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ON DETERMINISTIC SOLUTIONS FOR MULTI-MARGINAL OPTIMAL TRANSPORT WITH COULOMB COST

UGO BINDINI, LUIGI DE PASCALE, AND ANNA KAUSAMO

ABSTRACT. In this paper we study the three-marginal optimal mass transportation problem for the Coulomb cost on the plane \mathbb{R}^2 . The key question is the optimality of the so-called Seidl map, first disproved by Colombo and Stra. We generalize the partial positive result obtained by Colombo and Stra and give a necessary and sufficient condition for the radial Coulomb cost to coincide with a much simpler cost that corresponds to the situation where all three particles are aligned. Moreover, we produce an infinite class of regular counterexamples to the optimality of this family of maps.

1. INTRODUCTION

1.1. Multi-Marginal Optimal Mass Transportation Problem for Coulomb cost. We denote by $\mathcal{P}(\mathbb{R}^d)$ the set of all Borel probability measures on the space \mathbb{R}^d where $d \geq 1$ is the dimension of the space. In this paper we are interested in the Multi-Marginal Optimal Mass Transportation (MOT) problem for the Coulomb cost $\tilde{c}: (\mathbb{R}^d)^N \rightarrow \mathbb{R} \cup \{+\infty\}$,

$$\tilde{c}(x_1, \dots, x_N) = \sum_{1 \leq i < j \leq N} \frac{1}{|x_i - x_j|}.$$

We fix a marginal measure $\tilde{\rho} \in \mathcal{P}(\mathbb{R}^d)$ and seek for minimizing the quantity

$$\int_{(\mathbb{R}^d)^N} \tilde{c} d\gamma(x_1, \dots, x_N) \tag{1.1}$$

over all *couplings* $\gamma \in \mathcal{P}((\mathbb{R}^d)^N)$ of the marginal measures $\tilde{\rho}$, that is, over the set

$$\Pi_N(\tilde{\rho}) := \{\gamma \in \mathcal{P}(\mathbb{R}^d) \mid (pr_i)_\# \gamma = \tilde{\rho} \text{ for all } i \in \{1, \dots, N\}\},$$

where pr_i is the projection on the i -th coordinate:

$$pr_i(x_1, \dots, x_N) = x_i \text{ for all } (x_1, \dots, x_N) \in (\mathbb{R}^d)^N.$$

Finding the minimal γ for the problem (1.1) is often called solving the *Monge-Kantorovich* (MK) problem, in honor of the French mathematician Gaspard Monge

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(1746–1818) and the Russian mathematician Leonid Vitaliyevich Kantorovich (1912–1986), both of whom can be considered founders of the field of optimal mass transportation. The existence of minimizers for the problem (1.1) is easily proven (we are minimizing a linear functional on a compact set) and their structure is rather well-understood (see [11]). A much more challenging problem is the one of finding — or even proving the existence of — a *deterministic* optimal coupling. A deterministic optimal coupling is a solution γ_{opt} for the problem (1.1) of the type

$$\gamma_{opt} = (Id, T_1, \dots, T_{N-1})_{\#} \tilde{\rho}, \quad (1.2)$$

where $T_i: \mathbb{R}^d \rightarrow \mathbb{R}^d$ are Borel functions such that $(T_i)_{\#} \tilde{\rho} = \tilde{\rho}$ for all $i \in \{1, \dots, N-1\}$. This is equivalent to asking whether the equality

$$\begin{aligned} \min_{\gamma \in \Pi_N(\tilde{\rho})} \int_{(\mathbb{R}^d)^N} \tilde{c}(x_1, \dots, x_N) d\gamma(x_1, \dots, x_N) \\ = \min \left\{ \int_{\mathbb{R}^d} \tilde{c}(x, T_1(x), \dots, T_{N-1}(x)) d\tilde{\rho}(x) \mid (T_i)_{\#} \tilde{\rho} = \tilde{\rho} \right\} \end{aligned}$$

holds. If the answer is affirmative, we call any minimizing coupling of the type (1.2) a *Monge minimizer*.

Since the cost function \tilde{c} is symmetric with respect to permuting the coordinates and the density $\tilde{\rho}$ has no atoms, in view of the conjecture we are studying and also [7, 15, 17] we may restrict ourselves to seeking for Monge minimizers of the type

$$\gamma_{opt} = (Id, T, \dots, T^{N-1})_{\#} \tilde{\rho},$$

where $T: \mathbb{R}^d \rightarrow \mathbb{R}^d$ is a Borel measurable function such that $T_{\#} \tilde{\rho} = \tilde{\rho}$ and $T^N = Id$. Here and from now on we denote for all natural numbers k by T^k the k -fold composition of T with itself.

This paper concerns the case where $N = 3$, $d = 2$ and the density $\tilde{\rho}$ is radially symmetric, that is, $A_{\#} \tilde{\rho} = \tilde{\rho}$ for all $A \in SO(2)$. In this case (and also for general N and d as long as $\tilde{\rho}$ is radially symmetric) solving the MOT problem for Coulomb cost can be reduced to a one-dimensional problem where the underlying space is the positive halfline $\mathbb{R}_+ := [0, \infty)$. To make this notion precise, we define the *radial cost* $c: (\mathbb{R}_+)^3 \rightarrow \mathbb{R} \cup \{+\infty\}$,

$$\begin{aligned} c(r_1, r_2, r_3) = \min \{ \tilde{c}(v_1, v_2, v_3) \mid |v_i| = r_i \text{ for } i = 1, 2, 3 \} \\ \text{for all } (r_1, r_2, r_3) \in (\mathbb{R}_+)^3. \end{aligned}$$

For a given triple (r_1, r_2, r_3) there exist many differently-oriented vectors (v_1, v_2, v_3) that realize the above minimum. Once a triple of minimizers (v_1, v_2, v_3) has been fixed, the optimal configuration can be characterized by giving the radii and the angles between them. We may always assume that the vector v_1 lies along the positive x -axis. With this choice in mind we denote by θ_2 the angle between v_1 and v_2 and by θ_3 the angle between v_1 and v_3 . For this radial and angular data

that corresponds to the triple of vectors $(v_1, v_2, v_3) \in (\mathbb{R}^2)^3$ we will sometimes use the notation $C(r_1, r_2, r_3, \theta_2, \theta_3)$ for the Coulomb cost $\tilde{c}(v_1, v_2, v_3)$. This allows to rewrite the radial cost function c as

$$c(r_1, r_2, r_3) = \min_{(\theta_2, \theta_3) \in \mathbb{T}^2} C(r_1, r_2, r_3, \theta_2, \theta_3) \quad (1.3)$$

We also introduce *the radial density* $\rho = |\cdot|_{\mathbb{H}} \tilde{\rho}$.¹ Now solving the (MK) problem for the Coulomb cost and the marginal measure $\tilde{\rho}$ is equivalent to solving the one-dimensional (MK) problem in the class $\Pi_3(\rho)$ for the radial density ρ and the radial cost c , as will be made more rigorous in the next theorem, first proven by Pass (see [28, Section 3]).

Theorem 1.1. *The full (MK) problem for the Coulomb cost*

$$\min \left\{ \int_{(\mathbb{R}^2)^3} \tilde{c}(v_1, v_2, v_3) d\tilde{\gamma}(v_1, v_2, v_3) \mid \tilde{\gamma} \in \Pi_3(\tilde{\rho}) \right\} \quad (1.4)$$

and the corresponding radial problem

$$\min \left\{ \int_{(\mathbb{R}_+)^3} c(r_1, r_2, r_3) d\gamma \mid \gamma \in \Pi_3(\rho) \right\} \quad (1.5)$$

are equivalent in the following sense: the measure $\gamma \in \Pi_3(\rho)$ is optimal for the problem (1.5) if and only if the measure

$$\tilde{\gamma} := \gamma(r_1, r_2, r_3) \otimes \mu^{r_1, r_2, r_3}$$

is optimal for the problem (1.4). Above, μ^{r_1, r_2, r_3} is the singular probability measure on the 3-dimensional torus defined by

$$\mu^{r_1, r_2, r_3} = \frac{1}{2\pi} \int_0^{2\pi} \delta_t \delta_{\theta_2+t} \delta_{\theta_3+t} dt,$$

where (θ_2, θ_3) are minimizing angles $\theta_2 = \angle(v_1, v_2)$, $\theta_3 = \angle(v_1, v_3)$ for

$$c(r_1, r_2, r_3) = \min \{ \tilde{c}(v_1, v_2, v_3) \mid |v_i| = r_i \text{ for } i = 1, 2, 3 \}.$$

In [31] the authors conjectured the solution to the radial problem (1.5). The conjecture is stated for all d and N but for the sake of clarity we formulate it here for $N = 3$.

Conjecture 1.2 (Seidl). Let $\tilde{\rho} \in \mathcal{P}(\mathbb{R}^d)$ be radially-symmetric with radial density ρ . Let s_1 and s_2 be such that

$$\rho([0, s_1)) = \rho([s_1, s_2)) = \rho([s_2, \infty)) = \frac{1}{3}.$$

We define the map $T : [0, \infty)$ to be the unique map that sends, in the way that preserves the density ρ ,

¹Here $|\cdot|$ denotes the function $|\cdot| : \mathbb{R}^2 \rightarrow \mathbb{R}_+$ given by $|(x, y)| = \sqrt{x^2 + y^2}$.

- the interval $[0, s_1)$ to the interval $[s_1, s_2)$ decreasingly,
- the interval $[s_1, s_2)$ to the half-line $[s_2, \infty)$ decreasingly, and
- the half-line $[s_2, \infty)$ to the interval $[0, s_1)$ increasingly.

More formally, this map is defined as

$$T(x) = \begin{cases} F^{-1}\left(\frac{2}{3} - F(x)\right) & \text{when } x \in [0, s_1) \\ F^{-1}\left(\frac{4}{3} - F(x)\right) & \text{when } x \in [s_1, s_2) \\ F^{-1}(1 - F(x)) & \text{when } x \in [s_2, \infty), \end{cases}$$

where F is the cumulative distribution function of ρ , that is, $F(r) = \rho([0, r])$.

Then the map T is optimal for the radial problem (1.5).

The map introduced in Conjecture 1.2 is also called “The Seidl map” or “the *DDI* map” where the letters *DDI* stand for *Decreasing, Decreasing, Increasing*, identifying the monotonicities in which the first interval is mapped on the second, the second on the third, and finally the third back on the first. In an analogous manner one can define maps with different monotonicities: *III*, *IID*, *DDI* and so on. Since the marginals of our MOT problem are all the same and equal to ρ , the only maps T that make sense satisfy $T^3 = Id$, which leads us to the so-called $\mathcal{T} := \{I, D\}^3$ class, first introduced by Colombo and Stra in [8]:

$$\mathcal{T} := \{III, DDI, DID, IDD\}.$$

In [8] the authors were the first to disprove Seidl’s conjecture. They showed that for $N = 3$ and $d = 2$ the *DDI* map fails to be optimal if the marginal measure is concentrated on a very thin annulus. They also provided a positive example for the optimality of the *DDI* map: they constructed a density, concentrated on a union of three disjointed intervals the last of which is very far from the first two, so that the support of the transport plan given by the *DDI* map is c -cyclically monotone. On the other hand, in [12] De Pascale proved that also for the Coulomb cost the c -cyclical monotonicity implies optimality: this implication had been previously proven only for cost functions that can be bounded from above by a sum of ρ -integrable functions. Using these results and making the necessary passage between the radial problem (1.5) and the full problem (1.4) one gets the optimality of the *DDI* map for the example of Colombo and Stra. In [8] the authors also provided a counterexample for the non-optimality of all transport maps in the class \mathcal{T} .

In this paper we address the connection between the density ρ and the optimality or non-optimality of the Seidl map for $d = 2$ and $N = 3$. Our main results are the following:

Theorem 1.3. *Let $\rho \in \mathcal{P}(\mathbb{R}_+)$ such that*

$$r_2(r_3 - r_1)^3 - r_1(r_3 + r_2)^3 - r_3(r_1 + r_2)^3 \geq 0 \quad (1.6)$$

for ρ -a.e. $(r_1, r_2, r_3) \in [0, s_1] \times [s_1, s_2] \times [s_2, s_3]$. Then the DDI map T provides an optimal Monge solution $\gamma = (Id, T, T^2)_\#(\rho)$ to the problem (1.5).

This theorem makes more quantitative the positive result of Colombo and Stra (see Remarks 3.2 and 3.3 for a more detailed description). Its proof also gives a necessary and sufficient condition for the radial Coulomb cost to coincide with a much simpler cost that corresponds to the situation where all three particles are aligned. More precisely, we show that

Theorem 1.4. *Let $0 < r_1 < r_2 < r_3$. Then $(\theta_2, \theta_3) = (\pi, 0)$ is optimal in (1.3) if and only if*

$$r_2(r_3 - r_1)^3 - r_1(r_3 + r_2)^3 - r_3(r_1 + r_2)^3 \geq 0.$$

Moreover, if (1.6) holds, $(\theta_2, \theta_3) = (\pi, 0)$ is the unique minimum point.

We continue by using this new condition to construct a wide class of counterexamples for the optimality of the maps of the class \mathcal{T} . This class contains densities that are rather physical, for example positive, continuous and differentiable.

Theorem 1.5. *Let $\rho \in \mathcal{P}(\mathbb{R}_+)$ positive everywhere such that $\frac{s_1}{s_2} > \frac{1 + 2\sqrt{3}}{5}$ and*

$$T(x)(T^2(x) - x)^3 - x(T^2(x) + T(x))^3 - T^2(x)(x + T(x))^3 \geq 0 \quad (1.7)$$

for ρ -a.e. $x \in (0, s_1)$, where T is the DDI map. Then none of the maps S in the class $\{D, I\}^3$ provides an optimal Monge solution $\gamma = (Id, S, S^2)_\#(\rho)$ to the problem (1.5). Moreover, there exist smooth counterexample densities.

2. A STUDY OF THE c COST

Recall the definition of the radial cost function (1.1)

$$c(r_1, r_2, r_3) = \min \{ \tilde{c}(v_1, v_2, v_3) \mid |v_i| = r_i \text{ for all } i = 1, 2, 3 \}.$$

By rotational invariance, we can suppose that the minimum is always achieved for $v_1 = r_1 \hat{x}$, i.e., in polar coordinates, $\theta_1 = 0$. Hence we can say that

$$c(r_1, r_2, r_3) = \min \{ C(r_1, 0; r_2, \alpha; r_3, \beta) \mid (\alpha, \beta) \in \mathbb{T}^2 \}; \quad (2.1)$$

due to the dimension $d = 2$, the cost $C(r_1, 0; r_2, \alpha; r_3, \beta)$ has an explicit expression

$$\begin{aligned} C(r_1, 0; r_2, \alpha; r_3, \beta) &= \frac{1}{(r_1^2 + r_2^2 - 2r_1r_2 \cos \alpha)^{1/2}} + \frac{1}{(r_1^2 + r_3^2 - 2r_1r_3 \cos \beta)^{1/2}} \\ &\quad + \frac{1}{(r_2^2 + r_3^2 - 2r_2r_3 \cos(\alpha - \beta))^{1/2}} \end{aligned}$$

The main ingredient for the proof of Theorem 1.3 and Theorem 1.5 is the following result, already stated in the introduction, which we recall for the sake of reader.

Theorem 2.1. *Let $0 < r_1 < r_2 < r_3$. Then $(\alpha, \beta) = (\pi, 0)$ is optimal for the definition of the radial cost c if and only if the polynomial condition (1.6)*

$$r_2(r_3 - r_1)^3 - r_1(r_3 + r_2)^3 - r_3(r_1 + r_2)^3 \geq 0,$$

holds. Moreover, if the above holds, $(\alpha, \beta) = (\pi, 0)$ is the unique minimum point.

Proof of Theorem 2.1. Let $0 < r_1 < r_2 < r_3$ be fixed. In order to lighten the notation, we will omit the dependence on the radii when possible. We will also introduce the following functions for $i, j \in \{1, 2, 3\}$ and $\theta \in \mathbb{T}^1$:

$$D_{ij}(\theta) = r_i^2 + r_j^2 - 2r_i r_j \cos \theta, \quad F_{ij}(\theta) = \frac{1}{D_{ij}(\theta)^{1/2}}$$

It will be useful to compute the derivatives of F_{ij} , so we do it now:

$$\begin{aligned} F'_{ij}(\theta) &= -\frac{r_i r_j \sin \theta}{D_{ij}^{3/2}} \\ F''_{ij}(\theta) &= -\frac{r_i r_j \cos \theta}{D_{ij}^{3/2}} + \frac{3}{2} \frac{2r_i^2 r_j^2 \sin^2 \theta}{D_{ij}^{5/2}} \\ &= -\frac{r_i r_j (r_i r_j \cos^2 \theta + (r_i^2 + r_j^2) \cos \theta - 3r_i r_j)}{D_{ij}(\theta)^{5/2}} \end{aligned}$$

In order to simplify the notation even more, we denote

$$Q_{ij}(t) = r_i r_j t^2 + (r_i^2 + r_j^2)t - 3r_i r_j, \quad t \in [-1, 1],$$

so that

$$F''_{ij}(\theta) = -\frac{r_i r_j Q_{ij}(\cos \theta)}{D_{ij}(\theta)^{5/2}}.$$

Observe that $Q_{ij}(-1) = -(r_i + r_j)^2$ and $Q_{ij}(1) = (r_i - r_j)^2$, so that

$$F''_{ij}(0) = -\frac{r_i r_j}{|r_i - r_j|^3} \quad \text{and} \quad F''_{ij}(\pi) = \frac{r_i r_j}{(r_i + r_j)^3} \quad (2.2)$$

First we prove that if $(\alpha, \beta) = (\pi, 0)$ is optimal in (2.1), then (1.6) holds. Recall that the function to minimize is

$$f(\alpha, \beta) = F_{12}(\alpha) + F_{13}(\beta) + F_{23}(\alpha - \beta)$$

and notice that $f \in C^\infty(\mathbb{T}^2)$. Thus, if $(\pi, 0)$ is minimal, it must be a stationary point with positive-definite Hessian. Let us compute the gradient and the Hessian of f :

$$\begin{aligned} \nabla f(\alpha, \beta) &= (F'_{12}(\alpha) + F'_{23}(\alpha - \beta), F'_{13}(\beta) - F'_{23}(\alpha - \beta)), \\ Hf(\alpha, \beta) &= \begin{pmatrix} F''_{12}(\alpha) + F''_{23}(\alpha - \beta) & -F''_{23}(\alpha - \beta) \\ -F''_{23}(\alpha - \beta) & F''_{13}(\beta) + F''_{23}(\alpha - \beta) \end{pmatrix}. \end{aligned}$$

Using (2.2), we have

$$Hf(\pi, 0) = \begin{pmatrix} \frac{r_1 r_2}{(r_1 + r_2)^3} + \frac{r_2 r_3}{(r_2 + r_3)^3} & -\frac{r_2 r_3}{(r_2 + r_3)^3} \\ -\frac{r_2 r_3}{(r_2 + r_3)^3} & -\frac{r_1 r_3}{(r_3 - r_1)^3} + \frac{r_2 r_3}{(r_2 + r_3)^3} \end{pmatrix}$$

and

$$\begin{aligned} \det Hf(\pi, 0) &= -\frac{r_1^2 r_2 r_3}{(r_1 + r_2)^3 (r_3 - r_1)^3} - \frac{r_1 r_2 r_3^2}{(r_2 + r_3)^3 (r_3 - r_1)^3} \\ &\quad + \frac{r_1 r_2^2 r_3}{(r_1 + r_2)^3 (r_2 + r_3)^3} \\ &= \frac{r_1 r_2 r_3 [r_2 (r_3 - r_1)^3 - r_1 (r_3 + r_2)^3 - r_3 (r_1 + r_2)^3]}{(r_1 + r_2)^3 (r_2 + r_3)^3 (r_3 - r_1)^3}. \end{aligned}$$

The positivity of $\det Hf(\pi, 0)$ implies the condition (1.6), which proves the first part of Theorem 2.1.

Now we assume that (1.6) holds, and we want to get that $(\pi, 0)$ is the unique minimum point. The first (and most challenging) step is given by the following

Proposition 2.2. *Suppose that $0 < r_1 < r_2 < r_3$ satisfy (1.6). Then $(0, 0)$, $(0, \pi)$, $(\pi, 0)$, (π, π) are the only stationary points of $f(\alpha, \beta)$.*

The proof of Proposition 2.2 is quite technical and long. For the sake of clarity we postpone it to the end of this section, in order to keep focusing on the main result.

Since $\{0, \pi\}^2$ are the only stationary points, the global minimum of f must be between them. By direct comparison of the values $f(0, 0)$, $f(0, \pi)$, $f(\pi, 0)$, $f(\pi, \pi)$ we will conclude that $(\pi, 0)$ is the unique minimum point.

We compute

$$\begin{aligned} f(0, 0) &= \frac{1}{r_2 - r_1} + \frac{1}{r_3 - r_2} + \frac{1}{r_3 - r_1} \\ f(0, \pi) &= \frac{1}{r_2 - r_1} + \frac{1}{r_3 + r_2} + \frac{1}{r_3 + r_1} \\ f(\pi, 0) &= \frac{1}{r_2 + r_1} + \frac{1}{r_3 + r_2} + \frac{1}{r_3 - r_1} \\ f(\pi, \pi) &= \frac{1}{r_2 + r_1} + \frac{1}{r_3 - r_2} + \frac{1}{r_3 + r_1}, \end{aligned}$$

and observe that clearly $f(0, 0) > f(0, \pi)$. To deduce the other inequalities we observe that the function

$$h(x, y) = \frac{1}{x - y} - \frac{1}{x + y} \quad \text{for } 0 < y < x.$$

is decreasing in x and increasing in y , so $h(r_3, r_1) < h(r_2, r_1) \Rightarrow f(\pi, 0) < f(0, \pi)$ and $h(r_3, r_1) < h(r_3, r_2) \Rightarrow f(\pi, 0) < f(\pi, \pi)$, as wanted.

Proof of Proposition 2.2. A stationary point (α, β) must solve $\nabla f = 0$, i.e.,

$$\begin{cases} -\frac{r_1 r_2 \sin \alpha}{D_{12}(\alpha)^{3/2}} - \frac{r_2 r_3 \sin(\alpha - \beta)}{D_{23}(\alpha - \beta)^{3/2}} = 0 \\ -\frac{r_1 r_3 \sin \beta}{D_{13}(\beta)^{3/2}} + \frac{r_2 r_3 \sin(\alpha - \beta)}{D_{23}(\alpha - \beta)^{3/2}} = 0 \end{cases}$$

which we rewrite as

$$\begin{cases} \frac{r_1 r_2 \sin \alpha}{D_{12}(\alpha)^{3/2}} + \frac{r_1 r_3 \sin \beta}{D_{13}(\beta)^{3/2}} = 0 \\ \frac{r_1 r_3 \sin \beta}{D_{13}(\beta)^{3/2}} - \frac{r_2 r_3 \sin(\alpha - \beta)}{D_{23}(\alpha - \beta)^{3/2}} = 0. \end{cases} \quad (2.3)$$

Observe that the four points $(\alpha, \beta) \in \{0, \pi\}^2$ are always solutions for (2.3). We will study this system in detail for $\beta \in [0, \pi]$. The conclusions can then be derived for $\beta \in [-\pi, 0]$ by making use of the change of variables $\tilde{\alpha} = -\alpha$, $\tilde{\beta} = -\beta$. To proceed in the computations, we perform a finer study of the function

$$g_{ij}(\theta) = -F'_{ij}(\theta) = \frac{r_i r_j \sin \theta}{D_{ij}(\theta)^{3/2}},$$

so that the optimality conditions (2.3) will be rewritten in the form

$$\begin{cases} g_{12}(\alpha) = -g_{13}(\beta) \\ g_{13}(\beta) = g_{23}(\alpha - \beta). \end{cases} \quad (2.4)$$

We now prove that for every β in $[0, \pi]$ there exists at least one and at most two α 's such that each of the two equations is satisfied.

The derivative of g_{ij} is

$$g'_{ij}(\theta) = r_i r_j \frac{Q_{ij}(\cos \theta)}{D_{ij}(\theta)^{5/2}}$$

and it vanishes for

$$Q_{ij}(\cos \theta_{ij}) = 0 \Rightarrow \cos \theta_{ij} = \frac{-r_i^2 - r_j^2 + \sqrt{r_i^4 + 14r_i^2 r_j^2 + r_j^4}}{2r_i r_j} \in (0, 1).$$

By looking at the sign of the second degree polynomial Q_{ij} , we conclude that $g_{ij}(\theta)$ is increasing from 0 to its maximum on $[0, \theta_{ij}]$ and decreasing to 0 on $[\theta_{ij}, \pi]$

Lemma 2.3. *For every $\theta \in [0, \pi]$, $g_{13}(\theta) \leq g_{12}(\theta)$ and $g_{13}(\theta) \leq g_{23}(\theta)$. (See Figure 2.1.)*

Proof. We claim that $0 \leq g'_{13}(0) \leq g'_{12}(0)$ and $g'_{13}(\pi) \geq g'_{12}(\pi) \geq 0$. Indeed, using (2.2),

$$g'_{13}(0) = -F''_{13}(0) = \frac{r_1 r_3}{(r_3 - r_1)^3} \geq 0, \quad \text{and} \quad g'_{12}(0) = \frac{r_1 r_2}{(r_2 - r_1)^3},$$

thus

$$g'_{13}(0) \leq g'_{12}(0) \iff r_3(r_2 - r_1)^3 \leq r_2(r_3 - r_1)^3$$

which is weaker than (1.6).

On the other hand,

$$g'_{13}(\pi) = -F''_{13}(\pi) = -\frac{r_1 r_3}{(r_3 + r_1)^3} \leq 0, \quad \text{and} \quad g'_{12}(\pi) = -\frac{r_1 r_2}{(r_1 + r_2)^3},$$

thus

$$g'_{13}(\pi) \geq g'_{12}(\pi) \iff r_3(r_1 + r_2)^3 \leq r_2(r_3 + r_1)^3$$

which is once again weaker than (1.6).

Moreover, the equation $g_{13}(\theta) = g_{12}(\theta)$ has at most one solution in $(0, \pi)$, since we have the following chain of equivalent equalities:

$$\begin{aligned} g_{13}(\theta) &= g_{12}(\theta) \\ \frac{r_1 r_3}{D_{13}(\theta)^{3/2}} &= \frac{r_1 r_2}{D_{12}(\theta)^{3/2}} \\ r_3^{2/3}(r_1^2 + r_2^2 - 2r_2 r_3 \cos \theta) &= r_2^{2/3}(r_1^2 + r_3^2 - 2r_1 r_3 \cos \theta) \\ \cos \theta &= \frac{r_2^{2/3} r_3^{2/3}(r_3^{4/3} - r_2^{4/3}) - r_1^2(r_3^{2/3} - r_2^{2/3})}{2r_1 r_2^{2/3} r_3^{2/3}(r_3^{1/3} - r_2^{1/3})}. \end{aligned}$$

Recalling that both g_{13} and g_{12} vanish at the endpoints of $[0, \pi]$, we get the thesis. An analogous argument applies to the comparison between g_{13} and g_{23} . \square

Remark 2.4. It follows from the Lemma above that for every value of g_{13} , and so for every fixed β , there exists at least one α where $g_{12}(\alpha)$ takes the same value. If the value of g_{13} is not the maximal one then there are exactly two different α 's such that the value is achieved. The same holds for $g_{23}(\alpha - \beta)$. See figure below.

Lemma 2.5. *If $\cos \theta \in (\cos \theta_{ij}, 1)$ then*

$$g'_{ij}(\theta) < g'_{ij}(0) \frac{\cos \theta - \cos \theta_{ij}}{1 - \cos \theta_{ij}},$$

if $\cos \theta \in (-1, \cos \theta_{ij})$ then

$$g'_{ij}(\theta) < g'_{ij}(\pi) \frac{\cos \theta - \cos \theta_{ij}}{-1 - \cos \theta_{ij}}.$$

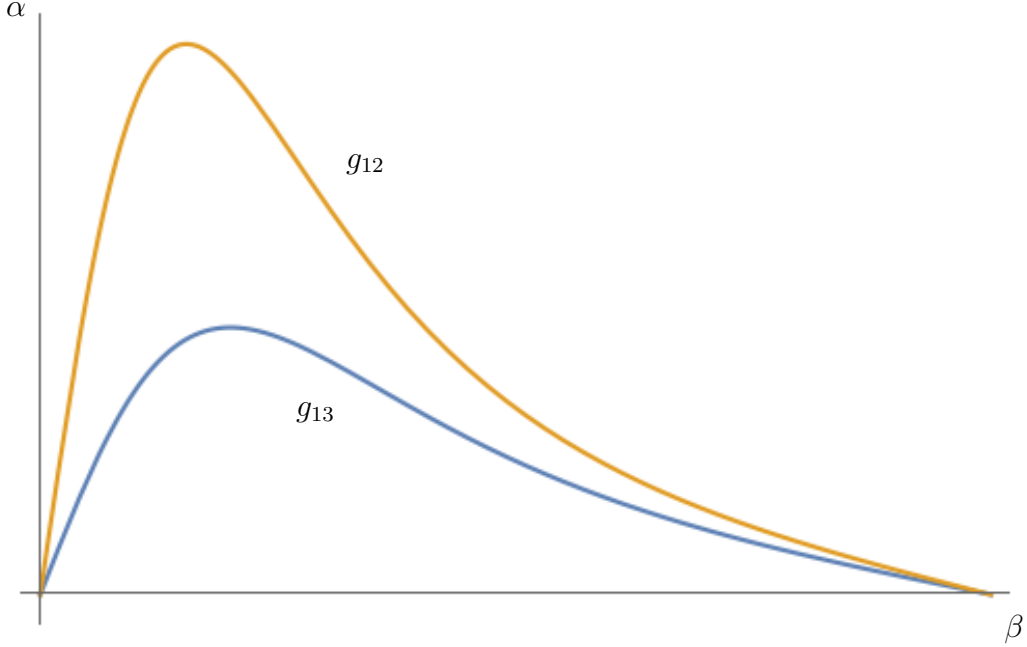


FIGURE 2.1. The relative position of the graphs of g_{12} and g_{13} on the interval $[0, \pi]$. However the strict inequality between the two maximal values is not proved. See Lemma 2.3

Proof. We omit for simplicity of notation the indices ij . Recall that

$$g'(\theta) = \frac{r_i r_j Q_{ij}(\cos \theta)}{(r_i^2 + r_j^2 - 2r_i r_j \cos \theta)^{5/2}} = h(\cos \theta),$$

where $h: [-1, 1] \rightarrow \mathbb{R}$, $h(t) = \frac{r_i r_j Q_{ij}(t)}{(r_i^2 + r_j^2 - 2r_i r_j t)^{5/2}}$.

The thesis is a weak version of the convexity of h : if h is convex, then the inequalities hold by applying the Jensen's inequality separately in the intervals $[-1, \cos \theta_{ij}]$ and $[\cos \theta_{ij}, 1]$. It could happen, however, that h has a concave part between -1 and a certain threshold ξ , and then it is convex. In this case we prove the following:

- h_{ij} is decreasing between -1 and a certain threshold σ , where it reaches the minimum;
- $\xi < \sigma$, i.e., in the interval $[\sigma, 1]$ the function is convex.

Then we deduce that, for $-1 \leq t \leq \sigma$,

$$h_{ij}(t) \leq h_{ij}(-1) \leq h_{ij}(-1) \frac{t - \cos \theta_{ij}}{-1 - \cos \theta_{ij}}$$

(recall that $h(-1)$ is negative).

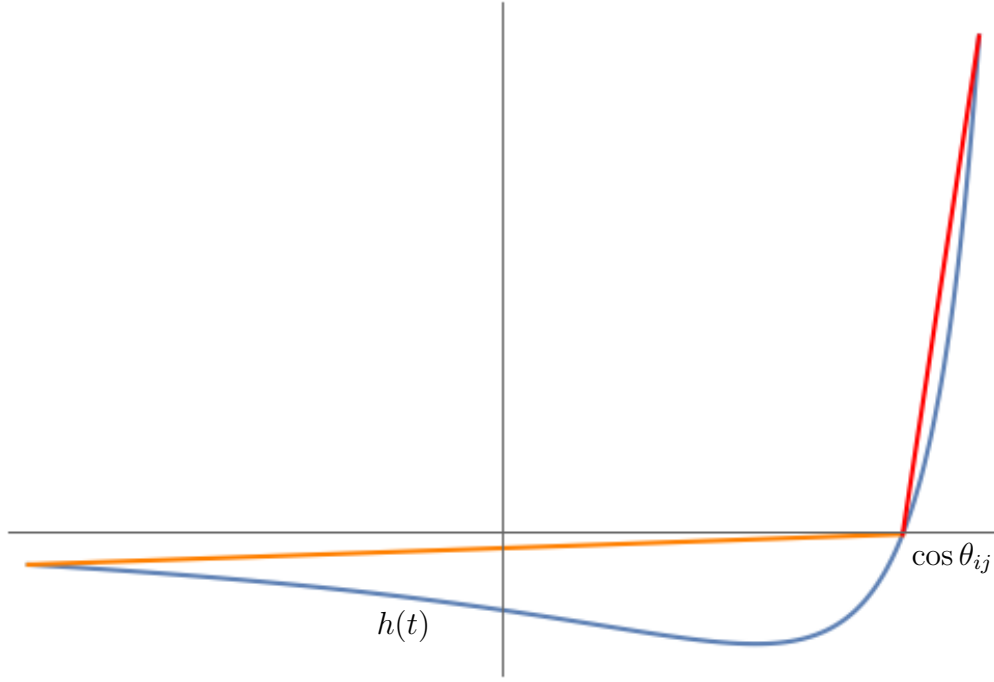


FIGURE 2.2. A graphical understanding of Lemma 2.5: the function $h(t)$ stays below two segments.

On the other hand, for $\sigma \leq t \leq \cos \theta_{ij}$,

$$\begin{aligned} h(t) &\leq \text{line joining } (\sigma, h(\sigma)) \text{ and } (\cos \theta_{ij}, 0) \\ &\leq \text{line joining } (-1, h(-1)) \text{ and } (\cos \theta_{ij}, 0) \end{aligned}$$

since σ is a minimum point. See Figure 2.2 for a more clear graphical meaning of the proof.

Here come the computations:

$$h'(t) = \frac{r_i^2 r_j^2 t^2 + 5r_i r_j (r_i^2 + r_j^2)t + r_i^4 - 13r_i^2 r_j^2 + r_j^4}{(r_i^2 + r_j^2 - 2r_i r_j t)^{7/2}}.$$

We have that $h'(t) = 0$ for

$$t = \frac{-5(r_i^2 + r_j^2) \pm \sqrt{21r_i^4 + 102r_i^2 r_j^2 + 21r_j^4}}{2r_i r_j}.$$

Observe that the smaller solution is always outside the interval $[-1, 1]$, since

$$-5(r_i^2 + r_j^2) - \sqrt{21r_i^4 + 102r_i^2 r_j^2 + 21r_j^4} < -\sqrt{102}r_i r_j < -2r_i r_j.$$

Denote by σ the bigger root.

We move on to the second derivative:

$$h''(t) = 3r_i r_j \frac{r_i^2 r_j^2 t^2 + 9r_i r_j (r_i^2 + r_j^2)t + 4r_i^4 - 27r_i^2 r_j^2 + 4r_j^4}{(r_i^2 + r_j^2 - 2r_i r_j t)^{9/2}}.$$

We have that $h''(t) = 0$ for

$$t = \frac{-9(r_i^2 + r_j^2) \pm \sqrt{65r_i^4 + 270r_i^2 r_j^2 + 65r_j^4}}{2r_i r_j}.$$

As above, the smaller root always lies outside the interval $[-1, 1]$. Denote by ξ the bigger root. Now we prove that $\sigma > \xi$ for any choice of the values $0 < r_i < r_j$. By homogeneity, denoting by $u = r_i^2/r_j^2 \in (0, 1)$, it suffices to prove that

$$-5(1+u) + \sqrt{21u^2 + 102u + 21} > -9(1+u) + \sqrt{65u^2 + 270u + 65},$$

i.e.,

$$\begin{aligned} 4(1+u) + \sqrt{21u^2 + 102u + 21} &> \sqrt{65u^2 + 270u + 65} \\ 37u^2 + 134u + 37u + 8(1+u)\sqrt{21u^2 + 102u + 21} &> 65u^2 + 270u + 65 \\ 8(1+u)\sqrt{3}\sqrt{7u^2 + 34u + 7} &> 28u^2 + 136u + 28 \\ 2\sqrt{3}(1+u) &> \sqrt{7u^2 + 34u + 7} \\ 12(1+u)^2 &> 7u^2 + 34u + 7 \\ 5(1-u)^2 &> 0, \end{aligned}$$

as wanted. \square

Now the idea is the following: in view of Lemma 2.3, the first equation of (2.3) implicitly defines two C^∞ functions $\alpha_0(\beta)$ and $\alpha_\pi(\beta)$ such that $\alpha_0(0) = 0, \alpha_\pi(0) = \pi$. Analogously, the second equation implicitly defines two functions $\hat{\alpha}_0(\beta)$ and $\hat{\alpha}_\pi(\beta)$ such that $\hat{\alpha}_0(0) = 0, \hat{\alpha}_\pi(0) = \pi$.

We want to prove that each curve $\alpha_{0,\pi}$ intersects each curve $\hat{\alpha}_{0,\pi}$ only in 0 or π . By sign considerations, we notice that the first equation implies $\alpha(\beta) \in [\pi, 2\pi]$ and the second equation implies $\hat{\alpha}(\beta) \in [\beta, \pi + \beta]$. Hence, the possible solutions lie in the region $\pi \leq \alpha \leq \pi + \beta$, and when considering the whole torus \mathbb{T}^2 the region has a “butterfly” shape.

This already shows that the curves $\alpha_0(\beta)$ and $\hat{\alpha}_0(\beta)$ do not produce solutions, since we have that $\beta - \pi \leq \alpha_0(\beta) \leq 0$ and $0 \leq \hat{\alpha}_0(\beta) \leq \pi$. Thus we can concentrate our attention on the curves α_π and $\hat{\alpha}_\pi$.

The key observation lies in the fact that

$$\pi \leq \alpha_\pi(\beta) \leq \pi + \alpha'_\pi(0)\beta,$$

i.e., the function $\alpha_\pi(\beta)$ stays below its tangent line at $\beta = 0$ (see Figure 2.4). Likewise, the function $\hat{\alpha}_\pi(\beta)$ stays above its tangent line at $\beta = 0$. This allows us

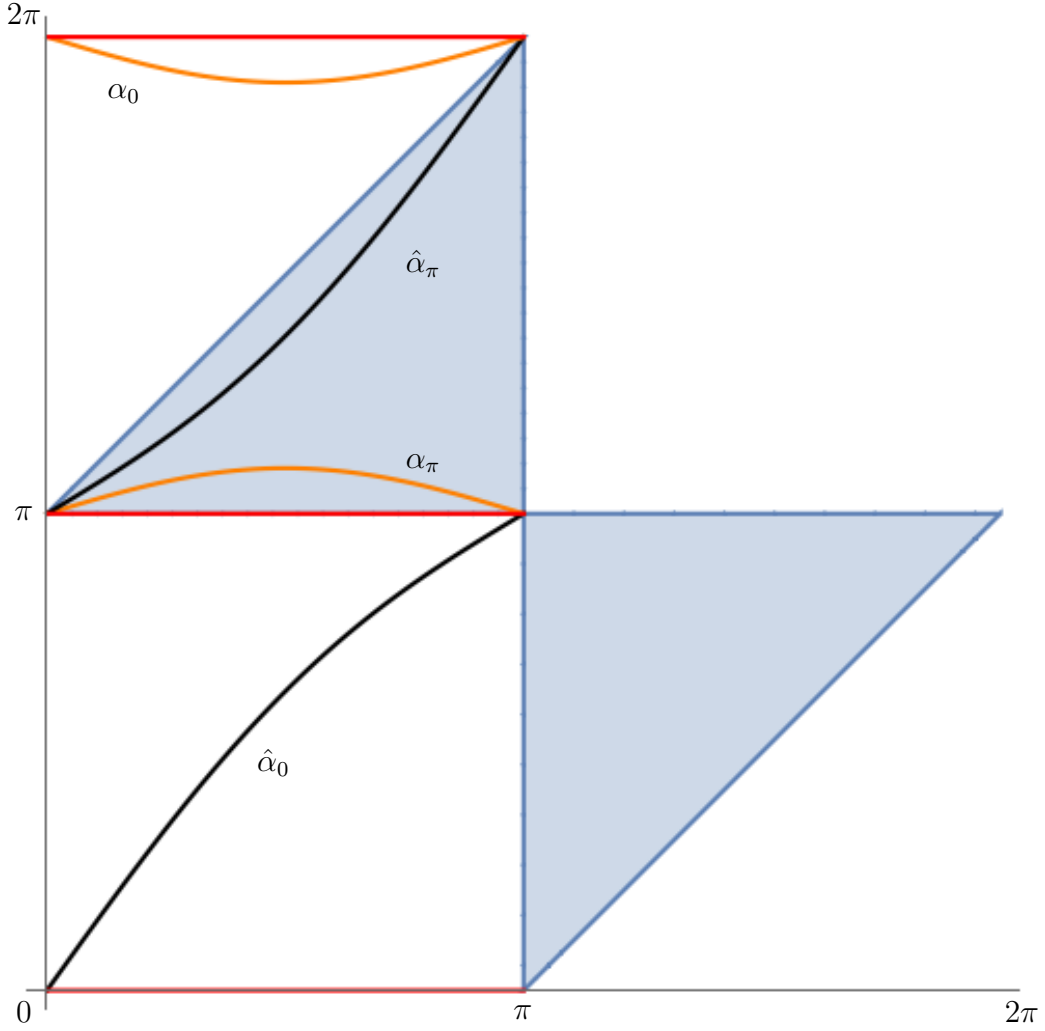


FIGURE 2.3. In blue, the “butterfly” region of admissible solutions to optimality conditions (2.3). In black and orange, a plot of the curves $\alpha_{0,\pi}$ and $\hat{\alpha}_{0,\pi}$ in the region $0 \leq \beta \leq \pi$.

to conclude that they do not intersect since, as we will see, the condition (1.6) is equivalent to $\alpha'_\pi(0) \leq \hat{\alpha}'_\pi(0)$.

Lemma 2.6. *For $\beta \in (0, \pi)$ let $\alpha(\beta)$ be the solution of*

$$\begin{cases} g_{13}(\beta) + g_{ij}(\alpha) = 0 \\ \alpha(0) = \alpha(\pi) = \pi. \end{cases}$$

Then

$$\pi \leq \alpha(\beta) < \pi + \alpha'(0)\beta.$$

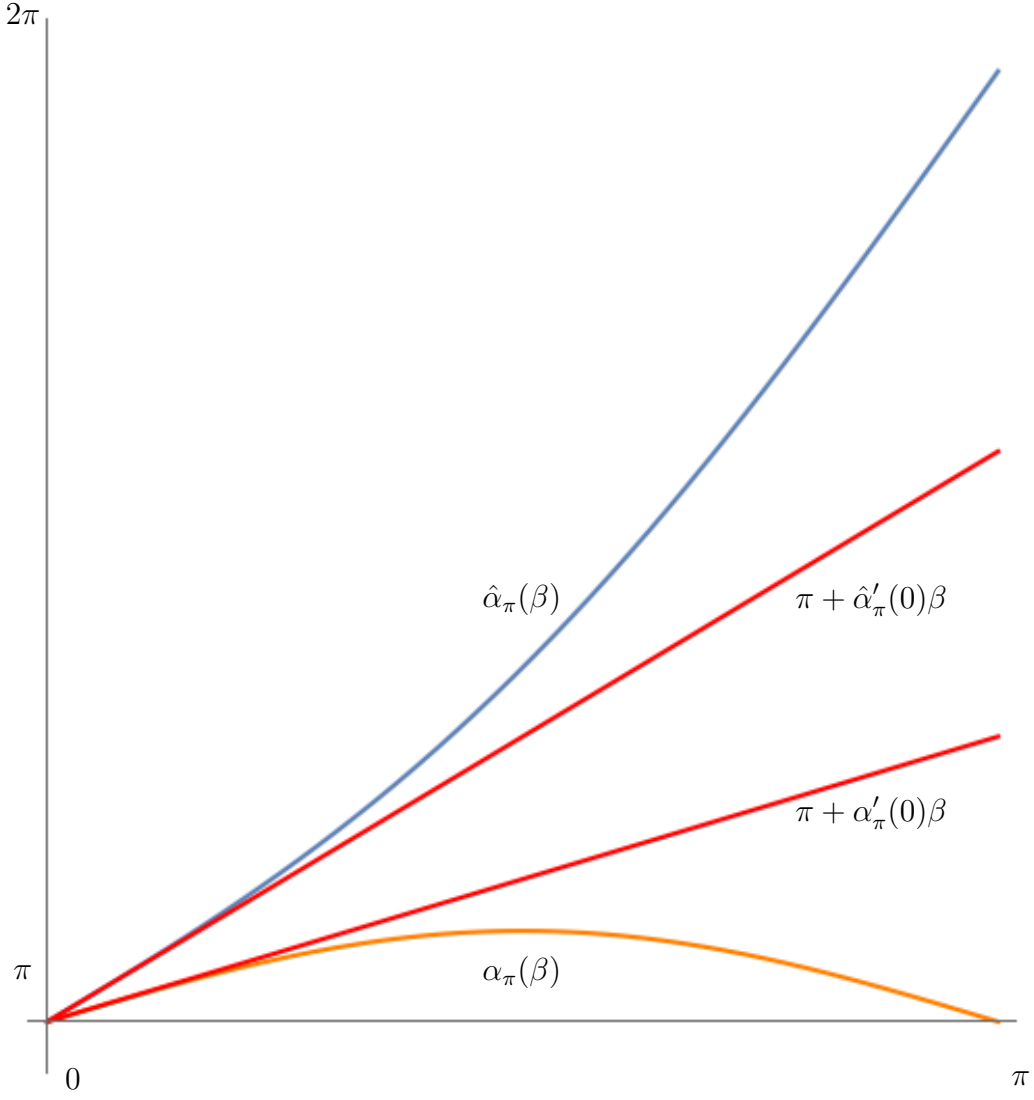


FIGURE 2.4. A graphical understanding of Lemma 2.6: the function $\alpha_\pi(\beta)$ is confined by $\pi \leq \alpha_\pi(\beta) \leq \pi + \alpha'_\pi(0)\beta$, and similarly $\pi + \hat{\alpha}'_\pi(0)\beta \leq \hat{\alpha}_\pi(\beta) \leq \pi + \beta$. This implies that the intersection between α_π and $\hat{\alpha}_\pi$ is only at $\beta = 0$.

(See Figure 2.4 for a graphical understanding.)

Proof. Differentiating in β we get

$$g'_{13}(\beta) + \alpha'(\beta)g'_{ij}(\alpha(\beta)) = 0 \implies \alpha'(\beta) = \frac{g'_{13}(\beta)}{-g'_{ij}(\alpha(\beta))}.$$

Take $\beta \in (0, \theta_{13})$, where θ_{13} is the critical value of g_{13} , so that $\cos \beta > \cos \theta_{13}$. By Lemma 2.3 we have that $\alpha \in [\pi, 2\pi - \theta_{ij}]$, because the equation $g_{13}(\beta) + g_{ij}(\alpha) = 0$ has two solutions in the interval $[\pi, 2\pi]$ and by definition α is the leftmost one. Using Lemma 2.5 we have

$$\alpha'(\beta) \leq \frac{g'_{13}(0)}{-g'_{ij}(\pi)} \frac{\cos \beta - \cos \theta_{13}}{1 - \cos \theta_{13}} \frac{-1 - \cos \theta_{ij}}{\cos \alpha(\beta) - \cos \theta_{ij}}.$$

Since $\frac{g'_{13}(0)}{-g'_{ij}(\pi)} = \alpha'(0) \geq 0$, it suffices to show that

$$\frac{\cos \beta - \cos \theta_{13}}{1 - \cos \theta_{13}} \frac{-1 - \cos \theta_{ij}}{\cos \alpha(\beta) - \cos \theta_{ij}} \leq 1.$$

Let $\tilde{\alpha} = \alpha(\beta) - \pi$, so that $0 \leq \tilde{\alpha} \leq \beta$. We must prove

$$\begin{aligned} & \frac{\cos \beta - \cos \theta_{13}}{1 - \cos \theta_{13}} \frac{1 + \cos \theta_{ij}}{\cos \tilde{\alpha} + \cos \theta_{ij}} \leq 1. \\ & (1 + \cos \theta_{ij})(\cos \beta - \cos \theta_{13}) \leq (1 - \cos \theta_{13})(\cos \tilde{\alpha} + \cos \theta_{ij}) \\ & (\cos \beta - \cos \tilde{\alpha}) + \cos \theta_{ij} \cos \beta + \cos \theta_{13} \cos \tilde{\alpha} \leq \cos \theta_{ij} + \cos \theta_{13}. \end{aligned}$$

But this is true, since $\tilde{\alpha} \leq \beta \implies \cos \beta - \cos \tilde{\alpha} \geq 0$ and clearly

$$\cos \theta_{ij} \cos \beta + \cos \theta_{13} \cos \tilde{\alpha} \leq \cos \theta_{ij} + \cos \theta_{13}.$$

We got the desired inequality for $\beta \in (0, \theta_{13})$. However, for $\beta \geq \theta_{13}$ we have $\alpha'(\beta) \leq 0$, hence the line $\alpha'(0)\beta$ is increasing and the function $\alpha(\beta)$ is decreasing, giving the inequality for every β . \square

By Lemma 2.6, we obtain that the function $\alpha_\pi(\beta)$ lies between the horizontal line $\alpha = \pi$ and the line $\alpha = \pi + \alpha'_\pi(0)\beta$ (strictly for $\beta > 0$). Recall that the function $\hat{\alpha}_\pi(\beta)$ satisfies the second equation of the stationary system ((2.3))

$$\frac{r_1 r_3 \sin \beta}{D_{13}(\beta)^{3/2}} - \frac{r_2 r_3 \sin(\hat{\alpha} - \beta)}{D_{23}(\hat{\alpha} - \beta)^{3/2}} = 0$$

with $\hat{\alpha}_\pi(0) = \pi$, $\hat{\alpha}_\pi(\pi) = 2\pi$.

By a change of variables $\tilde{\alpha}(\beta) = 2\pi + \beta - \hat{\alpha}_\pi(\beta)$, we get that $\tilde{\alpha}$ satisfies

$$\begin{cases} g_{13}(\beta) + g_{23}(\tilde{\alpha}) = 0 \\ \tilde{\alpha}(0) = \tilde{\alpha}(\pi) = 0, \end{cases}$$

hence $\pi < \tilde{\alpha}(\beta) < \pi + \tilde{\alpha}'(0)\beta$, i.e.,

$$\pi + \hat{\alpha}'_\pi(0)\beta < \hat{\alpha}_\pi(\beta) < \pi + \beta$$

for $\beta > 0$. So the idea is that the two lines provide a separation of the curves, so that no intersection can happen except at the starting point.

We conclude by observing that the condition (1.6) is equivalent to $\widehat{\alpha}'_\pi(0) \geq \alpha'_\pi(0)$: indeed we have

$$g_{13}(\beta) - g_{23}(\widehat{\alpha}_\pi(\beta) - \beta) = 0 \implies$$

$$\widehat{\alpha}'_\pi(0) = 1 + \frac{g'_{13}(0)}{g'_{23}(\pi)} = 1 - \frac{r_1 r_3}{(r_3 - r_1)^3} \frac{(r_2 + r_3)^3}{r_2 r_3} = \frac{r_2(r_3 - r_1)^3 - r_1(r_2 + r_3)^3}{r_2(r_3 - r_1^3)}$$

and

$$\alpha'_\pi(0) = \frac{g'_{13}(0)}{-g'_{12}(\pi)} = \frac{r_1 r_3}{(r_3 - r_1)^3} \frac{(r_1 + r_2)^3}{r_1 r_2} = \frac{r_3(r_1 + r_2)^3}{r_2(r_3 - r_1)^3}.$$

□

3. CONSEQUENCES OF THEOREM 2.1

When ρ satisfies the assumptions of Theorem 2.1, we know that

$$c(r_1, r_2, r_3) = \frac{1}{r_2 + r_1} + \frac{1}{r_3 + r_2} + \frac{1}{r_3 - r_1}$$

for ρ -a.e. $(r_1, r_2, r_3) \in [0, s_1] \times [s_1, s_2] \times [s_2, +\infty)$. The key observation lies in the fact that this can be viewed as a 1-dimensional Coulomb cost for points $-r_2, r_1, r_3 \in \mathbb{R}$. We can now rely on a somewhat well-established theory for the Coulomb cost in dimension $d = 1$.

This allows to prove Theorem 1.3.

Proof of Theorem 1.3. This is a direct consequence of the one-dimensional result presented in [6]. Indeed, we can consider the absolutely continuous measure $\tilde{\rho} \in \mathcal{P}(\mathbb{R})$ defined by

$$\tilde{\rho}(x) = \begin{cases} \rho(x) & x \in [0, s_1] \cup [s_2, +\infty) \\ \rho(-x) & x \in [-s_2, -s_1] \\ 0 & \text{otherwise} \end{cases}$$

and observe that the DDI map T for ρ corresponds to the optimal increasing map S defined in [6].

The optimality follows from the fact that $c(x, T(x), T^2(x)) = c_{1D}(y, S(y), S^2(y))$ for ρ -a.e. $x \in [0, s_1]$ and $\tilde{\rho}$ -a.e. $y \in [-s_2, -s_1]$, where c_{1D} is the Coulomb cost on the real line, as observed above. □

The idea of the first part of the the proof of Theorem 1.5 is to show that on the support of the DDI map, the c -cyclical monotonicity is violated. We prepare a couple of technical results.

Lemma 3.1. *Let $\frac{s_1}{s_2} > \frac{1 + 2\sqrt{3}}{5}$. Then there exist $\epsilon, M > 0$ such that*

$$\frac{2}{s_2 + \epsilon} + \frac{1}{2s_2 + \epsilon} + \frac{1}{2s_1 + \epsilon} > \frac{\sqrt{3}}{s_1 - \epsilon} + \frac{1}{s_1} + \frac{1}{M - \epsilon}. \quad (3.1)$$

Proof. When $\epsilon = 0$ and $M = +\infty$, the inequality (3.1) reads

$$\frac{2}{s_2} + \frac{1}{2s_2} + \frac{1}{2s_1} > \frac{\sqrt{3}}{s_1} + \frac{1}{s_1},$$

which is equivalent to $\frac{s_1}{s_2} > \frac{2\sqrt{3}+1}{5}$.

By continuity, there is a small ϵ such that

$$\frac{2}{s_2 + \epsilon} + \frac{1}{2s_2 + \epsilon} + \frac{1}{2s_1 + \epsilon} > \frac{\sqrt{3}}{s_1 - \epsilon} + \frac{1}{s_1}.$$

Now choose M big enough such that the desired inequality (3.1) holds. \square

Remark 3.2. We recall the polynomial condition (1.6):

$$r_2(r_3 - r_1)^3 - r_1(r_3 + r_2)^3 - r_3(r_1 + r_2)^3 \geq 0.$$

For fixed r_1 and r_2 , the cubic polynomial in r_3 that appears on the left-hand side of (1.6) has three real roots. They are given by the following expressions:

$$-r_2, \quad \frac{5r_1r_2 + r_2^2 \pm (r_1 + r_2)\sqrt{r_2^2 + 12r_1r_2 - 4r_1^2}}{2(r_2 - r_1)}.$$

Since we are only interested in the region where $r_3 > 0$ and since

$$\frac{5r_1r_2 + r_2^2 + (r_1 + r_2)\sqrt{r_2^2 + 12r_1r_2 - 4r_1^2}}{2(r_2 - r_1)}$$

is the only positive root for every value of $0 < r_1 < r_2$, the condition (1.6) can be rewritten as

$$\varphi(r_1, r_2) := \frac{5r_1r_2 + r_2^2 + (r_1 + r_2)\sqrt{r_2^2 + 12r_1r_2 - 4r_1^2}}{2(r_2 - r_1)} \leq r_3. \quad (3.2)$$

Remark 3.3. In [8], a crucial role was played by Lemma 4.1. In our framework this lemma can be obtained as a consequence of Theorem 2.1 by choosing (following the notation of [8])

$$r_3^- > \max_{[r_1^-, r_1^+] \times [r_2^-, r_2^+]} \varphi(r_1, r_2).$$

If $r_1^+ < r_2^-$, as assumed by the authors in [8], then the maximum above is a real number and the threshold r_3^- can be fixed. Thus our result gives a quantitative optimal version of their choice. Moreover, Theorem 2.1 allows us to deal with the case in which there is no gap between r_1^+ and r_2^- , since we have an explicit control of the growth of $\varphi(r_1, r_2)$ as $r_1 \rightarrow r_2$.

Before the next lemma we introduce the notation $c_\pi(r_1, r_2, r_3)$ for the Coulomb cost of the configuration where all three points are placed along the x -axis so that

the angle between v_1 and v_2 is π and the angle between v_1 and v_3 is 0; following our general line, the vector v_1 lies along the positive x -axis. In other words

$$c_\pi(r_1, r_2, r_3) = C(r_1, r_2, r_3, \pi, 0).$$

Lemma 3.4. *Let s_1, s_2, ε and M as in Lemma 3.1, and let $(r_1, r_2, r_3) \in (0, \varepsilon) \times (s_2 - \varepsilon, s_2) \times (s_2, s_2 + \varepsilon)$ and $(\ell_1, \ell_2, \ell_3) \in (s_1 - \varepsilon, s_1) \times (s_1, s_1 + \varepsilon) \times (M, +\infty)$. Suppose that the condition (3.2) is satisfied by both (r_1, r_2, r_3) and (ℓ_1, ℓ_2, ℓ_3) . Then*

$$c(r_1, r_2, r_3) + c(\ell_1, \ell_2, \ell_3) > c(\ell_1, r_2, r_3) + c(r_1, \ell_2, \ell_3).$$

Proof. Since the condition (3.2) is satisfied, we have

$$\begin{aligned} c(r_1, r_2, r_3) &= c_\pi(r_1, r_2, r_3) = \frac{1}{r_1 + r_2} + \frac{1}{r_2 + r_3} + \frac{1}{r_3 - r_1} \\ &\geq \frac{1}{s_2 + \varepsilon} + \frac{1}{2s_2 + \varepsilon} + \frac{1}{s_2 + \varepsilon} \end{aligned}$$

and

$$\begin{aligned} c(\ell_1, \ell_2, \ell_3) &= c_\pi(\ell_1, \ell_2, \ell_3) = \frac{1}{\ell_1 + \ell_2} + \frac{1}{\ell_2 + \ell_3} + \frac{1}{\ell_3 - \ell_1} \\ &\geq \frac{1}{2s_1 + \varepsilon} + \frac{1}{\ell_2 + \ell_3} + 0. \end{aligned}$$

Now we analyze the other side. Since (ℓ_1, ℓ_2, ℓ_3) satisfy (3.2) and $r_1 < \ell_1$, then also (r_1, ℓ_2, ℓ_3) satisfy (3.2)², so that

$$\begin{aligned} c(r_1, \ell_2, \ell_3) &= c_\pi(r_1, \ell_2, \ell_3) = \frac{1}{r_1 + \ell_2} + \frac{1}{\ell_2 + \ell_3} + \frac{1}{\ell_3 - r_1} \\ &\leq \frac{1}{s_1} + \frac{1}{\ell_2 + \ell_3} + \frac{1}{M - \varepsilon}. \end{aligned}$$

For the other term we have

$$c(\ell_1, r_2, r_3) \leq c_\Delta(\ell_1, r_2, r_3) \leq c_\Delta(\ell_1, \ell_1, \ell_1) = \frac{\sqrt{3}}{\ell_1} \leq \frac{\sqrt{3}}{s_1 - \varepsilon},$$

where $c_\Delta(r_1, r_2, r_3) = C(r_1, r_2, r_3, \frac{2\pi}{3}, \frac{4\pi}{3})$ denotes the cost when the angles are the ones of an equilateral triangle. The second inequality follows from the fact that we are keeping the angles fixed, but decreasing the size of the sides. By comparing the expressions and using Lemma 3.1 we get the desired inequality. \square

Finally we come to the proof of Theorem 1.5.

Proof of Theorem 1.5 We divide the proof in three steps: **1)** the non-optimality of the DDI map, **2)** the non-optimality of the other maps in the class $\{D, I\}^3$,

²It can be computed that $\varphi(r_1, r_2)$ is increasing in r_1 .

and **3)** the existence of smooth counterexample densities. In the first two steps we follow the ideas of [8, Proof of Counterexample 2.7].

Step 1) The non-optimality of the DDI map: We fix ε, M according to Lemma 3.1. Since ρ is fully supported and T is continuous, we have

$$T(x) \rightarrow s_2^- \text{ and } T^2(x) \rightarrow s_2^+ \text{ as } x \rightarrow 0,$$

and

$$T(x) \rightarrow s_1^+ \text{ and } T^2(x) \rightarrow +\infty \text{ as } x \rightarrow s_1^-.$$

This allows to choose triplets (r_1, r_2, r_3) and (ℓ_1, ℓ_2, ℓ_3) as in the hypothesis of Lemma 3.4 such that

$$(r_1, r_2, r_3) = (x, T(x), T^2(x)) \quad \text{and} \quad (\ell_1, \ell_2, \ell_3) = (y, T(y), T^2(y)).$$

Apply Lemma 3.4 to conclude that the support of the DDI map is not c -cyclically monotone.

Step 2) The non-optimality of the other maps in the class $\{D, I\}^3$ We assume that S is the DID map. The proof for the other maps of the class $\{D, I\}^3$ requires slightly different choices of intervals, but the idea is the same. It suffices to find two triples of radii $(l, S(l), S^2(l))$ and $(r, S(r), S^2(r))$ where $l, r \in [0, s_1]$ such that

$$c(l, S(l), S^2(r)) + c(r, S(r), S^2(l)) < c(l, S(l), S^2(l)) + c(r, S(r), S^2(r))$$

To this end, let us show that

$$\begin{aligned} &\text{There exist parameters } \tilde{\alpha} \in (0, s_1), \tilde{\beta} \in (s_1, s_2), \text{ and } \tilde{M} > s_2 \text{ such that} \\ &c = c_\pi \text{ on the set } (0, \tilde{\alpha}] \times [\tilde{\beta}, s_2] \times [\tilde{M}, \infty) \text{ and} \\ &\text{for all } r \in (0, \tilde{\alpha}) \text{ we have } S(r) \in [\tilde{\beta}, s_2] \text{ and } S^2(r) \in [\tilde{M}, \infty). \end{aligned} \quad (3.3)$$

Let us pick an $\alpha \in (0, s_1)$. We set $\beta = S(\alpha)$ and $M = S^2(\alpha)$. A comment: The DID map S maps the interval $(0, \alpha]$ first to the interval $[\beta, s_2]$ (by S) and then to the half-line $[M, \infty)$ (by S^2). By Lemma 4.1 in [8] we can fix a $\tilde{M} > s_2$ such that

$$c = c_\pi \text{ on the set } (0, \alpha] \times [\beta, s_2] \times [\tilde{M}, \infty).$$

If $\tilde{M} \leq M$, we can choose in (3.3) $\tilde{\alpha} = \alpha$ and $\tilde{\beta} = \beta$, and the claim follows. If $\tilde{M} > M$, we choose $\tilde{\alpha} = S(\tilde{M})$ and $\tilde{\beta} = S^2(\tilde{M})$, because now by the monotonicities of S we have that $(0, \tilde{\alpha}] \subset (0, \alpha)$ and $[\tilde{\beta}, s_2] \subset [\beta, s_2]$.

Now let us prove that the DID map is not optimal. We fix intervals $I \subset [0, s_1]$ and $J \subset [s_1, s_2]$ and a halfline $H \subset [s_2, \infty)$, given by Condition (3.3). We also fix points $r, l \in I$; without loss of generality we may assume that $l < r$. By the choice

of I , J and H we have $c = c_\pi$ on the Cartesian product $I \times J \times H$, and therefore we have

$$c(r, S(r), S^2(r)) = c_\pi(r, S(r), S^2(r)) \text{ and } c(l, S(l), S^2(l)) = c_\pi(l, S(l), S^2(l)). \quad (3.4)$$

Denoting

$$x_1 = -S(l), \quad x_2 = -S(r), \quad x_3 = l, \quad x_4 = r, \quad x_5 = S^2(r), \text{ and } x_6 = S^2(l),$$

we have six ordered points on the real line. As has been proved in [6], the optimal way of coupling these points is

$$(x_1, x_3, x_5) \text{ and } (x_2, x_4, x_6).$$

Therefore, denoting by c_{1D} the one-dimensional Coulomb cost, we have

$$c_{1D}(x_1, x_3, x_5) + c_{1D}(x_2, x_4, x_6) < c_{1D}(x_1, x_3, x_6) + c_{1D}(x_2, x_4, x_5).$$

By Condition (3.4) this is equivalent to

$$c_{1D}(x_1, x_3, x_5) + c_{1D}(x_2, x_4, x_6) < c(l, S(l), S^2(l)) + c(r, S(r), S^2(r)). \quad (3.5)$$

By our choices the points x_i we have

$$c_{1D}(x_1, x_3, x_5) = c_\pi(l, S(l), S^2(r)) \text{ and } c_{1D}(x_2, x_4, x_6) = c_\pi(r, S(r), S^2(l)).$$

Combining this with Condition (3.5) gives

$$c_\pi(l, S(l), S^2(r)) + c_\pi(r, S(r), S^2(l)) < c(l, S(l), S^2(l)) + c(r, S(r), S^2(r)). \quad (3.6)$$

The radial cost c is obviously majorized by the cost c_π for all radii, so we get

$$\begin{aligned} & c(l, S(l), S^2(r)) + c(r, S(r), S^2(l)) \\ & \leq c_\pi(l, S(l), S^2(r)) + c_\pi(r, S(r), S^2(l)) \stackrel{a)}{<} c(l, S(l), S^2(l)) + c(r, S(r), S^2(r)), \end{aligned}$$

where the inequality (a) is Condition (3.6). So all in all

$$c(l, S(l), S^2(r)) + c(r, S(r), S^2(l)) < c(l, S(l), S^2(l)) + c(r, S(r), S^2(r))$$

contradicting the c -cyclical monotonicity of the map S as we set out to prove. \square

Step 3) The existence of smooth counterexample densities: As noted in Remark 3.2, the polynomial condition (1.6) can be solved for r_3 and transformed into

$$r_3 \geq \varphi(r_1, r_2),$$

where

$$\varphi(r_1, r_2) = \frac{5r_1r_2 + r_2^2 + (r_1 + r_2)\sqrt{r_2^2 + 12r_1r_2 - 4r_1^2}}{2(r_2 - r_1)}.$$

If we study this condition on the ‘graph’ of the DDI -map

$$\mathcal{G} := \{(x, T(x), T^2(x)) \mid x \in [0, s_1]\},$$

that is, if we plug in $(r_1, r_2, r_3) = (x, T(x), T^2(x))$, we see that the main assumption (1.7) of this theorem can be written in the form:

$$T^2(x) \geq \varphi(x, T(x)) \text{ for } \rho\text{-a. e. } x \in (0, s_1).$$

This condition is satisfied whenever

$$T^2(x) = \varphi(x, T(x)) + h(x) \quad (3.7)$$

where $h : [0, s_1] \rightarrow \mathbb{R}$ is strictly positive with $h(0) = 0$. The expression (3.7) gives us an efficient way to construct counterexample densities. We can choose the densities ρ_1 and ρ_2 on the respective intervals $[0, s_1]$ and $[s_1, s_2]$ in any way we like. Then we define the tail for the measure (formally: $\rho|_{[s_2, \infty)} =: \rho_3$) by setting

$$\rho_3 = (\varphi + h)_\# \rho_1 = T_\#^2 \rho_1 \quad (3.8)$$

for a suitable ρ_1 . Above we have abbreviated $\varphi(x) = \varphi(x, T(x))$, and we will use the same abbreviation in the following. Note that once the densities ρ_1 , and ρ_2 have been chosen, the function $\varphi(x)$ is well-defined for all $x \in (0, s_1)$ because the *DDI* map T that maps the first interval to the second one is determined by the densities ρ_1 and ρ_2 .

In the beginning of this theorem, we have already assumed that the densities $\rho|_{[0, s_2]} := \rho_1 + \rho_2$ satisfy $\frac{s_1}{s_2} > \frac{1 + 2\sqrt{3}}{5}$. If we further assume that ρ_1, ρ_2 are smooth and satisfies the assumption $\frac{\rho(0)}{\rho(s_2)} > \frac{7}{2}$ (which will be motivated below), and then define the tail according to (3.7) choosing a specific h to be defined shortly, we actually get a smooth counterexample density.

First we illustrate how to generate a continuous density. We plug in the expression of φ the point $(x_1, x_2) = (x, T(x))$ and compute the derivative with respect to x . We omit the slightly tedious computations because they are not important for expressing the idea of the counterexample. At $x = 0$ the derivative reads

$$\varphi'(0) = \frac{1}{2}(5 + T'(0) + 1 + T'(0) + 8) = T'(0) + 7.$$

By choosing ρ_1, ρ_2 and h smooth, the continuity is clear everywhere except at the point s_2 . In particular, we must study the condition $\rho(s_2^-) = \rho(s_2^+)$.

Abbreviating for all $x \in (0, s_1)$ $\psi(x) = \varphi(x) + h(x)$ and using the Monge-Ampère equation for $T^2(x) = \psi(x)$ we get

$$\rho(x) = \psi'(x)\rho(\psi(x)). \quad (3.9)$$

Analogously, using Monge-Ampère for $T(x)$ we get

$$\rho(x) = -\rho(T(x))T'(x). \quad (3.10)$$

Putting $x = 0$ first of the two gives us $\rho(s_2^+)$ the second one gives us $\rho(s_2^-)$ and from the equality

$$\psi'(0)\rho(s_2^+) = -T'(0)\rho(s_2^-)$$

we get

$$h'(0) + 7 + T'(0) = -T'(0),$$

that is,

$$T'(0) = -\frac{1}{2}(h'(0) + 7). \quad (3.11)$$

Setting $x = 0$ in (3.10) gives $T'(0) = -\frac{\rho(0)}{\rho(s_2)}$, and combining this with (3.11) leads to the condition

$$\frac{\rho(0)}{\rho(s_2)} = \frac{1}{2}(h'(0) + 7),$$

that is,

$$h'(0) = 2\frac{\rho(0)}{\rho(s_2)} - 7.$$

This is the condition our auxiliary function h must satisfy to guarantee the continuity of the density ρ . As will be shown below, we will also need to assume that the first derivative of h is strictly positive, this is why the final assumption on the values $\rho(0)$ and $\rho(s_2)$ must read $\frac{\rho(0)}{\rho(s_2)} > \frac{7}{2}$ – that is, the inequality has to be strict.

About the differentiability of the counterexample densities

Let us see what the condition of ρ being differentiable at s_2 looks like, in terms of densities. The differentiability of the rest of the tail is guaranteed by the smoothness of ρ_1 , ρ_2 , and ψ .

We write the Monge-Ampere equation for ψ :

$$\psi'(x)\rho(\psi(x)) = \rho(x) \quad x \in (0, s_1).$$

We differentiate n -times both sides with respect to x :

$$\sum_{k=0}^n \binom{n}{k} \psi^{(n-k+1)}(x) \frac{d^k}{dx^k} \rho(\psi(x)) = \rho^{(n)}(x)$$

and we compute for $x = 0$

$$\sum_{k=0}^n \binom{n}{k} \psi^{(n-k+1)}(0) \left[\frac{d^k}{dx^k} \rho(\psi(x)) \right]_{x=0} = \rho^{(n)}(0).$$

Suppose that we already defined $h'(0), \dots, h^{(n)}(0)$. The only term containing $h^{(n+1)}(0)$ is obtained for $k = 0$ in the LHS, and reads $\psi^{(n+1)}(0)\rho(s_2)$. Hence we can isolate it and get

$$\psi^{(n+1)}(0)\rho(s_2) = \rho^{(n)}(0) - \sum_{k=1}^n \binom{n}{k} \psi^{(n-k+1)}(0) \left[\frac{d^k}{dx^k} \rho(\psi(x)) \right]_{x=0}.$$

Since ρ is positive everywhere, in particular $\rho(s_2) > 0$ and get a well-defined expression for $h^{(n+1)}(0)$ depending on $h'(0), \dots, h^{(n)}(0)$ (already previously defined by induction). The base step is given by $h(0) = 0$.

Now by Borel's lemma there exists a smooth function $f : \mathbb{R} \rightarrow \mathbb{R}$ such that $f^{(k)} = h^{(k)}$ for all natural numbers k . Because $h'(0) = f'(0) > 0$ and $h(0) = f(0) = 0$, there is a $\delta > 0$ and an interval $[0, \delta]$ such that $f(x) > 0$ for all $x \in [0, \delta]$. We now choose our h to coincide with f in the interval $[0, \frac{\delta}{2})$ and to be constant, equal to $f(\delta)$ on the interval $[\delta, \infty)$. On the interval $(\frac{\delta}{2}, \delta)$ we join these two parts smoothly, so that the function h is smooth on all of its domain $[0, \infty)$ – obviously at 0 we mean by smoothness the existence of all derivatives from the right. Now by using the h generated above and by defining the tail density ρ_3 according to (3.8) we get the existence of smooth counterexample densities. \square

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REFERENCES

- [1] Mathias Beiglböck, Christian Léonard, and Walter Schachermayer. A general duality theorem for the monge-kantorovich transport problem. *Studia Mathematica*, 209:151–167, 2012.
- [2] Andrea Braides et al. *Gamma-convergence for Beginners*, volume 22. Clarendon Press, 2002.
- [3] Giuseppe Buttazzo, Luigi De Pascale, and Paola Gori-Giorgi. Optimal-transport formulation of electronic density-functional theory. *Physical Review A*, 85(6):062502, 2012.
- [4] Guillaume Carlier. On a class of multidimensional optimal transportation problems. *Journal of convex analysis*, 10(2):517–530, 2003.
- [5] Guillaume Carlier, Chloé Jimenez, and Filippo Santambrogio. Optimal transportation with traffic congestion and wardrop equilibria. *SIAM Journal on Control and Optimization*, 47(3):1330–1350, 2008.
- [6] Maria Colombo, Luigi De Pascale, and Simone Di Marino. Multimarginal optimal transport maps for 1-dimensional repulsive costs. *Canad. J. Math*, 67:350–368, 2013.
- [7] Maria Colombo and Simone Di Marino. Equality between monge and kantorovich multi-marginal problems with coulomb cost. *Annali di Matematica Pura ed Applicata (1923-)*, 194(2):307–320, 2015.
- [8] Maria Colombo and Federico Stra. Counterexamples in multimarginal optimal transport with coulomb cost and spherically symmetric data. *Mathematical Models and Methods in Applied Sciences*, 26(06):1025–1049, 2016.

- [9] Codina Cotar, Gero Friesecke, and Claudia Klüppelberg. Density functional theory and optimal transportation with coulomb cost. *Communications on Pure and Applied Mathematics*, 66(4):548–599, 2013.
- [10] Gianni Dal Maso. *An introduction to Γ -convergence*, volume 8. Springer Science & Business Media, 2012.
- [11] Luigi De Pascale. Optimal transport with coulomb cost. approximation and duality. *ESAIM: Mathematical Modelling and Numerical Analysis*, 49(6):1643–1657, 2015.
- [12] Luigi De Pascale. On c-cyclical monotonicity for optimal transport problem with coulomb cost. *European Journal of Applied Mathematics*, 30(6):1210–1219, 2019.
- [13] Gero Friesecke, Christian B Mendl, Brendan Pass, Codina Cotar, and Claudia Klüppelberg. n -density representability and the optimal transport limit of the hohenberg-kohn functional. *The Journal of chemical physics*, 139(16):164109, 2013.
- [14] Wilfrid Gangbo and Andrzej Świech. Optimal maps for the multidimensional monge-kantorovich problem. *Communications on Pure and Applied Mathematics: A Journal Issued by the Courant Institute of Mathematical Sciences*, 51(1):23–45, 1998.
- [15] Nassif Ghoussoub and Bernard Maurey. Remarks on multi-marginal symmetric monge-kantorovich problems. *Discrete and Continuous Dynamical Systems - A*, 34, 2014.
- [16] Nassif Ghoussoub and Abbas Moameni. A self-dual polar factorization for vector fields. *Communications on Pure and Applied Mathematics*, 66(6):905–933, 2013.
- [17] Nassif Ghoussoub and Abbas Moameni. Symmetric monge-kantorovich problems and polar decompositions of vector fields. *Geometric and Functional Analysis*, 24(4):1129–1166, 2014.
- [18] Paola Gori-Giorgi and Michael Seidl. Density functional theory for strongly-interacting electrons: perspectives for physics and chemistry. *Physical Chemistry Chemical Physics*, 12(43):14405–14419, 2010.
- [19] Paola Gori-Giorgi, Michael Seidl, and Giovanni Vignale. Density-functional theory for strongly interacting electrons. *Physical review letters*, 103(16):166402, 2009.
- [20] Henri Heinrich. Problème de monge pour n probabilités. *Comptes Rendus Mathématique*, 334(9):793–795, 2002.
- [21] Pierre Hohenberg and Walter Kohn. Inhomogeneous electron gas. *Physical review*, 136(3B):B864, 1964.
- [22] Hans G Kellerer. Duality theorems for marginal problems. *Zeitschrift für Wahrscheinlichkeitstheorie und verwandte Gebiete*, 67(4):399–432, 1984.
- [23] Walter Kohn and Lu Jeu Sham. Self-consistent equations including exchange and correlation effects. *Physical review*, 140(4A):A1133, 1965.
- [24] Elliott H. Lieb. Density functionals for coulomb systems. In *Inequalities*, pages 269–303. Springer, 2002.
- [25] Christian B Mendl and Lin Lin. Kantorovich dual solution for strictly correlated electrons in atoms and molecules. *Physical Review B*, 87(12):125106, 2013.
- [26] Brendan Pass. Uniqueness and monge solutions in the multimarginal optimal transportation problem. *SIAM Journal on Mathematical Analysis*, 43(6):2758–2775, 2011.
- [27] Brendan Pass. On the local structure of optimal measures in the multi-marginal optimal transportation problem. *Calculus of Variations and Partial Differential Equations*, 43(3-4):529–536, 2012.
- [28] Brendan Pass. Remarks on the semi-classical hohenberg-kohn functional. *Nonlinearity*, 26(9):2731, 2013.
- [29] Svetlozar T Rachev and Ludger Rüschendorf. *Mass Transportation Problems: Volume I: Theory*, volume 1. Springer Science & Business Media, 1998.

- [30] Michael Seidl. Strong-interaction limit of density-functional theory. *Physical Review A*, 60(6):4387, 1999.
- [31] Michael Seidl, Paola Gori-Giorgi, and Andreas Savin. Strictly correlated electrons in density-functional theory: A general formulation with applications to spherical densities. *Physical Review A*, 75(4):042511, 2007.
- [32] Michael Seidl, John P Perdew, and Mel Levy. Strictly correlated electrons in density-functional theory. *Physical Review A*, 59(1):51, 1999.

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