\rho v) = 0, \\ \partial_t(\rho v) + \nabla\cdot(\rho v\otimes v) = -\rho\nabla p, \\ \Delta p = \rho. \end{cases} \tag{1.1}$$

The first equation is the conservation of mass, the second equation states that the acceleration field is given by $-\nabla p$, and the third equation is the gravitational Poisson coupling.

The reconstruction problem is to find a solution to (1.1) satisfying

$$\rho|_{t=0} = \rho_0, \quad \rho|_{t=T} = \rho_T,$$

i.e. given the initial and final densities, as opposed to the Cauchy (or initial-value) problem, where one is given the initial density and velocity. In [9] (see also [4] for the case of the incompressible Euler equations), the reconstruction problem was formulated as a minimization problem, minimizing the action of the Lagrangian, which is a convex functional of properly chosen variables. Through this variational formulation, the reconstruction problem becomes very similar to the time-continuous formulation of the optimal transport problem of Benamou and Brenier [5]. Moreover, through the study of a dual problem, reminiscent of Monge–Kantorovich duality, partial regularity results for the velocity and the density were obtained.

The optimal transport problem of [9] was formulated as finding minimizers of the action

$$I(\rho, v, p) = \frac{1}{2}\int_0^T \int_{\mathbb{T}^d} \rho(t,x)|v(t,x)|^2 + |\nabla p(t,x)|^2 \, dxdt, \tag{1.2}$$

over all ρ, p and v satisfying

$$\partial_t \rho + \nabla \cdot (\rho v) = 0,$$

$$\rho(0) = \rho_0, \quad \rho(T) = \rho_T,$$

$$\Delta p = \rho - 1,$$

where $\mathbb{T}^d$ denotes the d-dimensional torus, as the study in [9] was performed in the space-periodic case.

1.3. *Goal of the paper*

In this paper we address the problem of finding minimizers for the action

$$I(\rho, v) = \int_0^T \left(\int_{\mathbb{R}^d} \frac{1}{2}\rho(t,x)|v(t,x)|^2 dx + \mathcal{F}(t, \rho(t)) \right) dt, \tag{1.3}$$

for a certain class of *internal energy* $\mathcal{F}$, and we will obtain some partial results in that direction.

Apart from the application in cosmology, several authors have looked at continuous optimal transport with or without interaction, notably through their natural connections with mean-field games. We refer the reader to the work [14] and the references therein, where the connection is explored. Again, we also refer to the book [11] where the notion of gradient flows on space of measures and its relation to optimal transport are addressed.

This work is about the study of regularity of minimizers to (1.3). In [10], Lee and McCann address the case where

$$\mathcal{F}(t,\rho) = \int \rho(t,x)Q(t,x)dx,$$

which is obviously linear in ρ. This Lagrangian corresponds to the case of a continuum of matter evolving in an external acceleration field given by $\nabla Q(t,x)$. We call this the noninteracting case for obvious reasons. This can be recast as an optimal transport problem where the cost function is given by

$$c(x,y) = \inf_{\gamma(0)=x,\gamma(T)=y} \int_0^T \frac{1}{2}|\dot{\gamma}(t)|^2 + Q(t,\gamma(t))dt, \tag{1.4}$$

where γ is a smooth curve connecting x and y. By assuming that $Q(t,x) = \varepsilon V(x)$ for some V satisfying the structure condition

$$-\int_0^1\int_0^\tau \langle u,(1-t)\partial_s^2 \text{ Hess } V_{x+t(v+sw)}u\rangle|_{s=0}dtd\tau \geq C,$$

for a constant $C > 0$, for all (x,v) in the tangent bundle $T\mathbb{T}^d$, and for all unit tangent vectors u,w in the tangent space $T_x\mathbb{T}^d$ that are orthogonal to each other, Lee and McCann obtain that for a small enough $\varepsilon > 0$, the cost c satisfies the conditions found in [15] to ensure the regularity of the optimal map. (Note that in order to be consistent with our notations, here we changed the sign of the potential actually considered in [10].)

1.3.1. *The noninteracting, discrete case*

In this paper we will restrict ourselves to the case where the force field only acts at a single discrete time between 0 and T:

$$Q(t,x) = \delta_{t=T/2}Q(x).$$

The minimization problem therefore becomes

$$I(\rho,v) = \int_0^T\int_{\mathbb{R}^d} \frac{1}{2}\rho(t,x)|v(t,x)|^2dxdt + \int_{\mathbb{R}^d} \rho(T/2,x)Q(x)dx, \tag{1.5}$$

for some potential Q. This restriction will allow us to remove the smallness condition on Q.

1.3.2. *The mean-field case*

We will be able to extend our result to the nonlinear situation where the force field is given by

$$\nabla Q(x) = \int \rho(t,y)\nabla\kappa(x-y)dy, \tag{1.6}$$

still acting at a single intermediate time. This corresponds to the case where a particle located at y accelerates another particle located at x with an acceleration equal to $\nabla\kappa(x-y)$. In this case we will show that the action to minimize becomes

$$I(\rho, v) = \frac{1}{2}\int_0^T\int_{\mathbb{R}^d} \rho|v|^2 dxdt + \frac{1}{2}\int_{\mathbb{R}^d}\int_{\mathbb{R}^d} \rho(T/2, x)\kappa(x-y)\rho(T/2, y)dxdy. \tag{1.7}$$

Reasoning formally, one sees straightaway that on $[0, T/2]$ we are solving the usual optimal transport problem in its "Benamou–Brenier" formulation [5], as well as on $[T/2, T]$, and therefore particles will travel with constant velocity in those two intervals. At $t = T/2$, the velocity v will be discontinuous. We will give a sufficient condition on κ to ensure a smooth transport map and intermediate density. Unfortunately, the gravitational case, which corresponds to the Coulomb kernel

$$\kappa(x-y) = \frac{c_d}{|x-y|^{d-2}}, \tag{1.8}$$

does not satisfy our condition.

1.4. *The time discretization*

A natural approximation of the time-continuous problem is to partially discretize in time (1.3) into

$$I(\rho, v) = \int_0^T\int_{\mathbb{R}^d} \frac{1}{2}\rho(t,x)|v(t,x)|^2 dxdt + \frac{T}{N}\sum_{i=1}^{N-1} \mathcal{F}(t_i, \rho(t_i)), \tag{1.9}$$

for $t_i = \frac{iT}{N}$, $i = 0, \ldots, N$, a discretization of the time interval $[0, T]$. Then, on each subinterval $[t_{i-1}, t_{i+1}]$, having set $\rho(t_{i-1})$ and $\rho(t_{i+1})$, one has to solve a problem of the form (1.5). For this reason, the study of the problem (1.5) seems a natural starting point. Our results show regularity on $\rho(T/2)$ assuming $\rho(0)$ and $\rho(T)$ are regular [loosely speaking, $\rho(T/2)$ has the same regularity as $\rho(0)$ and $\rho(T)$]. It would be a natural extension of our work to deal with multiple time steps, however we do not see a straightforward way to tackle this problem.

1.5. *Organization of the paper*

The paper is organized as follows: In Sec. 2 we state the problem formally, our main assumptions, and our results. In Sec. 3, we derive Eq. (2.17) formally by straightforward computations. In Sec. 4, we introduce a two-step optimal transport problem and prove Theorem 2.1. By assuming the conditions (H0)–(H1) we have the existence and uniqueness of the velocity potential ϕ. Moreover, we provide an interpretation of the cost function from a natural mechanical point of view. In Sec. 5, we introduce the condition (H2), which is crucial in obtaining the regularity of ϕ. In Sec. 6, upon formulating our reconstruction problem into an optimal transport problem, we have the regularity of ϕ and conclude Theorem 2.2. In Sec. 7, we consider the mean-field case under the condition (H2c), which is preserved by convex combinations, and then prove Theorems 2.4 and 2.5.

2. Problem Statement, Assumptions and Results

2.1. *Equivalent formulation of the problem*

We start by giving three formulations of the problem that will turn out to be equivalent.

Problem 1. *We consider $\mathcal{P}_2(\mathbb{R}^d)$ (in short $\mathcal{P}_2$) the set of probability measures on $\mathbb{R}^d$ with finite second moment, and a functional $\mathcal{F} : \mathcal{P}_2 \to \mathbb{R} \cup \{+\infty\}$. For a given curve $\rho(t) : [0,T] \to \mathcal{P}_2$ and a vector field $v(t) \in L^2([0,T] \times \mathbb{R}^d, dt \times d\rho(t))$ we consider the action*

$$I(\rho, v) = \int_{[0,T]\times\mathbb{R}^d} \frac{1}{2} d\rho(t,x)|v(t,x)|^2 dt + \mathcal{F}(\rho(T/2)) \tag{2.1}$$

and the constraints

$$\partial_t \rho + \nabla \cdot (\rho v) = 0, \tag{2.2}$$

$$\rho(0) = \rho_0, \quad \rho(T) = \rho_T. \tag{2.3}$$

Problem 1 is to minimize I among all ρ, v satisfying (2.2)–(2.3).

Problem 2. *Consider the space of continuously differentiable curves $\Gamma = C^1([0,T]; \mathbb{R}^d)$. To each $x \in \mathbb{R}^d \cap$ support (ρ_0) we associate $\gamma(t,x) \in \Gamma$ such that $\gamma(0,x) = x$. We consider*

$$J(\gamma) = \int_0^T \frac{1}{2} |\partial_t \gamma(t,x)|^2 dt\, d\rho_0(x) + \mathcal{F}(\rho(T/2)), \tag{2.4}$$

where[a]

$$\rho(T/2) = \gamma(T/2)_{\#}\rho_0, \tag{2.5}$$

and under the constraint

$$\rho_T = \gamma(T)_{\#}\rho_0. \tag{2.6}$$

Problem 2 is to minimize J among all γ satisfying (2.5)–(2.6).

Problem 3. *For $\mu, \nu \in \mathcal{P}_2$, letting $\Gamma_{\mu,\nu}$ to be the set of probability measures on $\mathbb{R}^d \times \mathbb{R}^d$ with marginals μ and ν, we recall that the Wasserstein distance* (*of order* 2) *between μ and ν is given by*

$$W_2^2(\mu, \nu) = \inf_{\pi \in \Gamma_{\mu,\nu}} \int_{\mathbb{R}^d\times\mathbb{R}^d} \frac{1}{2}|x-y|^2 d\pi(x,y). \tag{2.7}$$

We define

$$K(\rho) = \frac{2}{T} W_2^2(\rho_0, \rho) + \mathcal{F}(\rho) + \frac{2}{T} W_2^2(\rho, \rho_T). \tag{2.8}$$

[a]The subscript # classically means that $\gamma(T/2)$ pushes forward ρ_0 onto $\rho(T/2)$.

Problem 3 *is to minimize* K *among all* $\rho \in \mathcal{P}_2$. *It coincides with the notion of Wasserstein Barycenters, see* [16, 17], *when*

$$\mathcal{F}(\rho) = CW_2^2(\rho_I, \rho), \quad C > 0,$$

for some intermediate measure $\rho_I \in \mathcal{P}_2$.

From the classical results of optimal transport (see [12, 13, 11]), in the case where $\mathcal{F}(\rho)$ is convex and lower-semi-continuous (l.s.c.) in ρ there holds the following proposition.

Proposition 2.1. *Let* $\rho_0, \rho_T \in \mathcal{P}_2 \cap L^1(\mathbb{R}^d)$. *Assume that* $\mathcal{F}(\rho)$ *is convex and l.s.c. in* ρ, *and that Problem* 1, 2, *or* 3 *has at least one admissible solution, then Problems* 1–3 *are equivalent, and moreover there holds*

$$v(0, x) = \partial_t \gamma(0, x) = \frac{2}{T}(\nabla \Phi^*(x) - x) =: \nabla \phi(x), \tag{2.9}$$

where v, γ *are respectively from Problems* 1 *and* 2, Φ^* *is a convex potential such that* $\nabla \Phi^*_{\#} \rho_0 = \rho$, *and* ρ *is the optimizer in Problem* 3.

Proposition 2.2 gives the Euler–Lagrange equation characterizing the optimizer. It is based on the Riemannian metric induced on $\mathcal{P}_2$ by W_2 (see again the above references for a complete coverage).

Proposition 2.2. *Let* ρ *be the optimizer in Problem* 3. *There exists a vector field* $w = \nabla \Xi \in L^2(d\rho)$ *and two convex potentials* Φ, Ψ *such that*[b]

$$\nabla \Phi_{\#} \rho = \rho_0, \tag{2.10}$$

$$\nabla \Psi_{\#} \rho = \rho_T, \tag{2.11}$$

$$\nabla \Psi + \nabla \Phi = 2x + \frac{T}{2} \nabla \Xi, \tag{2.12}$$

moreover, $\nabla \Xi$ *can be identified to be the gradient of* $\mathcal{F}$ *with respect to the Wasserstein metric, i.e. for all curves* $\rho_t \subset \mathcal{P}_2 \cap \mathrm{Dom}(\mathcal{F})$ *passing through* ρ *at* $t = 0$, *and such that*

$$\partial_t \rho_t + \nabla \cdot (\rho_t v_t) = 0,$$

for some $v_t \in L^\infty([0, T]; L^2(d\rho_t))$ *there holds*

$$\frac{d}{dt} \mathcal{F}(\rho_t) \bigg|_{t=0} = \int d\rho \, \nabla \Xi \cdot v_0.$$

We will denote $\nabla \Xi = \nabla_W \mathcal{F} \Big|_\rho$.

We next characterize Ξ in the two cases of interest for this paper.

[b]Note that Φ^* above is the Legendre transform of Φ.

Proposition 2.3. (i) *Assume that* $\mathcal{F}(\rho)$ *is as in* (1.5). *Then*

$$\Xi = \frac{Q}{T}.$$

(ii) *If* $\mathcal{F}(\rho)$ *is as in* (1.7) *then*

$$\Xi = \frac{1}{T}\int_{\mathbb{R}^d} \kappa(\cdot - y)d\rho(y) =: \frac{Q_\rho}{T}.$$

We can also completely characterize the optimal velocity: With ϕ *as in Proposition* 2.1, *we have the following:*

(i) *When* $t \in [0, \frac{T}{2})$, $v(t,x) = \nabla\phi(x_0)$, *where* $x = x_0 + t\nabla\phi(x_0)$; $\rho(t) = (x + t\nabla\phi)_{\#}\rho_0$.
(ii) *When* $t \in (\frac{T}{2}, T]$, $v(t,x) = \nabla\phi(x_0) + \nabla Q(z)$, *where* $x = z + (t - \frac{T}{2})(\nabla\phi(x_0) + \nabla Q(z))$ *and* $z = x_0 + \frac{T}{2}\nabla\phi(x_0)$.

Finally, we characterize the optimal map: $\mathbf{m}(x)$ *such that* $\mathbf{m}(\gamma(0,x)) = \gamma(T,x)$ (*for* γ *the optimizer in Problem* 2) *will be given by*

$$\mathbf{m}(x) = x + T\nabla\phi + \frac{T}{2}\nabla Q\left(x + \frac{T}{2}\nabla\phi\right), \tag{2.13}$$

and there also holds

$$\mathbf{m}(x) = \nabla\Psi(\nabla\Phi^*(x)). \tag{2.14}$$

2.2. *Assumptions*

From the previous observations, and in order to motivate our assumptions, let us derive formally the equation giving the initial velocity potential ϕ. Let the initial density ρ_0 be supported on a bounded domain $\Omega_0 \subset \mathbb{R}^d$, and the final density ρ_T be supported on a bounded domain $\Omega_T \subset \mathbb{R}^d$, satisfying the balance condition

$$M := \int_{\Omega_0} \rho_0(x)\,dx = \int_{\Omega_T} \rho_T(y)dy. \tag{2.15}$$

Starting from the definition (2.13), we introduce the modified potential functions

$$\tilde{\phi}(x) := \frac{T}{2}\phi(x) + \frac{1}{2}|x|^2, \quad \text{and} \quad \tilde{Q}(z) := \frac{T}{2}Q(z) + |z|^2. \tag{2.16}$$

By computing the determinant of the Jacobian $D\mathbf{m}$ and noting that $\mathbf{m}_{\#}\rho_0 = \rho_T$, i.e. that $\mathbf{m}$ pushes forward the measure ρ_0 onto the measure ρ_T, one can derive the Monge–Ampère-type equation (see Sec. 3 for detailed computation)

$$\det[D^2\tilde{\phi} - (D^2\tilde{Q}(\nabla\tilde{\phi}))^{-1}] = \left(\frac{1}{\det D^2\tilde{Q}(\nabla\tilde{\phi})}\right)\frac{\rho_0}{\rho_T \circ \mathbf{m}}, \tag{2.17}$$

with a natural boundary condition

$$\mathbf{m}(\Omega_0) = \Omega_T. \tag{2.18}$$

To ensure the regularity of the solution $\tilde{\phi}$ (equivalently that of ϕ) to the boundary-value problem (2.17) and (2.18), it is necessary to impose certain conditions on the potential function $\tilde{Q}$ (equivalently on Q) and the domains Ω_0, Ω_T. In this paper we assume $\tilde{Q}$ satisfies the following conditions:

(H0) The potential function $\tilde{Q}$ belongs to $C^4(\mathbb{R}^d)$.

(H1) The potential function $\tilde{Q}$ is uniformly convex, namely $D^2\tilde{Q} \geq \varepsilon_0 I$ for some $\varepsilon_0 > 0$.

(H2) The potential function $\tilde{Q}$ satisfies for all $\xi, \eta \in \mathbb{R}^d$, with $\xi \perp \eta$,

$$\sum_{i,j,k,l,p,q,r,s} (\tilde{Q}_{ijrs} - 2\tilde{Q}^{pq}\tilde{Q}_{irp}\tilde{Q}_{jsq})\tilde{Q}^{rk}\tilde{Q}^{sl}\xi_k\xi_l\eta_i\eta_j \leq -\delta_0|\xi|^2|\eta|^2, \tag{2.19}$$

where $\{\tilde{Q}^{ij}\}$ is the inverse of $\{\tilde{Q}_{ij}\}$, and δ_0 is a positive constant. When $\delta_0 = 0$, we call it (H2w), a weak version of (H2).

Note that the conditions (H0) and (H1) imply that the inverse matrix $(D^2\tilde{Q})^{-1}$ exists, and ensure that Eq. (2.17) is well defined. Condition (H2) is an analog of the Ma–Trudinger–Wang (MTW) condition in optimal transportation, which is necessary for regularity results (note the factor 2 however). We shall give more detailed interpretations and examples in Sec. 5.

2.3. *Results*

Our first main result is the following.

Theorem 2.1. *Under the assumptions* (H0) *and* (H1) *Problems* 1–3 *are equivalent to solving an optimal transport problem with cost function* $c(x, y) = \tilde{Q}^*(x + y)$, *where* $\tilde{Q}^*$ *is the Legendre transform of* $\tilde{Q}$ *given in* (2.16). *There exists a potential* $\tilde{\phi}$ *such that the optimal transport map of* ρ_0 *onto* ρ_T *with cost* c *will be given by* $T(x) = y$ *such that* $D_xQ^*(x + y) = D_x\tilde{\phi}(x)$. *Then* $\phi = \frac{2}{T}(\tilde{\phi} - |x|^2/2)$ *will be the initial velocity potential as in Proposition* 2.1.

Our next result is a regularity result.

Theorem 2.2. *Let* ϕ *be the initial velocity potential as above. Assume the potential function* $\tilde{Q}$ *satisfies conditions* (H0)–(H2), Ω_T *is q-convex with respect to* Ω_0 *(defined in* Sec. 6*). Assume that* $\rho_T \geq c_0$ *on* Ω_T *for some positive constant* c_0, $\rho_0 \in L^p(\Omega_0)$ *for some* $p > \frac{d+1}{2}$, *and the balance condition* (2.15) *is satisfied. Then, the velocity potential* ϕ *is* $C^{1,\alpha}(\overline{\Omega}_0)$ *for some* $\alpha \in (0, 1)$.

If furthermore, Ω_0, Ω_T *are* C^4 *smooth and uniformly q-convex with respect to each other,* $\rho_0 \in C^2(\overline{\Omega}_0)$, *and* $\rho_T \in C^2(\overline{\Omega}_T)$, *then* $\phi \in C^3(\overline{\Omega}_0)$, *and higher regularity follows from the theory of linear elliptic equations. In particular, if* $\tilde{Q}, \Omega_0, \Omega_T, \rho_0, \rho_T$ *are* C^∞, *then the velocity potential* ϕ *is in* $C^\infty(\overline{\Omega}_0)$.

The proof of Theorem 2.2 follows from Theorem 2.1, and from the observation that condition (H2) is equivalent to $\tilde{Q}^*$ satisfying the MTW condition. Under this formulation, the regularity results then follow from the results in [9, 18, 15, 19]. For $C^{1,\alpha}$ regularity results under the condition (H2w) and some additional conditions on domains, we refer the reader to [20, 21]. See also [22, 23] for related results.

As a byproduct of those two results we obtain the following:

Theorem 2.3. *Consider the optimal transport problem with cost $c(x,y) = R(x+y)$ for some $R : \mathbb{R}^d \to \mathbb{R}$ convex. Then this problem is equivalent to the minimization problem* (1.5) *with potential $Q(z) = \frac{2}{T}(R^*(z) - |z|^2)$, for R^* being the Legendre–Fenchel transform of R.*

For the mean-field case, we have the following existence and uniqueness result.

Theorem 2.4. *Assume that $\kappa \in C^4(\mathbb{R}^d; \mathbb{R}^+)$ is convex. There exists a minimizer to problem* (1.7). *Moreover, once $\rho(T/2)$ is known, letting $\bar\rho = \rho(T/2)$, the minimizer will be the same as the solution of non-interacting problem* (1.5) *where Q is given by*

$$Q(x) = \int_{\mathbb{R}^d} \bar\rho(y)\kappa(x-y)dy. \tag{2.20}$$

Under additional assumptions on the kernel κ and the domains, we have the following regularity result.

Theorem 2.5. *Let $\Omega_{T/2} := \nabla\tilde\phi(\Omega_0)$ with $\tilde\phi$ given in* (2.16). *Assume moreover that κ satisfies the following*:

(H2c) *For any $\xi, \eta \in \mathbb{R}^d$, $x, y \in \Omega_{T/2}$,*

$$\sum_{i,j,k,l,p,q,r,s} (D^4_{ijrs}\kappa(x-y))\tilde\kappa^{rk}\tilde\kappa^{sl}\xi_k\xi_l\eta_i\eta_j \le 0,$$

where $\{\tilde\kappa^{ij}\}$ is the inverse of $\{\kappa_{ij} + \frac{2}{T}I\}$.

Assume that Ω_0, Ω_T are smooth convex domains. Let $\varphi \in C^2(\overline{\Omega}_0)$ and $\psi \in C^2(\overline{\Omega}_T)$ be convex defining functions of Ω_0 and Ω_T, respectively. Suppose that for any $z, w \in \Omega_{T/2}$,

$$\left[\varphi_{ij}(x) + \frac{TM}{8}\kappa_{ijk}(z-w)\varphi_k(x)\right] \ge b_0\delta_{ij}, \quad \forall\, x \in \partial\Omega_0, \tag{2.21}$$

and

$$\left[\psi_{ij}(y) + \frac{TM}{8}\kappa_{ijk}(z-w)\psi_k(y)\right] \ge b_1\delta_{ij}, \quad \forall\, y \in \partial\Omega_T, \tag{2.22}$$

where b_0, b_1 are two constants, and M is the total mass in (2.15).

If $b_1 \ge 0$, Ω_T is q-convex with respect to Ω_0, where Q is given by (2.20), *then the first conclusion of Theorem* 2.2 *holds. If furthermore, $b_0, b_1 > 0$ are positive and Ω_0 and Ω_T, are uniformly q-convex with respect to each other, then the second conclusion of Theorem* 2.2 *holds, namely the initial velocity potential ϕ is smooth provided $\kappa, \Omega_0, \Omega_T, \rho_0$ and ρ_T are smooth, which in turn implies that the intermediate density $\rho(T/2)$ is smooth.*

The proof of Theorem 2.5 relies on the observation that the q-convexity and the condition (H2c) are preserved under convex combinations, and therefore by convolution with the density $\rho(T/2)$, and on some *a priori* C^1 estimates on the potential. We remark that the condition (H2c) is related to the condition (B4) in [21] where the cost function satisfies the MTW condition without the orthogonal restriction.

3. Formal Derivation of Eq. (2.17)

Throughout the following context, unless mentioned otherwise, the function ϕ always denotes the initial velocity potential, namely at time $t = 0$, the velocity

$$v(0, x) = \nabla\phi(x), \quad \text{for } x \in \Omega_0. \tag{3.1}$$

In order to derive the equation for ϕ, let us track a single point $x \in \Omega_0$.

Recalling that at $t = T/2$, the potential ∇Q affects the velocity $v = \nabla\phi$, the final point $y = \mathbf{m}(x)$ is given by

$$\mathbf{m}(x) = x + T\nabla\phi + \frac{T}{2}\nabla Q\left(x + \frac{T}{2}\nabla\phi\right). \tag{3.2}$$

The Jacobian matrix of $\mathbf{m}$ is

$$\begin{aligned} D\mathbf{m} &= I + TD^2\phi + \frac{T}{2}D^2Q\cdot\left[I + \frac{T}{2}D^2\phi\right] \\ &= \left[I + \frac{T}{2}D^2Q\right]\cdot\left[I + \frac{T}{2}D^2\phi\right] + \frac{T}{2}D^2\phi, \end{aligned}$$

where I is the $d\times d$ identity matrix, and the matrix (D^2Q) is taken at $(x+T/2\nabla\phi)$.

Define

$$A := \left[I + \frac{T}{2}D^2Q\right],$$

and assume that the matrix $(I + A)$ is invertible. Then

$$\begin{aligned} D\mathbf{m} &= A\cdot\left[I + \frac{T}{2}D^2\phi\right] + \frac{T}{2}D^2\phi = [I + A]\cdot\frac{T}{2}D^2\phi + A \\ &= [I + A]\cdot\frac{T}{2}D^2\phi + (I + A) - I \\ &= [I + A]\left[\frac{T}{2}D^2\phi + I - (I + A)^{-1}\right]. \end{aligned} \tag{3.3}$$

Computing the determinant of $D\mathbf{m}$, we have

$$\begin{aligned} \det D\mathbf{m} &= \det[I + A]\det\left[\frac{T}{2}D^2\phi + I - (I + A)^{-1}\right] \\ &= \det[I + A]\det\left[\frac{T}{2}D^2\phi + I - \left(2I + \frac{T}{2}D^2Q\left(x + \frac{T}{2}\nabla\phi(x)\right)\right)^{-1}\right]. \end{aligned}$$

Recall that the modified velocity potential $\tilde{\phi}$ and potential function $\tilde{Q}$ are given by

$$\tilde{\phi}(x) = \frac{T}{2}\phi(x) + \frac{1}{2}|x|^2 \quad \text{and} \quad \tilde{Q}(z) = \frac{T}{2}Q(z) + |z|^2,$$

we have $D^2\tilde{Q} = (I + A)$ and

$$\det D\mathbf{m} = \det D^2\tilde{Q} \det[D^2\tilde{\phi} - (D^2\tilde{Q}(\nabla\tilde{\phi}))^{-1}].$$

Therefore, we obtain the Monge–Ampère equation

$$\det\,[D^2\tilde{\phi} - (D^2\tilde{Q}(\nabla\tilde{\phi}))^{-1}] = \frac{\det D\mathbf{m}}{\det D^2\tilde{Q}}.$$

Note that $\mathbf{m}_{\#}\rho_0 = \rho_T$ [defined in (3.6)], thus $|\det D\mathbf{m}(x)| = \rho_0(x)/\rho_T(\mathbf{m}(x))$. Then we obtain Eq. (2.17),

$$\det\,[D^2\tilde{\phi} - (D^2\tilde{Q}(\nabla\tilde{\phi}))^{-1}] = \left(\frac{1}{\det D^2\tilde{Q}}\right)\frac{\rho_0}{\rho_T \circ \mathbf{m}}, \tag{3.4}$$

with an associated natural boundary condition

$$\mathbf{m}(\Omega_0) = \Omega_T. \tag{3.5}$$

Remark 3.1. In the continuous case (1.1), Loeper obtained in [9] partial regularity for ϕ, that holds only in the interior (with respect to time) of the domain. In particular, there was no result regarding the initial velocity. In this paper, we obtain the regularity of ϕ over the whole domain in the discrete case by using the regularity in optimal transportation.

We need to introduce a notion of weak solutions for Eq. (3.4).

Definition 3.1. A function $\tilde{\phi}$ is said to be a weak *Brenier* solution to (3.4) whenever $\mathbf{m}$ defined from $\tilde{\phi}$ as in (3.2) is such that

$$\mathbf{m}_{\#}\rho_0 = \rho_T, \tag{3.6}$$

namely, for all $B \subset \mathbb{R}^d$ Borel, there holds $\rho_0(\mathbf{m}^{-1}(B)) = \rho_T(B)$ (this is also mentioned as $\mathbf{m}$ pushes forward ρ_0 onto ρ_T).

Remark 3.2. It is known that, depending on the geometry of the support of ρ_T, the notion of *Brenier* solution might be equivalent to the notion of *Aleksandrov* solution.

4. A Two-Step Transport

Problem (1.5) falls into the class of optimal transport problems with a general cost function

$$c_T(x, y) = \inf \int_0^T L(\gamma(t), \dot{\gamma}(t))dt, \tag{4.1}$$

where the infimum is taken over all smooth curves $\gamma(\cdot)$ satisfying $\gamma(0) = x$ and $\gamma(T) = y$, as considered in [10]. In our case the Lagrangian is defined by $L(x, v) = \frac{1}{2}|v|^2 + \delta_{t=T/2}Q(x)$. Moreover, we can compute explicitly the optimal path γ by dividing the transport map $\mathbf{m} = \mathbf{m_2} \circ \mathbf{m_1}$ such that at $t = \frac{T}{2}$,

$$z = \mathbf{m_1}(x) = x + \frac{T}{2}\nabla\phi(x) = \nabla\tilde{\phi}(x), \tag{4.2}$$

and at $t = T$,

$$y = \mathbf{m_2}(z) = z + \frac{T}{2}\nabla Q(z) + \frac{T}{2}\nabla\phi(x) = 2z + \frac{T}{2}\nabla Q(z) - x = \nabla\tilde{Q}(z) - x. \tag{4.3}$$

Correspondingly,

$$\begin{aligned} c_T(x, y) &= \inf_z \left\{ \frac{1}{2}\left|\frac{z-x}{T/2}\right|^2 \cdot \frac{T}{2} + \frac{1}{2}\left|\frac{y-z}{T/2}\right|^2 \cdot \frac{T}{2} + Q(z) \right\} \\ &= \inf_z \left\{ \frac{1}{T}\left(|z-x|^2 + |y-z|^2\right) + Q(z) \right\}. \end{aligned} \tag{4.4}$$

Formally at the minimizer by taking $0 = \frac{\partial c_T(x,y)}{\partial z}$ one can recover the equality (4.3), namely

$$\frac{y-z}{T/2} = \frac{z-x}{T/2} + \nabla Q(z).$$

Furthermore, through a straightforward computation, one has

$$\begin{aligned} c_T(x, y) &= \inf_z \left\{ \frac{2}{T}|z|^2 - \frac{2}{T}z \cdot (x+y) + Q(z) \right\} + \frac{1}{T}\left(|x|^2 + |y|^2\right) \\ &= \frac{2}{T}\inf_z \left\{ |z|^2 - z \cdot (x+y) + \frac{T}{2}Q(z) \right\} + \frac{1}{T}(|x|^2 + |y|^2). \end{aligned}$$

Now, let $\tilde{\phi}^*, \tilde{Q}^*$ be Legendre transforms of convex functions $\tilde{\phi}, \tilde{Q}$, respectively, i.e.

$$\begin{cases} (x, \nabla\tilde{\phi}(x)) = (\nabla\tilde{\phi}^*(z), z), \\ (z, \nabla\tilde{Q}(z)) = (\nabla\tilde{Q}^*(p), p), \end{cases}$$

where

$$p := \nabla\tilde{Q}(z) = y + x. \tag{4.5}$$

These agree with (4.2) and (4.3) as well. Recall that $\tilde{Q}(z) = \frac{T}{2}Q(z) + |z|^2$ defined in (2.16), one has

$$\begin{aligned} c_T(x, y) &= \frac{2}{T}\inf_z\{\tilde{Q}(z) - z \cdot p\} + \frac{1}{T}(|x|^2 + |y|^2) \\ &= -\frac{2}{T}\sup_z\{z \cdot p - \tilde{Q}(z)\} + \frac{1}{T}(|x|^2 + |y|^2) \\ &= -\frac{2}{T}\tilde{Q}^*(p) + \frac{1}{T}(|x|^2 + |y|^2), \end{aligned}$$

where $\tilde{Q}^*$ is exactly the Legendre transform of $\tilde{Q}$ as defined above (4.5). Note that $\tilde{Q}^*$ is well defined and C^4 smooth under the assumptions (H0) and (H1).

Note that the terms involving only x or y do not affect the optimal transport map, therefore, we will look at an optimal transport problem with cost

$$c(x,y) = \tilde{Q}^*(x+y), \tag{4.6}$$

and seek to maximize the cost functional

$$\mathcal{C}(\mathbf{s}) = \int_{\Omega_0} \rho_0(x)\tilde{Q}^*(x+\mathbf{s}(x))dx,$$

among all maps $\mathbf{s} : \Omega_0 \to \Omega_T$ such that $\mathbf{s}_\# \rho_0 = \rho_T$. Note that here we consider the maximization instead of the minimization problem as in [24, 15].

When the cost function c is strictly convex as is the case for $\tilde{Q}^*$ in (4.6) satisfying (H0)–(H1), it was proved [25, 26] that a unique optimal mapping can be determined by the potential functions, that leads to the Monge–Ampère equation

$$\det[D^2\tilde{\phi}(x) - D^2\tilde{Q}^*(p)] = (\det D^2\tilde{Q}^*(p))\frac{\rho_0(x)}{\rho_T \circ \mathbf{m}(x)}, \tag{4.7}$$

with the natural boundary condition (3.5), where $p = x + y$. Note that the matrix $(D^2\tilde{\phi} - D^2\tilde{Q}^*)$ is nonnegative, and $D^2\tilde{Q}^*$ is positive definite by condition (H1), which makes Eq. (4.7) elliptic. Note also that in the absence of regularity, one has to understand the solution to (4.7) in the weak "Brenier" sense in Definition 3.1 (see [24]).

In our case,

$$\nabla\tilde{Q}^*(x+y) = \nabla\tilde{\phi}(x), \tag{4.8}$$

and using the properties of the Legendre transform

$$\begin{aligned} y &= \nabla\tilde{Q}(\nabla\tilde{\phi}(x)) - x \\ &= \frac{T}{2}\nabla Q(\nabla\tilde{\phi}(x)) + 2\nabla\tilde{\phi}(x) - x. \end{aligned}$$

From the above computations, the initial velocity is given by $\frac{2}{T}(z-x)$ where $z = \nabla\tilde{Q}^*(x+y)$, hence following (4.8) we recover that

$$v(0,x) = \nabla\phi(x) = \frac{2}{T}(\nabla\tilde{\phi}(x) - x), \tag{4.9}$$

while $\nabla\tilde{\phi}(x) = z$, where z is the mid-point of the trajectory at $t = T/2$.

Lemma 4.1 (C^1-bound). *Let Ω_0, Ω_T be two bounded domains and $\tilde{\phi}$ be a solution of* (4.7) *and* (3.5). *Assume that the potential $\tilde{Q}$ satisfies* (H0) *and* (H1). *Then*

$$|\nabla\tilde{\phi}(x)| \le C, \tag{4.10}$$

for all $x \in \overline{\Omega}_0$, where the constant C depends on Ω_0, Ω_T, and $\tilde{Q}$. Furthermore, at time $t = T/2$, the intermediate domain $\Omega_{T/2} := \mathbf{m_1}(\Omega_0) = \nabla\tilde{\phi}(\Omega_0)$ is bounded.

Proof. From (4.8) and $p = x + y$,

$$\nabla\tilde{\phi}(x) = \nabla\tilde{Q}^*(x + y),$$

where $\tilde{Q}^* = \tilde{Q}^*(p)$ is the Legendre transform of $\tilde{Q} = \tilde{Q}(z)$, thus is smooth and strictly convex. As $x \in \Omega_0$ and $y \in \Omega_T$, $x + y \in B_R(0)$ for a bounded constant R. Hence $|\nabla\tilde{Q}^*(x + y)| \leq C$, and (4.10) is obtained.

Recall that from (4.2), at time $t = \frac{T}{2}$, $z = \mathbf{m_1}(x) = \nabla\tilde{\phi}(x)$. The inequality (4.10) implies that the intermediate domain $\Omega_{T/2} = \mathbf{m_1}(\Omega_0)$ is bounded. □

We remark that from the uniqueness of v in [9] [in fact, from the duality argument of [9, §3.2] two optimal solutions must have the same density $\rho(T/2)$, thus the uniqueness of v follows since $I(\rho, v)$ is strictly convex in v], a solution of (4.7) is thus the velocity potential $\tilde{\phi}$. Therefore, we have the following.

Proposition 4.1. *The two-step gravitational transport problem is an optimal transportation associated with the cost function* (4.6). *By assuming conditions* (H0) *and* (H1), *we have the existence and uniqueness* (*up to a constant*) *of solution* $\tilde{\phi}$ *to the boundary-value problem* (4.7) *and* (3.5) *in the weak "Brenier" sense.*

Also in turn by (2.16), *we have the existence and uniqueness* (*up to a constant*) *of the initial velocity potential* ϕ.

Theorem 2.1 follows then directly from Proposition 4.1. Additionally, to prove Theorem 2.2 it is equivalent to obtain the regularity of solutions of (4.7) in optimal transportation, that requires appropriate convexity conditions on domains Ω_0, Ω_T, and more importantly some structure conditions on the potential function $\tilde{Q}$ to be described in the following sections.

5. Conditions on the Potential Function

From Proposition 4.1, in order to obtain the regularity of the velocity potential $\tilde{\phi}$, it suffices to consider the optimal transportation with the cost function (4.6). From the results of [24], it is now well understood that the so-called MTW condition (introduced in [15]) is necessary (at least in its weak form) for the regularity of optimal mappings.

First, let us recall the MTW condition in optimal transportation. For a general cost function $c(x, y) : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, use the notation

$$c_{ij,\ldots,kl\cdots} = \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_j}\cdots\frac{\partial}{\partial y_k}\frac{\partial}{\partial y_l}\cdots c,$$

and let $[c^{i,j}]$ denote the inverse of $[c_{i,j}]$. The MTW condition is that

$$\mathrm{MTW} := (c_{ij,rs} - c^{p,q}c_{ij,p}c_{q,rs})c^{r,k}c^{s,l}\xi_k\xi_l\eta_i\eta_j \geq c_0|\xi|^2|\eta|^2, \tag{5.1}$$

for any $\xi, \eta \in \mathbb{R}^d$ and $\xi \perp \eta$, where $c_0 > 0$ is a constant. When $c_0 = 0$, it is called the weak MTW condition.

In our case, the cost function is given by the potential function $\tilde{Q}^*$ in (4.6). To introduce the analogous MTW condition, denote the matrix

$$D^2\tilde{Q}^*(p) = (D^2\tilde{Q}(\nabla\tilde{\phi}))^{-1} =: \mathcal{A}(z), \tag{5.2}$$

where $p = x + y$ and $z = \nabla\tilde{\phi}$, as in (4.5) and (4.2), respectively. Since $c(x, y) = \tilde{Q}^*(x + y)$, by differentiation we have

$$\mathrm{MTW} = (\tilde{Q}^*_{ijrs} - \tilde{Q}^{*pq}\tilde{Q}^*_{ijp}\tilde{Q}^*_{qrs})\tilde{Q}^{*rk}\tilde{Q}^{*sl}\xi_k\xi_l\eta_i\eta_j. \tag{5.3}$$

From the Legendre transform and (5.2), one has

$$z = \nabla\tilde{Q}^*(p), \quad \frac{\partial z_i}{\partial p_j} = D^2_{ij}\tilde{Q}^*(p) = \mathcal{A}_{ij}(z).$$

Hence, using Einstein summation one has

$$\begin{aligned} D^3_{ijr}\tilde{Q}^* &= \frac{\partial z_k}{\partial p_r}D_k\mathcal{A}_{ij} = \mathcal{A}_{kr}D_k\mathcal{A}_{ij}, \\ D^4_{ijrs}\tilde{Q}^* &= D_l\mathcal{A}_{kr}\left(\frac{\partial z_l}{\partial p_s}\right)D_k\mathcal{A}_{ij} + \mathcal{A}_{kr}D^2_{kl}\mathcal{A}_{ij}\left(\frac{\partial z_l}{\partial p_s}\right) \\ &= (D_l\mathcal{A}_{kr})\mathcal{A}_{ls}(D_k\mathcal{A}_{ij}) + \mathcal{A}_{kr}(D^2_{kl}\mathcal{A}_{ij})\mathcal{A}_{ls}, \end{aligned} \tag{5.4}$$

and thus

$$\begin{aligned} \mathrm{MTW} &= [\mathcal{A}^{rk}(\mathcal{A}_{kr}(D^2_{kl}\mathcal{A}_{ij})\mathcal{A}_{ls} + (D_l\mathcal{A}_{kr})\mathcal{A}_{ls}(D_k\mathcal{A}_{ij}) \\ &\quad - \mathcal{A}^{pq}\mathcal{A}_{kp}(D_k\mathcal{A}_{ij})\mathcal{A}_{ls}(D_l\mathcal{A}_{qr}))\mathcal{A}^{sl}]\xi_k\xi_l\eta_i\eta_j \\ &= D^2_{kl}\mathcal{A}_{ij}\xi_k\xi_l\eta_i\eta_j. \end{aligned}$$

Therefore, the MTW condition in our case is that

$$D^2_{z_k z_l}\mathcal{A}_{ij}(z)\xi_i\xi_j\eta_k\eta_l \geq c_0|\xi|^2|\eta|^2, \tag{5.5}$$

for any $\xi, \eta \in \mathbb{R}^d$, with $\xi \perp \eta$, where $c_0 > 0$ is a constant.

Next, we shall formulate the condition (5.5) in terms of the original potential function $\tilde{Q}$. From (5.2), $\mathcal{A}^{ij} = D^2_{ij}\tilde{Q}$. By differentiating $I = \mathcal{A}\mathcal{A}^{-1}$, we have

$$\begin{aligned} D_k\mathcal{A}_{ij} &= -\mathcal{A}_{ir}(D_k\mathcal{A}^{rs})\mathcal{A}_{sj}, \\ D^2_{kl}\mathcal{A}_{ij} &= -\mathcal{A}_{ir}(D^2_{kl}\mathcal{A}^{rs})\mathcal{A}_{sj} + \mathcal{A}_{im}(D_l\mathcal{A}^{mn})\mathcal{A}_{nr}(D_k\mathcal{A}^{rs})\mathcal{A}_{sj} \\ &\quad + \mathcal{A}_{ir}(D_k\mathcal{A}^{rs})\mathcal{A}_{sm}(D_l\mathcal{A}^{mn})\mathcal{A}_{nj} \\ &= -\mathcal{A}_{ir}(D^2_{kl}\mathcal{A}^{rs})\mathcal{A}_{sj} + \mathcal{A}_{im}(D_l\mathcal{A}^{mn})\mathcal{A}_{nr}(D_k\mathcal{A}^{rs})\mathcal{A}_{sj} \\ &\quad + \mathcal{A}_{im}(D_k\mathcal{A}^{mn})\mathcal{A}_{nr}(D_l\mathcal{A}^{rs})\mathcal{A}_{sj} \\ &= -\mathcal{A}_{ir}(D^2_{kl}\mathcal{A}^{rs})\mathcal{A}_{sj} + (D_l\mathcal{A}_{ir})\mathcal{A}^{rs}(D_k\mathcal{A}_{sj}) \\ &\quad + (D_k\mathcal{A}_{ir})\mathcal{A}^{rs}(D_l\mathcal{A}_{sj}). \end{aligned} \tag{5.6}$$

Hence, the left-hand side of (5.5) is

$$D^2_{\eta\eta}\mathcal{A}_{\xi\xi} = -\big(D^2_{\eta\eta}\tilde{Q}_{ij}\big)(\mathcal{A}\xi)_i(\mathcal{A}\xi)_j + 2(\mathcal{A}\xi)_i\big(D_\eta\tilde{Q}_{ir}\big)\tilde{Q}^{rs}\big(D_\eta\tilde{Q}_{sj}\big)(\mathcal{A}\xi)_j.$$

Letting $\tilde{\xi} := \mathcal{A}\xi$ and recalling that $\tilde{Q} = \tilde{Q}(z)$ is a scalar function, one has

$$\begin{aligned} D^2_{\eta\eta}\mathcal{A}_{\xi\xi} &= -D^2_{\eta\eta}\tilde{Q}_{\tilde{\xi}\tilde{\xi}} + 2\big(D_\eta\tilde{Q}_{\tilde{\xi}r}\big)\tilde{Q}^{rs}\big(D_\eta\tilde{Q}_{s\tilde{\xi}}\big) \\ &= -D^4_{\tilde{\xi}\tilde{\xi}\eta\eta}\tilde{Q} + 2\big\langle\nabla\tilde{Q}_{\tilde{\xi}\eta}, \nabla\tilde{Q}_{\tilde{\xi}\eta}\big\rangle_{\mathcal{A}}, \end{aligned} \tag{5.7}$$

where $\langle\xi,\xi\rangle_{\mathcal{A}} := \xi_i\xi_j\tilde{Q}^{ij}$.

Combining (5.5) and (5.7), we obtain the following result.

Proposition 5.1. *The MTW condition in our case can be expressed directly in terms of the potential function* $\tilde{Q}$:

(H2) *The potential function* $\tilde{Q}$ *satisfies for all* $\xi,\eta \in \mathbb{R}^d$, *with* $\xi\perp\eta$,

$$\sum_{i,j,k,l,p,q,r,s} (\tilde{Q}_{ijrs} - 2\tilde{Q}^{pq}\tilde{Q}_{ijp}\tilde{Q}_{qrs})\tilde{Q}^{rk}\tilde{Q}^{sl}\xi_k\xi_l\eta_i\eta_j \le -\delta_0|\xi|^2|\eta|^2, \tag{5.8}$$

where $\{\tilde{Q}^{ij}\}$ *is the inverse matrix of* $\{\tilde{Q}_{ij}\}$, *and* δ_0 *is a positive constant. When* $\delta_0 = 0$, *we call it* (H2w), *a weak version of* (H2).

Comparing with (5.3), one can see that (5.8) is in a similar form in spite of the factor 2.

6. Regularity of the Potential

It is well known that in order to guarantee some regularity for Eq. (4.7), one needs some notion of convexity of domains. In optimal transport, it has been proved that if the target domain is not c-convex, there exist some smooth densities ρ_0, ρ_T such that the optimal mapping is not even continuous, see [15, §7.3]. For global regularity, one needs both the initial and the target domains to be uniformly c-convex in [19].

In our case, the cost function is $c(x,y) = \tilde{Q}^*(x+y)$. Similarly to the c-convexity in optimal transportation, we introduce the following q-convexity for domains.

Definition 6.1 (The q-exponential map). Assume the potential function $\tilde{Q}$ satisfies conditions (H0) and (H1). For $x \in \Omega_0$ we define the *q-exponential map* at x, denoted by $\mathfrak{I}_x : \mathbb{R}^n \to \mathbb{R}^n$, such that

$$\mathfrak{I}_x(z) = \nabla\tilde{Q}(z) - x.$$

Note that this is reminiscent of the mapping $\mathbf{m_2}$ in (4.3), namely for $z \in \Omega_{T/2} = \nabla\tilde{\phi}(\Omega_0)$, $\mathfrak{I}_x(z) = y \in \Omega_T$. We rename it in order to follow the lines of optimal transportation.

Definition 6.2. The domain Ω_T is *q-convex* with respect to Ω_0 if the pre-image $\mathfrak{I}_x^{-1}(\Omega_T)$ is convex for all $x \in \Omega_0$, where $\mathfrak{I}_x$ is the q-exponential map in Definition 6.1.

If the pre-image $\mathfrak{I}_x^{-1}(\Omega_T)$ is uniformly convex for all $x \in \Omega_0$, then we call Ω_T is *uniformly q-convex* with respect to Ω_0.

By duality we can also define the (uniform) q-convexity for Ω_0 with respect to Ω_T.

Remark 6.1. (i) Similarly to [27], in the smooth case we have an analytic formulation of the q-convexity of Ω_0 with respect to Ω_T. Let $\varphi \in C^2(\overline{\Omega}_0)$ be a defining function of Ω_0. That is $\varphi = 0$, $|\nabla\varphi| \neq 0$ on $\partial\Omega_0$, and $\varphi < 0$ in Ω_0. Ω_0 is q-convex with respect to Ω_T if

$$[\varphi_{ij}(x) - \tilde{Q}^{*}{}^{kl} D_k \tilde{Q}^*_{ij}(x+y)\varphi_l(x)] \geq 0, \quad \forall\, x \in \partial\Omega_0,\;\; y \in \Omega_T. \tag{6.1}$$

If the matrix in (6.1) is uniformly positive, Ω_0 is uniformly q-convex with respect to Ω_T. Note that this analytic formulation is independent of the choice of φ, and by exchanging x and y, we also have the analytic formulation of the q-convexity of Ω_T with respect to Ω_0.

(ii) Even though Ω_0 and Ω_T are uniformly q-convex, the intermediate domain $\Omega_{T/2} = \nabla\tilde{\phi}(\Omega_0)$ may not be q-convex. See [28] for the counterexamples in the optimal transportation case.

Upon formulating our reconstruction problem to optimal transportation in Sec. 4 and assuming appropriate conditions on the potential function $\tilde{Q}$ and the domains, the regularity of the velocity potential $\tilde{\phi}$ will follow from the established results in optimal transportation. In particular, we have the following results that together compose the proof of Theorem 2.2.

Theorem 6.1 (From [18, 24]). *Let ϕ be the velocity potential in the reconstruction problem* (1.5). *Assume that the potential function $\tilde{Q}$ satisfies the conditions* (H0)–(H2), *that Ω_T is q-convex with respect to Ω_0. Assume that $\rho_T \geq c_0$ on Ω_T for some positive constant c_0, $\rho_0 \in L^p(\Omega_0)$ for some $p > \frac{d+1}{2}$, and the balance condition* (2.15) *is satisfied. Then, we have*

$$\|\phi\|_{C^{1,\alpha}(\overline{\Omega}_0)} \leq C,$$

for some $\alpha \in (0,1)$, where C is a positive constant. When $p = \frac{d+1}{2}$, the velocity potential ϕ belongs to $C^1(\overline{\Omega}_0)$.

Theorem 6.2 (From [19]). *If furthermore, Ω_0, Ω_T are C^4 smooth and uniformly q-convex with respect to each other, $\rho_0 \in C^2(\overline{\Omega}_0)$, and $\rho_T \in C^2(\overline{\Omega}_T)$, then $\phi \in C^3(\overline{\Omega}_0)$, and higher regularity follows from the theory of linear elliptic equations. Particularly, if $\tilde{Q}, \Omega_0, \Omega_T, \rho_0$ and ρ_T are C^∞, then the velocity potential $\phi \in C^\infty(\overline{\Omega}_0)$.*

Similarly to [19], we are able to reduce the condition (H2) to (H2w) in Theorem 6.2 by assuming an additional condition called *c-boundedness* on Ω_0 in [19]. Namely, there exists a global barrier function h on Ω_0 such that

$$[D_{ij}h - \tilde{Q}^{*lk}\tilde{Q}^*_{ijl}D_k h]\xi_i\xi_j \geq \delta_1|\xi|^2,$$

for some constant $\delta_1 > 0$. In the recent work of Jiang and Trudinger [29] for the case of generated prescribed Jacobian equations, the above c-boundedness condition can also be removed. We refer the reader to [29, 19] for more details, and also [30] for a simpler proof of the essential barrier construction.

7. The Mean-Field Case

7.1. *Convexity of the space of MTW potentials*

The potential function $\tilde{Q}$ in our two-step gravitational transport problem is a scalar function defined on the intermediate domain $\Omega_{T/2} = \nabla\tilde{\phi}(\Omega_0)$, which only takes effect at time $t = T/2$. In the general reconstruction problem considered by Loeper in [9], the gravitational function p actually solves the Poisson equation in the system (1.1), and takes effect for all $t \in (0, T)$. In fact, at each $t \in (0, T)$, p is a convolution of the density ρ and the Coulomb kernel (1.8). One can see the convolution as a continuous convex combination with weights $\rho(t, x)$, and a Kernel satisfying (H2) would lead, by convolution, to a potential also satisfying (H2). Therefore, in order to study the general case, a natural question one may ask is that:

Is the set of potential functions satisfying (H2) *convex*?

The answer is "No" in general as shown in the following examples.

Example 7.1. Let the dimension $d = 3$ and

$$\tilde{Q}(z) := z_2^2 z_3^2 + z_1 z_3^2 + z_1 z_2^2 + A|z|^2,$$
$$\tilde{Q}'(z) := z_2^2 z_3^2 - z_1 z_3^2 - z_1 z_2^2 + A|z|^2,$$

where $z \in \Omega_{T/2}$ that is a bounded domain due to Lemma 4.1, and A is a positive constant.

By differentiating we have

$$D^2\tilde{Q} \text{ (or } D^2\tilde{Q}') = \begin{bmatrix} 2A, & \pm 2z_2, & \pm 2z_3 \\ \pm 2z_2, & 2A + 2z_3^2 \pm 2z_1, & 4z_2z_3 \\ \pm 2z_3, & 4z_2z_3, & 2A + 2z_2^2 \pm 2z_1 \end{bmatrix}.$$

Choosing A sufficiently large such that $A \gg \operatorname{diam}(\Omega_{T/2})$, we have

$$D^2\tilde{Q} \text{ (and } D^2\tilde{Q}') \geq AI,$$

where I is the 3×3 identity matrix. Hence, $\tilde{Q}$ and $\tilde{Q}'$ satisfy the conditions (H0) and (H1).

By further computations one can easily verify that both $\tilde{Q}$ and $\tilde{Q}'$ satisfy the condition (H2w) as well. Choose $\xi = (0,1,0)$, $\eta = (0,0,1)$, and let $\mathrm{MTW}(\tilde{Q})$ denote the left-hand side of (5.8) for this choice of ξ, η. We have

$$\mathrm{MTW}(\tilde{Q}) \text{ (and MTW } (\tilde{Q}')) \approx \left(D^4_{2233}\tilde{Q} - 2D^3_{331}\tilde{Q}D^3_{122}\tilde{Q}\right) \le -2.$$

However, let $\tilde{Q}'' := \frac{1}{2}(\tilde{Q} + \tilde{Q}') = z_2^2 z_3^2 + A|z|^2$. As the third-order terms vanish, one can see that

$$\mathrm{MTW}(\tilde{Q}'') \approx D^4_{2233}\tilde{Q}'' = 4,$$

which contradicts with (5.8), namely $\tilde{Q}''$ does not satisfy the condition (H2).

One can further modify the above example to show that $\tilde{Q}$, $\tilde{Q}'$ satisfy (H2) but their convex combination does not. Define

$$\tilde{Q}(z) := F(z) + T(z) + A|z|^2,$$
$$\tilde{Q}'(z) := F(z) - T(z) + A|z|^2,$$

where $F(z)$ denotes the fourth-order terms satisfying $F_{ijkl}\xi_i\xi_j\eta_k\eta_l > 0$, and $T(z)$ denotes the third-order terms such that the quadratic product of $T_{ijs}T_{skl}\xi_i\xi_j\eta_k\eta_l$ is strictly larger than $F_{ijkl}\xi_i\xi_j\eta_k\eta_l$. Then by choosing $A > 0$ sufficiently large one has $\tilde{Q}, \tilde{Q}'$ satisfying (H0)–(H2). On the other hand, it is easily seen that $\tilde{Q}'' := \frac{1}{2}(\tilde{Q} + \tilde{Q}') = F(z) + A|z|^2$ does not satisfy (H2).

Inspired by the above example, we may consider the following variety of (H2) by removing the third-order terms and the orthogonality.

(H2c) The potential function $\tilde{Q}$ satisfies for all $\xi, \eta \in \mathbb{R}^d$,

$$\sum_{i,j,k,l,p,q,r,s} (D^4_{ijrs}\tilde{Q})\tilde{Q}^{rk}\tilde{Q}^{sl}\xi_k\xi_l\eta_i\eta_j \le 0, \tag{7.1}$$

where $\{\tilde{Q}^{ij}\}$ is the inverse of $\{\tilde{Q}_{ij}\}$.

Note that the second term on the left-hand side of (5.8) is always nonpositive. Obviously, (H2c) implies (H2w), but not the other way around.

Lemma 7.1. *The set $\mathcal{S}$ of potential functions $\tilde{Q}$ satisfying* (H0), (H1), *and* (H2c) *is convex.*

Proof. For any $\tilde{Q} \in \mathcal{S}$, define the vector $\tilde{\xi}$ by $\tilde{\xi}_i = \tilde{Q}^{ik}\xi_k$. From (H0) and (H1), one has $|\tilde{\xi}| \approx |\xi|$, namely there exist two universal constants C_1, C_2 such that

$$C_1|\xi| \le |\tilde{\xi}| \le C_2|\xi|.$$

Hence, (7.1) is equivalent to

$$\sum_{i,j,k,l,p,q,r,s} (D^4_{ijrs}\tilde{Q})\xi_k\xi_l\eta_i\eta_j \le 0. \tag{7.2}$$

Now the convexity of $\mathcal{S}$ follows naturally from the linearity of (7.2). In fact, let $\tilde{Q}, \tilde{Q}' \in \mathcal{S}$ satisfy (7.2). One can easily check that $\tau\tilde{Q} + (1-\tau)\tilde{Q}'$ also satisfies the same inequality (7.2), for all $\tau \in [0,1]$. Therefore, $\tau\tilde{Q} + (1-\tau)\tilde{Q}' \in \mathcal{S}$. □

7.2. *Proof of Theorem* 2.4

Going back to the notations of [9], define $J = \rho v$ and then the functional we want to minimize is

$$I(\rho, J) = \int_0^T \int_{\mathbb{R}^d} \frac{|J|^2}{2\rho} dxdt + \frac{1}{2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \rho(T/2, x)\kappa(x-y)\rho(T/2, y)dxdy.$$

From the assumptions of Theorem 2.4, the existence of a minimizer can be obtained by the direct method as in [9, §3.1]. It also falls easily that trajectories of minimizers will have constant velocity on $[0, T/2^-)$ and on $(T/2^+, T]$, and that $v(T/2^+, x) - v(T/2^-, x) = \nabla Q(x)$ where Q is given by

$$Q(x) = \int_{\mathbb{R}^d} \rho(T/2, y)\kappa(x-y)dy.$$

Therefore, once the $\rho(T/2)$ has been found, the problem can be treated equivalently as in the noninteracting problem, with Q as above.

7.3. *Proof of Theorem* 2.5

In order to obtain the global regularity, we need to show the following q-convexity of domains.

Lemma 7.2. *Assume that κ is C^4 and convex. Assume Ω_0 is convex, and let $\varphi \in C^2(\overline{\Omega}_0)$ be a convex defining function of Ω_0, namely $\varphi < 0$ in Ω_0, $\varphi = 0$, and $|\nabla\varphi| \neq 0$ on $\partial\Omega_0$. Suppose that*

$$\left[\varphi_{ij}(x) + \frac{TM}{8}\kappa_{ijk}(z-w)\varphi_k(x)\right] \geq c_0\delta_{ij}, \quad \forall\, x \in \partial\Omega_0, \quad \forall\, z, \quad w \in \Omega_{T/2}, \tag{7.3}$$

for a constant $c_0 \geq 0$, where κ_{ijk} are partial derivatives in z and M is the total mass in (2.15)*. Then, Ω_0 is uniformly q-convex with respect to Ω_T if $c_0 > 0$; and Ω_0 is q-convex with respect to Ω_T if $c_0 = 0$.*

Proof. It suffices to verify the inequality (6.1). In this case, the modified potential is

$$\tilde{Q}(z) = \frac{T}{2} \int_{\Omega_{T/2}} \bar{\rho}(w)\kappa(z-w)dw + |z|^2, \tag{7.4}$$

where $\bar{\rho}(w) = \rho(T/2, w)$. From the proof of Lemma 4.1, the intermediate domain $\Omega_{T/2}$ is bounded. From [24], the density $\bar{\rho}$ is bounded, namely $0 \leq \bar{\rho} \leq C$ for a constant $C > 0$. Since κ is convex in z, the potential $\tilde{Q}$ is uniformly convex, namely the matrix

$$\tilde{Q}_{ij}(z) \geq 2\delta_{ij}, \quad \forall\, z \in \Omega_{T/2}. \tag{7.5}$$

Now, we convert (6.1) in terms of $\tilde{Q}$. Note that since $\tilde{Q}^*$ is the Legendre transform of $\tilde{Q}$, from (5.2), ${\tilde{Q}^*}{}^{kl}(p) = \tilde{Q}_{kl}(z) = \mathcal{A}^{kl}(z)$, where $p = x + y$. Combining

(5.4) and (5.6) one has

$$\begin{aligned}D^3_{ijk}\tilde{Q}^*(z) &= \mathcal{A}_{kr}D_r\mathcal{A}_{ij}(z)\\ &= -\mathcal{A}_{kr}\mathcal{A}_{im}D_r\mathcal{A}^{mn}\mathcal{A}_{nj}(z).\end{aligned}$$

Hence, (6.1) is equivalent to, for any vector $\xi \in \mathbb{S}^{n-1}$,

$$[\varphi_{ij}(x) + \tilde{Q}^{ir}(D_k\tilde{Q}_{rs})\tilde{Q}^{sj}(z)\varphi_k(x)]\xi_i\xi_j \geq 0, \quad \forall\, x \in \partial\Omega_0,\ \ z \in \Omega_{T/2}.$$

Similarly as for (5.7), letting $\tilde{\xi} := \mathcal{A}\xi$, namely $\tilde{\xi}_i = \tilde{Q}^{ir}\xi_r$, one has

$$[\tilde{Q}_{ir}\varphi_{rs}(x)\tilde{Q}_{sj} + (D_k\tilde{Q}_{ij}(z))\varphi_k(x)]\tilde{\xi}_i\tilde{\xi}_j \geq 0, \quad \forall\, x \in \partial\Omega_0,\ \ z \in \Omega_{T/2}. \tag{7.6}$$

Therefore, in order to show Ω_0 is q-convex with respect to Ω_T, it suffices to verify (7.6).

By differentiating (7.4),

$$D_k\tilde{Q}_{ij}(z) = \frac{T}{2}\int_{\Omega_{T/2}} \bar{\rho}(w)\kappa_{ijk}(z-w)dw.$$

From (2.15) and the conservation of mass, one has

$$\int_{\Omega_{T/2}} \bar{\rho}(w)dw = M.$$

Then, one can easily see that for any $z \in \Omega_{T/2}$,

$$\min_{w\in\overline{\Omega}_{T/2}} \frac{TM}{2}\kappa_{ijk}(z-w) \leq D_k\tilde{Q}_{ij}(z) \leq \max_{w\in\overline{\Omega}_{T/2}} \frac{TM}{2}\kappa_{ijk}(z-w). \tag{7.7}$$

Since φ is convex, combining (7.5) and (7.7) into (7.6) we obtain

$$\begin{aligned}[\tilde{Q}_{ir}\varphi_{rs}(x)\tilde{Q}_{sj} + (D_k\tilde{Q}_{ij}(z))\varphi_k(x)] &\geq \min_{w\in\overline{\Omega}_{T/2}} 4\left[\varphi_{ij}(x) + \frac{TM}{8}\kappa_{ijk}(z-w)\varphi_k(x)\right]\\ &\geq 4c_0,\end{aligned}$$

where the last step was due to the assumption (7.3). Note that the matrix $(\tilde{Q}_{ij}(z))$ is positive definite and bounded for all $z \in \Omega_{T/2}$. So, there is a constant $C > 0$ such that $C^{-1}|\xi| \leq |\tilde{\xi}| \leq C|\xi|$ for any vector $\xi \in \mathbb{R}^n$. Therefore, the lemma is proved. □

Remark 7.1. (i) Similarly to the above proof, by exchanging x and y, we can also obtain the q-convexity of Ω_T with respect to Ω_0 under the assumption (2.22)

(ii) Note that the convexity assumption on Ω_0 can be dropped by imposing a more involved condition on the kernel κ comparing to (7.3). Here, Lemma 7.2 only provides a sufficient condition for Ω_0 to be q-convex.

Proof of Theorem 2.5. Thanks to Lemma 7.2, from the assumptions (2.21) and (2.22) we know that Ω_T is q-convex with respect to Ω_0 if $b_1 \geq 0$, and Ω_0, Ω_T are uniformly q-convex with respect to each other if $b_0, b_1 > 0$. Therefore, it suffices to verify that the modified potential function

$$\tilde{Q}(z) = |z|^2 + \frac{T}{2}\int_{\Omega_{T/2}} \rho(T/2, y)\kappa(z-y)dy$$

satisfies the conditions (H0), (H1), and (H2c). The condition (H0) follows from the smoothness of the kernel κ; the condition (H1) follows from the convexity of κ. From the assumption that κ satisfies the condition (H2c) and Lemma 7.1, the potential function $\tilde{Q}$ satisfies (H2c). Hence, the proof follows from Theorem 2.2. $\square$

Unfortunately, the Coulomb kernel (1.8) $\kappa(x-y) = \frac{c_d}{|x-y|^{d-2}}$ does not satisfy the condition (H2c). By direct computation we can verify that it satisfies the condition (H2). However, since the space of potential function satisfying (H2) is not convex, as shown in Example 7.1, Theorem 2.5 does not apply to that case.

Lemma 7.3. *The Coulomb kernel κ in* (1.8) *satisfies the condition* (H2), *if* $c_d > 0$.

Proof. It suffices to consider $\kappa(z) = |z|^{2-d}$. By differentiation we have

$$\nabla\kappa(z) = (2-d)|z|^{-d}z =: p.$$

Let κ^* be the Legendre transform of κ, then $\kappa(z) + \kappa^*(p) = z\cdot p$, thus

$$\begin{aligned}\kappa^*(p) &= z\cdot p - \kappa(z)\\ &= (1-d)|z|^{2-d}\\ &= \frac{1-d}{(d-2)^{(2-d)/(1-d)}}|p|^{\frac{2-d}{1-d}}.\end{aligned}$$

In the discrete case, from (4.6) we obtain that the cost function is

$$c(x,y) = \frac{d-1}{(d-2)^m}|x+y|^m, \quad m = \frac{2-d}{1-d} \in (0,1). \tag{7.8}$$

By computation in optimal transportation (5.1), we have the LHS of (5.5) as

$$\begin{aligned}\mathrm{LHS}(z,\xi,\eta) = \frac{d-1}{(d-2)^m}\left(\frac{m-2}{m-1}\right)|z|^{-\frac{m}{m-1}}\Bigg\{1 - \frac{m}{m-1}\left(\frac{z\cdot\eta}{|z|}\right)^2 - m\left(\frac{z\cdot\xi}{|z|}\right)^2\\ + \frac{m(3m-2)}{m-1}\left(\frac{z\cdot\xi}{|z|}\right)^2\left(\frac{z\cdot\eta}{|z|}\right)^2 + (m-1)(\xi\cdot\eta)^2\Bigg\},\end{aligned}$$

for any ξ, η with $|\xi| = |\eta| = 1$.

Since $0 < m < 1$, the coefficient $\frac{d-1}{(d-2)^m}\left(\frac{m-2}{m-1}\right) > 0$. For the terms in the bracket, we have

$$I := 1 - m\left(\frac{z \cdot \xi}{|z|}\right)^2 + (m-1)(\xi \cdot \eta)^2 \geq 0,$$

with the equality holding if and only if $\xi = \eta = z/|z|$, and

$$\begin{aligned} II &:= \frac{m}{1-m}\left(\frac{z \cdot \eta}{|z|}\right)^2 - \frac{m(3m-2)}{1-m}\left(\frac{z \cdot \xi}{|z|}\right)^2\left(\frac{z \cdot \eta}{|z|}\right)^2 \\ &= \frac{m}{1-m}\left(\frac{z \cdot \eta}{|z|}\right)^2\left[1 - (3m-2)\left(\frac{z \cdot \xi}{|z|}\right)^2\right]. \end{aligned}$$

If $m \in (0, \frac{2}{3}]$, then $(3m-2) \leq 0$, thus

$$II \geq \frac{m}{1-m}\left(\frac{z \cdot \eta}{|z|}\right)^2 \geq 0,$$

with the last equality holding if and only if $z \perp \eta$.

If $m \in (\frac{2}{3}, 1)$, then

$$1 - (3m-2)\left(\frac{z \cdot \xi}{|z|}\right)^2 > 1 - (3m-2) = 3 - 3m > 0.$$

We also have $II \geq 0$ with the last equality holding if and only if $z \perp \eta$.

Therefore, we obtain

$$\mathrm{LHS}(z, \xi, \eta) > 0,$$

for all unit vectors ξ, η. □

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