OPTIMAL TRANSPORT WITH COULOMB COST. APPROXIMATION AND DUALITY *, **, ***

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Abstract. We revisit the duality theorem for multimarginal optimal transportation problems. In particular, we focus on the Coulomb cost. We use a discrete approximation to prove equality of the extremal values and some careful estimates of the approximating sequence to prove existence of maximizers for the dual problem (Kantorovich's potentials). Finally we observe that the same strategy can be applied to a more general class of costs and that a classical results on the topic cannot be applied here.

1. Introduction

This paper deals with the following variational problem. Let $\rho \in \mathcal{P}(\mathbb{R}^3)$ be a probability measure (ρ will be called electronic density) and let

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

be the Coulomb cost. Consider the set $\Pi(\rho) = \{P \in \mathcal{P}(\mathbb{R}^{3N}) \mid \pi^i_\sharp P = \rho\}$, where π^i denotes the projection on the ith copy of $\mathbb{R}^3$ and $\pi^i_\sharp P$ is the push-forward measure. We aim to minimize

$$\min_{\Pi(\rho)} \int_{\mathbb{R}^{Nd}} c(x_1, \ldots, x_N) \mathrm{d}P(x_1, \ldots, x_N). \tag{1.1}$$

This problem fits in the general framework of multimarginal optimal transportation problems. In particular it is the multimarginal optimal transportation problem with all the N marginals coinciding with ρ and with Coulomb cost.

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In contrast with the classical two-marginal optimal transportation problems, the theory of multimarginal optimal transportation problems is still at the beginning and many relevant open problems need to be studied. Some general results are available in [4, 17, 21–23], results for special costs are available, for example in [11] for the quadratic cost with some generalization in [15], and in [5] for the determinant. Some new applications are emerging for example in [12].

In the particular case of the Coulomb cost there are also many other questions related to the applications. Recent results on the topic are contained in [3, 6–8, 10] and some of them will be described better in subsequent sections.

The literature quoted so far is not at all exaustive and we refer the reader to the bibliographies of the cited papers for a more detailed picture. However, in the author's opinion, at the moment the wealth of problems obscures the body of known results. In this paper we will focus on the Kantorovich duality for problem (1.1). We denote by ρ^N the product measure $\underbrace{\rho \otimes \ldots \otimes \rho}_{N-times}$. We will prove that

$$\min_{\Pi(\rho)} \int_{\mathbb{R}^{Nd}} c(x_1, \ldots, x_N) \mathrm{d}P(x_1, \ldots, x_N)$$

$$= \sup \left\{ N \int u \mathrm{d}\rho \ : \ u \in L^1_\rho, u(x_1) + \ldots + u(x_N) \leq c(x_1, \ldots, x_N), \ \rho^N - \text{a.e.} \right\} \quad (1.2)$$

and that the right-hand side of (1.2) admits a maximizer which is, in particular, bounded. Thanks to the symmetries of the problem we also have that the right-hand side of (1.2) coincide with

$$\sup \left\{ \sum_{i=1}^N \int u_i \mathrm{d}\rho \ : \ u_i \in L^1_\rho, \ u_1(x_1) + \ldots + u_N(x_N) \leq c(x_1, \ldots, x_N), \ \rho^N - \text{a.e.} \right\}.$$

Infact, this last sup is *a priori* bigger then (1.2). Since for any admissible N-tuple $(u_1, \ldots, u_N)$ the function $u(x) = \frac{1}{N} \sum_{i=1}^N u_i(x)$ is admissible for the previous problem, equality holds.

Some of the basic ideas originated in the paper [17]. However, in Remark 3.14, we will show that Theorem 2.21 of [17] does not apply to the Coulomb cost in order to prove that a maximizer of the dual problem exists. The tools will be Γ-convergence and some careful estimates of the maximizers of the approximating problems.

We remark that a necessary but not sufficient *assumption* for (1.1) to be finite is that ρ is not concentrated on a set of cardinality $\leq N - 1$. We will assume this whenever needed.

We will adopt the notations $\mathbf{x} = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}$ so that $x_i \in \mathbb{R}^3$ for each $i \in \{1, \ldots, N\}$. And $\rho - \inf$ will denote both the essential ρ infimum or the essential ρ^{N-1} infimum depending on the number of variables involved.

1.1. Motivations

The main object in the quantum mechanical modeling of a particle with N electrons is a wave-function ψ, *i.e.* an element of

$$\mathcal{A} := \left\{ \psi \in H^1((\mathbb{R}^3 \times \mathbb{Z}_2)^N, \mathbb{C}) \ : \ \|\psi\|_{L^2} = 1 \right\}.$$

The space $(\mathbb{R}^3 \times \mathbb{Z}_2)^N$ is the configuration space for the N electrons. In fact, the state of each electron is individuated by the position in $\mathbb{R}^3$ and the spin in $\mathbb{Z}_2$. While it is easy to understand the interpretation of the position variable, the notion of spin is slightly more difficult to grasp. We may roughly explain it as follows: when a magnetic field is applied to the electron of position x_0 velocity v_0, the electron may be deflected in two different ways which are characterized by the two possible spins. The name is then reminiscent of the behavior of a spinning top which hits a wall with a certain translational velocity in a point p_0 and may rebound in two

different directions depending on the whirling direction. However this analogy, although suggestive, is not the historical one nor can be considered physically meaningful.

It is easy, once we free ourself from this last analogy, to imagine the possibility of a spin variable with values in $\mathbb{Z}_k$ or other spaces.

The quantity

$$|\psi((x_1, \alpha_1), \ldots, (x_N, \alpha_N))|^2$$

represents the probability that the N electrons occupy the state $((x_1, \alpha_1), \ldots, (x_N, \alpha_N))$ and then, since the electrons are indistinguishable ψ satisfies

$$|\psi((x_{\sigma(1)}, \alpha_{\sigma(1)}), \ldots, (x_{\sigma(N)}, \alpha_{\sigma(N)}))|^2 = |\psi((x_1, \alpha_1), \ldots, (x_N, \alpha_N))|^2$$

for all permutations σ of the N electrons. This brings to introduce the distinction between Fermionic and Bosonic particles, however such distinction will not have relevance here since we will discuss duality for a relaxed problem. The distinction may be instead relevant when discussing the relaxation process. A particle is *Fermionic* if

$$\psi((x_{\sigma(1)}, \alpha_{\sigma(1)}), \ldots, (x_{\sigma(N)}, \alpha_{\sigma(N)})) = \mathrm{sgn}(\sigma)\psi((x_1, \alpha_1), \ldots, (x_N, \alpha_N)),$$

and *Bosonic* if

$$\psi((x_{\sigma(1)}, \alpha_{\sigma(1)}), \ldots, (x_{\sigma(N)}, \alpha_{\sigma(N)})) = \psi((x_1, \alpha_1), \ldots, (x_N, \alpha_N)).$$

Since the spin will not play any role in the rest of the paper we will consider wave-functions depending only on the positions of the electrons. Including the dependence on the spin is just a matter of adding a summation over the two possible values in the formulas (below we give an example in the case of kinetic energy). In the simplest situation the electrons move with a certain velocity while interacting with the nuclei (or, equivalently, with an external potential) and with each other. The interaction with the nuclei and the interaction between electrons are of Coulombian nature. So if we assume that there are M nuclei with charge Z_i and position R_i the interaction potential in the position x will be $v(x) = -\sum_{i=1}^{M} \dfrac{Z_i}{|x - R_i|}$. Then the energy of a particular state of the particle is made of three parts:

the *Kinetic energy*[2]

$$T[\psi] = \frac{1}{2} \int_{\mathbb{R}^{3N}} |\nabla \psi(x_1), \ldots, x_N)|^2 \mathrm{d}x_1 \ldots \mathrm{d}x_N,$$

the *electron-nuclei* interaction energy

$$V_{ne}[\psi] = \sum_{i=1}^{N} \int_{\mathbb{R}^{3N}} v(x_i)|\psi(x_1, \ldots x_N)|^2 \mathrm{d}x_1 \ldots \mathrm{d}x_N,$$

the *electron-electron* interaction energy

$$V_{ee}[\psi] = \sum_{1 \leq i < j \leq N} \int_{\mathbb{R}^{3N}} \frac{1}{|x_i - x_j|}|\psi(x_1, \ldots, x_N)|^2 \mathrm{d}x_1 \ldots \mathrm{d}x_N.$$

A relevant quantity in quantum mechanics, quantum chemistry and other disciplines is the ground state energy of an atom

$$E_0 = \min_{\psi \in \mathcal{A}} T[\psi] + V_{ee}[\psi] + V_{ne}[\psi].$$

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[2]If we want to include the "spin coordinate" in the state of the particle then

$$T[\psi] = \sum_{\alpha_1, \ldots, \alpha_n = 0}^{1} \frac{1}{2} \int_{\mathbb{R}^{3N}} |\nabla \psi((x_1, \alpha_1), \ldots, (x_N, \alpha_N))|^2 \mathrm{d}x_1 \ldots \mathrm{d}x_N.$$

Remark 1.1. The special form of the electron-nuclei interaction is widely irrelevant in the expression of V_{ee} above. So one could just include a term of the same form with an external potential v.

In order to compute (numerically) E_0 one needs to solve the Schrödinger equation in $3N$ dimensions and this is very costly even for a small number of electrons. A less costly alternative is represented by the *Density-Functional Theory* introduced first by Hohenberg and Kohn in [16] and then Kohn and Sham in [18]. At the beginning of the theory the mathematical foundations of DFT were very weak. The paper which started to put DFT on solid mathematical foundations is, to my knowledge, [19].

The main object in DFT is the electronic density ρ which is obtained by integrating out $N - 1$ particles

$$\rho(x) = \int_{\mathbb{R}^{3(N-1)}} |\psi(x, x_2, \ldots, x_N)|^2 \mathrm{d}x_2 \ldots \mathrm{d}x_N$$

and it represents the probability distribution of a single electron. The relation between ψ and ρ will be denoted by $\psi \downarrow \rho$. In particular ρ is always a probability density on $\mathbb{R}^3$ independently of the number of electrons. The basic idea of DFT is to express everything in term of the electronic density ρ instead of the wave function ψ. It is easy to express the *electron-nuclei* interaction energy in terms of ρ. We have

$$V_{ne}[\psi] = N \int_{\mathbb{R}^3} v(x)\mathrm{d}\rho(x).$$

Then, following Hohenberg and Kohn, we write

$$E_0 = \min_{\rho} \left\{ F_{HK}(\rho) + N \int_{\mathbb{R}^3} v(x)\mathrm{d}\rho(x) \right\} \tag{1.3}$$

where

$$F_{HK}(\rho) = \min_{\psi \downarrow \rho} \left\{ T[\psi] + V_{ee}[\psi] \right\},$$

is called the universal Hohenberg−Kohn functional (*universal* since it does not depends on the specific particle). At the beginning of the DFT several mathematical questions needed to be settled in order to have a meaningful mathematical theory. For example: which is the correct minimization domain? Does the functional F_{HK} enjoy some properties which make the variational problem amenable? And so on. As we said, Lieb in [19] started to look at these questions. In particular, Lieb described the set of admissible ρ

$$H = \left\{ \rho \mid 0 \le \rho, \ \int \rho = 1, \ \sqrt{\rho} \in H^1(\mathbb{R}^3) \right\}.$$

Writing explicitly F_{HK} is not possible, then Kohn and Sham considered

$$F_{KS}(\rho) = \min_{\psi \downarrow \rho} \{T[\psi]\}.$$

In the Bosonic case it is possible to express

$$F_{KS}(\rho) = N \int |\nabla \sqrt{\rho}|^2 \mathrm{d}x.$$

In the fermionic case

$$\int |\nabla \sqrt{\rho}|^2 \mathrm{d}x \le \frac{1}{N} F_{KS}(\rho) \le (4\pi)^2 N^2 \int |\nabla \sqrt{\rho}|^2 \mathrm{d}x$$

(But the optimal constant in the inequality above, to my knowledge is still not known). Then one may rewrite

$$F_{HK} = F_{KS} + F_{xc}$$

where F_{xc} is called *exchange-correlation energy* it needs to be determined or at least approximated and it is the term which keeps into account the interaction between electrons.

Let us denote by $\mathfrak{C}(\rho)$ the minimal value in (1.1). Since for every $\psi \downarrow \rho$ the measure $|\psi|^2 \mathrm{d}x_1 \ldots \mathrm{d}x_N \in \Pi(\rho)$ we have

$$\mathfrak{C}(\rho) \leq V_{ee}[\psi].$$

The functional $\mathfrak{C}(\rho)$ appear in DFT in several ways. The first and perhaps the most elementary appearance is in the estimate from below

$$F_{KS}(\rho) + \mathfrak{C}(\rho) \leq F_{HK}(\rho).$$

This estimate is useful in the variational study of DFT and is is also the basis for the so called KS-SCE DFT (Kohn and Sham, Strictly Correlated Electrons Density-Functional Theory) in which $\mathfrak{C}(\rho)$ is interpreted as an approximation of F_{xc} for particles in which the *electron-electron* interaction is relevant. This is a very rapidly developing domain started in [24] (see also [14, 25, 26] but we are far from being exhaustive).

Again $\mathfrak{C}(\rho)$ appear when considering the SCE-DFT (Strictly Correlated Electrons-Density-Functional Theory), which is the analogous of DFT in a regime in which the *electron-electron* interaction is preponderant. This means writing

$$F_{HK} = \mathfrak{C} + F_{kd},$$

where F_{kd} is called *kinetic-decorrelation energy*, it needs to be determined and it is the term which keeps into account the kinetic energy of the particle (see, for example, [13, 14]).

The third appearance is given in [8] where the authors proved that $\mathfrak{C}$ is the semiclassical limit of the DFT in the case of a two electrons particle. It is not clear if this last result also holds for more than two electrons.

Finally we quote a direct application of the duality theorem we are considering. In the numerical approximations of all the problems above one need to compute $\mathfrak{C}(\rho)$. Before the link with Optimal Transport problems was discovered this approximation was done by computing the co-motion functions which are the analogue of the optimal transport maps. However, more recently, Mendl and Lin in [20] introduced a numerical method which use the Kantorovich potential to compute the value.

2. PRELIMINARY RESULTS AND TOOLS

2.1. Definition of Γ-convergence and basic results

A crucial tool that we will use throughout this paper is Γ-convergence. All the details can be found, for instance, in Braides's book [2] or in the classical book by Dal Maso [9]. In what follows, (X, d) is a metric space or a topological space equipped with a convergence.

Definition 2.1. Let $(F_n)_n$ be a sequence of functions $X \mapsto \bar{\mathbb{R}}$. We say that $(F_n)_n$ Γ-converges to F and we write $F_n \xrightarrow[n]{\Gamma} F$ if for any $x \in X$ we have

- for any sequence $(x_n)_n$ of X converging to x

$$\liminf_n F_n(x_n) \geq F(x) \qquad (\Gamma\text{-liminf inequality});$$

- there exists a sequence $(x_n)_n$ converging to x and such that

$$\limsup_n F_n(x_n) \leq F(x) \qquad (\Gamma\text{-limsup inequality}).$$

This definition is actually equivalent to the following equalities for any $x \in X$:

$$F(x) = \inf \left\{ \liminf_n F_n(x_n) : x_n \to x \right\} = \inf \left\{ \limsup_n F_n(x_n) : x_n \to x \right\}$$

The function $x \mapsto \inf\{\liminf_n F_n(x_n) : x_n \to x\}$ is called Γ-liminf of the sequence $(F_n)_n$ and the other one its Γ-limsup. A useful result is the following (which for instance implies that a constant sequence of functions does not Γ-converge to itself in general).

Proposition 2.2. *The Γ-liminf and the Γ-limsup of a sequence of functions $(F_n)_n$ are both lower semicontinuous on X.*

The main interest of Γ-convergence resides in its consequences in terms of convergence of minima:

Theorem 2.3. *Let $(F_n)_n$ be a sequence of functions $X \to \bar{\mathbb{R}}$ and assume that $F_n \xrightarrow[n]{\Gamma} F$. Assume moreover that there exists a compact and non-empty subset K of X such that*

$$\forall n \in N, \; \inf_X F_n = \inf_K F_n$$

(we say that $(F_n)_n$ is equi-mildly coercive on X). Then F admits a minimum on X and the sequence $(\inf_X F_n)_n$ converges to $\min F$. Moreover, if $(x_n)_n$ is a sequence of X such that

$$\lim_n F_n(x_n) = \lim_n (\inf_X F_n)$$

and if $(x_{\phi(n)})_n$ is a subsequence of $(x_n)_n$ having a limit x, then $F(x) = \inf_X F$.

Since we will deal also with dual problems we need the analogue of Γ-convergence for maxima, which is sometimes called Γ^+-convergence.

Definition 2.4. Let $(F_n)_n$ be a sequence of functions $X \mapsto \bar{\mathbb{R}}$. We say that $(F_n)_n$ Γ^+-converges to F, and we write $F_n \xrightarrow[n]{\Gamma^+} F$ if for any $x \in X$ we have

- for any sequence $(x_n)_n$ of X converging to x

$$\limsup_n F_n(x_n) \leq F(x) \qquad (\Gamma^+\text{-limsup inequality});$$

- there exists a sequence $(x_n)_n$ converging to x and such that

$$\liminf_n F_n(x_n) \geq F(x) \qquad (\Gamma^+\text{-liminf inequality}).$$

The natural generalizations of Proposition 2.2 and Theorem 2.3 hold with upper semicontinuity, maximum values and maximum points replacing lower semicontinuity, minimum values and minimum points.

2.2. Permutation invariant costs

The Coulomb cost c as well as the approximations that we will consider are permutation invariant in the sense that

$$c(x_{\sigma(1)}, \dots, x_{\sigma(N)}) = c(x_1, \dots, x_N), \quad \forall \sigma \in \mathcal{S}^N.$$

Several simplifications are permitted by this invariance.

3. DUALITY

Denote by

$$\chi_K(x) = \begin{cases} 1 \text{ if } x \in K, \\ 0 \text{ otherwise.} \end{cases}$$

Introduce the set of *elementary* functions

$$\mathcal{E}(\mathbb{R}^{3N}) = \left\{ \varphi : \mathbb{R}^{3N} \to \mathbb{R} \text{ measurable } : \varphi(x) = \sum_{i=1}^{k} a_i \chi_{A_i^1 \times \ldots \times A_i^N} \right\}$$

for suitables constants a_i and Borel sets $A_k^i \subset \mathbb{R}^3$. We consider the following approximation of c.

Proposition 3.1. *There exists a sequence of costs c_n such that*

(1) $0 \leq c_n \leq c$;
(2) $c_n \in \mathcal{E}(\mathbb{R}^{3N})$;
(3) $c_n \nearrow c$;
(4) c_n *is l.s.c.;*
(5) c_n *is permutation invariant.*

Proof. Let $(a_1, \ldots, a_N) \in \mathbb{Z}^{3N}$ and define $a - 1 := (k - 1, p - 1, q - 1)$ for $a = (k, p, q) \in \mathbb{Z}^3$ and (with a slight abuse of notations) $(x, y) := (x_1, y_1) \times (x_2, y_2) \times (x_3, y_3)$ for $x, y \in \mathbb{R}^3$. Then $\forall n \in \mathbb{N}$ define the interior of the diadyc cube by

$$Q^n(a_1, \ldots, a_N) = \left(\frac{a_1 - 1}{2^n}, \frac{a_1}{2^n} \right) \times \ldots \times \left(\frac{a_N - 1}{2^n}, \frac{a_N}{2^n} \right).$$

and for all positives R

$$\mathbf{Q}(R) = \underbrace{[-R, R] \times \ldots \times [-R, R]}_{3N-\text{times}}.$$

Define c_n as follows

$$c_n(\mathbf{x}) = \begin{cases} \inf_{Q^n(a_1, \ldots, a_N)} c(\mathbf{x}) \text{ if } \mathbf{x} \in Q^n(a_1, \ldots, a_N) \text{ and } Q^n(a_1, \ldots, a_N) \subset \mathbf{Q}(n), \\ 0 \qquad\qquad\qquad \text{if } \mathbf{x} \notin \mathbf{Q}(n). \end{cases}$$

Then extend c_n to the entire space by relaxation *i.e.*

$$c_n(\mathbf{x}) = \inf \left\{ \liminf_{k \to \infty} c(\mathbf{x}^k) : \lim_{k \to \infty} \mathbf{x}^k = \mathbf{x}, \quad \text{and} \quad \forall k, \mathbf{x}^k \in Q^n(a_1, \ldots, a_N) \quad \text{for some} \quad (a_1, \ldots, a_N) \in \mathbb{Z}^{3N} \right\}.$$

With this definition properties (1), (3) and (4) above are straightforward. To prove (2) it is enough to remark that c_n is constant on i dimensional, relatively open faces of $Q^n(a_1, \ldots, a_N)$ and that such faces are products of intervals (which may degenerate to a point). Finally (5) holds since

$$\inf_{Q^n(a_1, \ldots, a_N)} c = \inf_{Q^n(a_{\sigma(1)}, \ldots, a_{\sigma(N)})} c$$

for every $\sigma \in \mathcal{S}^N$. □

Remark 3.2. Without loss of generality we can write

$$c_n(\mathbf{x}) = \sum_{i=1}^{k_n} a_i \chi_{A_i^1}(x_1) \ldots \chi_{A_i^N}(x_N)$$

with sets A_i^k such that if $A_i^k \cap A_j^k \neq \emptyset$ then $A_i^k = A_j^k$, for all $k \in \{1, \ldots, N\}$.

Define $K(c_n, \cdot) : \mathcal{P}(\mathbb{R}^{3N}) \to [0, +\infty]$ as

$$K(c_n, P) = \begin{cases} \displaystyle\int c_n dP \text{ if } P \in \Pi(\rho), \\ +\infty \qquad \text{otherwise}, \end{cases}$$

and $D(c_n, \cdot) : L_\rho^1 \to \overline{\mathbb{R}}$ as

$$D(c_n, v) = \begin{cases} N \displaystyle\int v \mathrm{d}\rho \text{ if } v(x_1) + \ldots + v(x_N) \leq c_n(x_1, \ldots, x_N), \ \rho^N - \text{a.e.} \\ -\infty \qquad \text{otherwise}. \end{cases}$$

Also in this case, maximizing $D(c_n, v)$ is equivalent to maximize

$$\begin{cases} \displaystyle\sum_{i=1}^{N} \int v_i \mathrm{d}\rho \text{ if } v_1(x_1) + \ldots + v_N(x_N) \leq c_n(x_1, \ldots, x_N), \ \rho^N - \text{a.e.} \\ -\infty \qquad \text{otherwise}. \end{cases}$$

Proposition 3.3. *The functionals $K(c_n, \cdot)$ are equicoercive and*

$$K(c_n, \cdot) \xrightarrow{\Gamma} K(c, \cdot),$$

with respect to the w^*-convergence of measures.

Proof. Equicoercivity follows from the fact that $\Pi(\rho)$ is w^*-compact. Since $K(c_n, \grave{)}$ is non-decreasing (in n) and $K(c, \cdot)$ is l.s.c., Γ-convergence is a standard fact. We report the proof for the sake of completeness. Let $P_n \xrightarrow{*} P$ and fix $m \in \mathbb{N}$. For $m < n$

$$K(c_m, P_n) \leq K(c_n, P_n).$$

Since c_m is lower semi-continuous

$$K(c_m, P) \leq \liminf_{n \to \infty} K(c_m, P_n) \leq \liminf_{n \to \infty} K(c_n, P_n).$$

And since $K(c_m, P) \to K(c, P)$ we obtain

$$K(c, P) \leq \liminf_{n \to \infty} K(c_n, P_n).$$

For what concerns the Γ-lim sup inequality, since $c_n \nearrow c$ it is enough to consider $P_n = P$ for all $n \in \mathbb{N}$ and to apply the Monotone Convergence Theorem. $\qquad\square$

Lemma 3.4. *Assume that ρ is not concentrated on a set of cardinality $\leq N - 1$. If $u \in L_\rho^1$ and*

$$u(x_1) + \ldots + u(x_N) \leq c(x_1, \ldots, x_N), \qquad \rho^N - \text{a.e.},$$

then there exists $k \in \mathbb{R}$ such that $u \leq k$ ρ-a.e.

Proof. We have

$$u(x) \leq \rho - \inf_{x_2, \ldots, x_N} \{c(x, x_2, \ldots, x_N) - u(x_2) - \ldots - u(x_N)\}, \quad \rho - a.e.$$

Since $u \in L_\rho^1$ and ρ has not $\leq N - 1$ atoms, we may consider $\underline{x}_1, \ldots, \underline{x}_N$ with $\underline{x}_i \neq \underline{x}_j$ if $i \neq j$ such that $u(\underline{x}_i) \in \mathbb{R}$. We denote $l = \min\{u(\underline{x}_1), \ldots, u(\underline{x}_N)\}$. Consider $0 < r$ such that $B(\underline{x}_i, r) \cap B(\underline{x}_j, r) = \emptyset$ if $i \neq j$. Then any $x \in \mathbb{R}^3$ can belong to $B(\underline{x}_i, r)$ for at most one i. We may suppose without loss of generality that $i = 1$. It follows that

$$u(x) \leq c(x, \underline{x}_2, \ldots, \underline{x}_N) - u(\underline{x}_2) - \ldots - u(\underline{x}_N) \leq \frac{N(N-1)}{2}\frac{1}{r} - Nl := k. \qquad\square$$

Remark 3.5. In the previous proof k clearly depends on u through the constant l and on ρ through the constant r.

Proposition 3.6. *The functionals*

$$D(c_n, \cdot) \xrightarrow{\Gamma^+} D(c, \cdot),$$

with respect to the weak-L^1 convergence.

Proof. We start with the Γ^+-$\liminf$ inequality. Let $u \in L_\rho^1$ such that $-\infty < D(c, u)$ then

$$u(x_1) + \ldots + u(x_N) \le c(x_1, \ldots, x_N), \quad \rho^N - \text{a.e.}$$

and by Lemma 3.4 u is bounded above. For an arbitrary $0 < \varepsilon$ there holds

$$D(c, u) - \varepsilon < N \int_{\mathbb{R}^3} u \mathrm{d}\rho.$$

Moreover by Lusin's theorem there exists $K \subset \mathbb{R}^3$ compact such that $u_{|K}$ is continuous, $\rho(\mathbb{R}^3 \setminus K) < \varepsilon$ and

$$D(c, u) - \varepsilon < N \int_K u \mathrm{d}\rho.$$

Since $c_n \nearrow c$ and are l.s.c we may apply a Dini's type theorem and we obtain that there exists n_0 such that if $n_0 < n$ then

$$u(x_1) + \ldots + u(x_N) - \varepsilon < c_n(x_1, \ldots, x_N), \quad \rho^N - \text{a.e.} \tag{3.1}$$

on $K \times \ldots \times K$. We consider

$$\overline{u}(x) := u(x) - \frac{\varepsilon}{N} - N(\sup u)\chi_{\mathbb{R}^3 \setminus K}(x).$$

Since $0 \le c_n$ and (3.1) holds we have, for $n_0 < n$,

$$\overline{u}(x_1) + \ldots + \overline{u}(x_N) \le c_n(x_1, \ldots, x_N), \quad \rho^N - \text{a.e.}$$

Moreover if $M \in \mathbb{N}$ and $N^2 \sup u < M$ then

$$D(c, u) - (2 + M)\varepsilon < N \int_{\mathbb{R}^3} u \mathrm{d}\rho - \varepsilon - N^2 \varepsilon \sup u \le N \int_{\mathbb{R}^3} u \mathrm{d}\rho - \varepsilon - N^2 \rho(\mathbb{R}^3 \setminus K) \sup u = N \int_{\mathbb{R}^3} \overline{u} \mathrm{d}\rho. \tag{3.2}$$

For what concernes the Γ^+-$\limsup$ inequality assume that $u_n \rightharpoonup u$ in L_ρ^1 and assume without loss of generality that

$$u_n(x_1) + \ldots + u_n(x_N) \le c_n(x_1, \ldots, x_N), \quad \rho^N - \text{a.e.}$$

Then

$$u_n(x_1) + \ldots + u_n(x_N) \le c(x_1, \ldots, x_N)$$

and

$$\lim_{n \to \infty} N \int u_n \mathrm{d}\rho = N \int u \mathrm{d}\rho. \qquad \square$$

In the next subsection we will prove the needed compactness property.

3.1. Estimates of the approximating Kantorovich potentials and conclusions

Lemma 3.7. *For all $n \in \mathbb{N}$*

$$\max D(c_n, \cdot) = \min K(c_n, \cdot). \tag{3.3}$$

Moreover $D(c_n, \cdot)$ admits a maximizer $(u_1^n, \ldots, u_N^n)$

Proof. The proof is revisited from [17].

Since we have written $c_n(\mathbf{x}) = \sum_{i=1}^{k_n} a_i \chi_{A_i^1}(x_1) \ldots \chi_{A_i^N}(x_N)$ we may find sets $X_1, \ldots, X_N$ each of $k_n + 1$ elements,

$$\varphi_i : \mathbb{R}^3 \to X_i$$

and

$$\tilde{c}_n : X_1 \times \ldots \times X_N \to \mathbb{R}$$

such that

$$c_n(\mathbf{x}) = \tilde{c}_n(\varphi_1(x_1), \ldots, \varphi_N(x_N)).$$

If we define $\varphi : \mathbb{R}^{3N} \to X_1 \times \ldots \times X_N$ by $\varphi = \otimes_{i=1}^N \varphi_i$ and $\rho_i = \varphi_i \sharp \rho \in \mathcal{P}(X_i)$, then we have that for all $\gamma \in \Pi(\rho)$ we may consider $\tilde{\gamma} := \varphi_\sharp \gamma \in \Pi(\rho_1, \ldots, \rho_N)$ and

$$\int_{\mathbb{R}^{3N}} c_n \mathrm{d}\gamma = \int_{\mathbb{R}^{3N}} \tilde{c}_n(\varphi(\mathbf{x})) \mathrm{d}\gamma = \int_{X_1 \times \ldots \times X_N} \tilde{c}_n \mathrm{d}\tilde{\gamma}.$$

We remark that since $\tilde{c}_n$ and $\tilde{\gamma}_n$ may be identified with elements of $\mathbb{R}^{k_n+1} \times \cdots \times \mathbb{R}^{k_n+1}$ and ρ_i with an element of $\mathbb{R}^{k_n+1}$, the problem may be reformulated as follows:

$$\begin{cases} \min \tilde{c} \cdot \tilde{\gamma}, \\ P_i \tilde{\gamma} = \rho_i, \\ 0 \le \tilde{\gamma}, \end{cases} \tag{3.4}$$

where the P_i form the projection matrix. Thus the problem is a linear programming problem whose minimum value coincides with the maximum value of the dual problem

$$\begin{cases} \max \tilde{\rho}^T \cdot \tilde{u}, \\ P^T \tilde{u} \le \tilde{c}^T. \end{cases} \tag{3.5}$$

It remains to identify $\tilde{u}$ with a N-tuple $(u_1, \ldots, u_N)$ of *elementary* functions in $\mathcal{E}(\mathbb{R}^{3N})$ which maximises

$$\max \left\{ \sum_{i=1}^N \int u_i \mathrm{d}\rho \ : \ u_i \in L_\rho^1, \ u_1(x_1) + \ldots + u_N(x_N) \le c_n(x_1, \ldots, x_N) \right\}. \tag{3.6}$$

$\square$

We now prove a first property of minimiser P of $K(c, \cdot)$. This requires additional assumptions on ρ.

Since the pointwise transportation cost diverges when two (3-dimensional) coordinates get too close it is useful to introduce the following notations:

$$D_\alpha := \{\mathbf{x} = (x_1, \ldots, x_N) \ : \ |x_i - x_j| \le \alpha \text{ for some } i, j\},$$

will be the closed strip around the diagonals,

$$G := \{\mathbf{x} = (x_1, \ldots, x_N) \ : \ x_i \ne x_j \text{ if } i \ne j\}.$$

For simplicity we pose $D_0 = D$. Then $G = \mathbb{R}^{3N} \setminus D$. Finally we introduce a notation for a "cube" with rounds 3-dimensional faces

$$Q(\mathbf{x}, r) := \{\mathbf{y} = (y_1, \ldots, y_N) \; : \; \max_i |y_i - x_i| < r\},$$

we will omit the center $\mathbf{x}$ when it is the origin.

Proposition 3.8. *Assume that ρ does not have atoms. Let $P \in \Pi(\rho)$ be a minimizer. Then, for all $r > 0$ there exists $\alpha(r)$ such that*

$$P\left(D_{\alpha(r)} \cap Q(r)\right) = 0$$

We first prove an elementary lemma

Lemma 3.9. *Assume that ρ does not have atoms. Let $P \in \Pi(\rho)$ be a plan with finite cost and let $\mathbf{x} \in sptP$. Then there exist $\mathbf{x}^2, \ldots, \mathbf{x}^N \in sptP$ such that*

(1) $\mathbf{x}^2, \ldots, \mathbf{x}^N \in G$;
(2) $x_j^i \neq x_\sigma^k$ *if $k \neq i$ or $\sigma \neq j$.*

Proof. First remark that if P has finite cost then $P(D) = 0$ and then P-a.a. points belong to G. Then fix a vector $\overline{a} \in \mathbb{R}^3$ and consider the set $X_{\overline{a}}^i = \{\mathbf{x} \in \mathbb{R}^{3N} \; : \; x_i = \overline{a}\}$. By definition of marginals and since ρ does not have atoms

$$P(X_{\overline{a}}^i) = \rho\left(\{\overline{a}\}\right) = 0.$$

Then, starting from $\mathbf{x}^1 = \mathbf{x}$ we may choose

$$\mathbf{x}^j \in sptP \setminus \left(D \cup \left(\cup_{k<j} \cup_{\substack{i=1,\ldots,N \\ \sigma=1,\ldots,N}} X_{x_\sigma^k}^i\right)\right). \qquad \square$$

Proof of Proposition 3.8. Assume that $\mathbf{x}^1 = (x_1^1, \ldots, x_N^1) \in D \cap sptP$ and choose points $\mathbf{x}^2, \ldots, \mathbf{x}^N$ in $sptP$ as in Lemma 3.9. For all choices of positive radii $r_1 \ldots, r_N$

$$P(Q(\mathbf{x}^i, r_i)) > 0.$$

And later on we will choose suitable r_i's. Denote by $P_i = P_{|Q(x^i, r_i)}$ and choose constants $\lambda_i \in (0, 1]$ such that

$$\lambda_1 |P_1| = \ldots = \lambda_N |P_N|.$$

We then write

$$P = \lambda_1 P_1 + \ldots + \lambda_N P_N + P_R \quad (P_R \text{ is the remainder}).$$

We estimate from below the cost of P as follows

$$C(P) = C(P_R) + \sum_{i=1}^{N} \lambda_i C(P_i) \geq C(P_R) + \sum_{i=1}^{N} \lambda_i \left(\sum_{k=1}^{N} \sum_{k<j} \frac{1}{|x_k^i - x_j^i| + 2r_i}\right) |P_i|.$$

Consider now the marginals $\nu_1^i, \ldots, \nu_N^i$ of $\lambda_i P_i$ and build the new local plans

$$\tilde{P}_1 = \nu_1^1 \times \nu_2^2 \times \ldots \nu_N^N, \; \tilde{P}_2 = \nu_1^2 \times \nu_2^3 \times \ldots \nu_N^1, \ldots \tilde{P}_N = \nu_1^N \times \nu_2^1 \times \ldots \nu_N^{N-1}.$$

To write the estimates from below it is convenient to remark that we may also write: $\tilde{P}_i = \nu_1^i \times \ldots \nu_k^{i+k-1} \times \ldots \nu_N^{i+N-1}$ where we consider the upper index (mod N). Then consider the new transport plan

$$\tilde{P} := P_R + \tilde{P}_1 + \ldots + \tilde{P}_N.$$

It is straightforward to check that the marginals of $\tilde{P}$ are the same as the marginals of P. Moreover $|\tilde{P}_i| = \lambda_i |P_i|$. So we can estimate the cost of $\tilde{P}$ from above.

$$C(\tilde{P}) = C(P_R) + \sum_{i=1}^{N} C(\tilde{P}_i) \leq C(P_R) + \sum_{i=1}^{N} \left(\sum_{k=1}^{N} \sum_{k<j} \frac{1}{|x_{k+i-1}^k - x_{j+i-1}^j| - r_k - r_j} \right) |\tilde{P}_i|.$$

The final step is to choose r_i for $i = 1, \ldots, N$ so that the 3-dimensional faces of the cubes $Q(\mathbf{x}^i, r_i)$ do not overlap and

$$\sum_{i=1}^{N} \left(\sum_{k=1}^{N} \sum_{k<j} \frac{1}{|x_{k+i-1}^k - x_{j+i-1}^j| - r_k - r_j} \right) < \sum_{i=1}^{N} \left(\sum_{k=1}^{N} \sum_{k<j} \frac{1}{|x_k^i - x_j^i| + 2r_i} \right).$$

This final condition contradicts the minimality of P and it is feasible because, since $x_i^1 = x_j^1$ for some i and j the right hand side is unbounded for $r_1 \to 0$ while the left hand side is bounded above for r_i sufficiently small.

It follows that the diagonal D and the $sptP$ do not intersect and since both sets are compact inside $\overline{Q(r)}$, they must have positive distance in $Q(r)$ □

Let P_n denote a sequence of minimisers of $K(c_n, \cdot)$ converging to a minimiser P of $K(c, \cdot)$. We choose $0 < \mathcal{R}$ such that $P(Q(\mathcal{R})) = M > 0$ and we consider $\alpha(\mathcal{R})$ according to Proposition 3.8 above. Since $Q(\mathcal{R})$ is open we have,

$$\liminf_{n \to \infty} P_n(Q(\mathcal{R})) \geq M$$

and then for n big enough $P_n(Q(\mathcal{R})) \geq \frac{M}{2}$. Since $D_{\alpha(\mathcal{R})} \cap \overline{Q(\mathcal{R})}$ is closed we have

$$\lim_{n \to \infty} P_n(D_{\alpha(\mathcal{R})} \cap \overline{Q(\mathcal{R})}) = 0.$$

Then for n big enough

$$\frac{M}{4} < P_n(Q(\mathcal{R}) \setminus D_{\alpha(\mathcal{R})}). \tag{3.7}$$

Proposition 3.10. *Assume that ρ does not have atoms and let n satisfies* (3.7) *above, then there exists a maximiser u of $D(c_n, \cdot)$ and two positive constants r_n and k_n such that*

$$|u| \leq \frac{2N(N-1)^2}{r_n} - (N-1)^2 k_n.$$

We will later show that we can control r_n and k_n uniformly in n.

Proof. Consider a point $(\overline{x}_1, \ldots, \overline{x}_N) \in sptP_n \setminus D_{\alpha(\mathcal{R})}$ and in $Q(\mathcal{R})$.

We start from a maximiser $(u_1, \ldots, u_N)$ of (3.6) and we remark that without loss of generality we may assume that $u_i(\overline{x}_i) = \dfrac{c(\overline{x}_1, \ldots, \overline{x}_N)}{N} := k_n$ for all i and that

$$u_i(x) = \inf \left\{ c(y_1, \ldots, x, y_{i+1} \ldots, y_N) - \sum_{k \neq i} u_k(y_k) \right\},$$

for all i and x. Then we begin by choosing $r_n < \dfrac{\alpha(\mathcal{R})}{2}$ and we have the following estimate. If $x \notin \cup_{i=2}^{N} B(\overline{x}_i, r_n)$ then

$$\begin{aligned} u_1(x) &\leq c_n(x, \overline{x}_2, \ldots, \overline{x}_N) - u_2(\overline{x}_2) - \ldots - u_N(\overline{x}_N) \\ &\leq c(x, \overline{x}_2, \ldots, \overline{x}_N) - u_2(\overline{x}_2) - \ldots - u_N(\overline{x}_N) \\ &\leq \frac{N(N-1)}{r_n} - (N-1)k_n. \end{aligned} \tag{3.8}$$

We now select a, possibly smaller, r_n so that

$$\rho(B(\overline{x}_1, r_n)) + \ldots + \rho(B(\overline{x}_N, r_n)) < \varepsilon \ll \frac{M}{4}. \tag{3.9}$$

It follows that the set

$$\{\mathbf{y} \in Q(\mathcal{R}) \cap spt P_n \mid \mathbf{y} \notin D_{\alpha(\mathcal{R})}, \ y_i \notin B(\overline{x}_j, r_n) \text{ for } i, j = 1, \ldots, N\}$$

has positive P_n measure. Next, take $(\overline{y}_1, \ldots, \overline{y}_N)$ in this last set. Since $\overline{y}_1$ does not belong to the balls centered at $\overline{x}_i$ the estimate above holds and then

$$u_2(\overline{y}_2) + \ldots + u_N(\overline{y}_N) = c_n(\overline{y}_1, \ldots, \overline{y}_N) - u_1(\overline{y}_1) \geq - \left(\frac{N(N-1)}{r_n} - (N-1)k_n \right).$$

Finally, up to a division by 2 of r_n we have that for all $x \in \cup_{i=2}^{N} B(\overline{x}_i, r_n)$

$$\begin{aligned}
u_1(x) &\leq c_n(x, \overline{y}_2, \ldots, \overline{y}_N) - u_2(\overline{y}_2) - \ldots - u_N(\overline{y}_N) \\
&\leq c(x, \overline{y}_2, \ldots, \overline{y}_N) - u_2(\overline{y}_2) - \ldots - u_N(\overline{y}_N) \\
&\leq \frac{N(N-1)}{r_n} + \frac{N(N-1)}{r_n} - (N-1)k_n.
\end{aligned} \tag{3.10}$$

This completes the estimate from above of u_1. The same computation holds for the other u_i. The estimate from above of the u_i given by (3.8) and (3.10) translates in an estimates from below which holds ρ-a.e.. Indeed for ρ-a.e. x there holds

$$u_1(x) = \inf\{c_n(x, x_2, \ldots, x_n) - u_2(x_2) - \ldots - u_N(x_N)\} \geq (N-1)^2 k_n - \frac{2N(N-1)^2}{r_n}.$$

It remains to remark that

$$u(x) = \frac{1}{N} \sum_{i=1}^{N} u_i(x)$$

is a Kantorovich potential for c_n and it satisfies the required estimate. $\qquad\square$

Proposition 3.11. *The constants r_n and k_n in Proposition 3.10 can be controlled uniformly in n.*

Proof. Consider a point $\mathbf{x} = (\overline{x}_1, \ldots, \overline{x}_N) \in spt P \setminus D_{\alpha(\mathcal{R})}$ and in $Q(\mathcal{R})$. Then consider r such that

(1) $r < \dfrac{\alpha(\mathcal{R})}{2}$,

(2) $N \displaystyle\sum_i \rho(B(\overline{x}_i, r)) < \dfrac{M}{4}$.

Now we will show that in the construction of Proposition 3.10 we may choose $k_n \to \dfrac{c(\overline{x}_1, \ldots, \overline{x}_N)}{N}$ and $r_n = \dfrac{r}{4}$. Infact, since $P_n \overset{*}{\rightharpoonup} P$ we may choose in the estimates of Proposition 3.10 a sequence of points $\mathbf{x}^n = (\overline{x}_1^n, \ldots, \overline{x}_N^n) \to (\overline{x}_1, \ldots, \overline{x}_N)$. The convergence of $\mathbf{x}^n$ to $\mathbf{x}$ already gives the required convergence of k_n. Moreover, we also have that for n big enough $B(\overline{x}_i^n, \frac{r}{2}) \subset B(\overline{x}_i, r)$ for all i and then (3.9) is satisfied. Finally in Proposition 3.10 we divided r_n by 2 to have some distance between $\overline{x}_i$ and $\overline{y}_j$ and this last division brings us to $r_n = \dfrac{r}{4}$. $\qquad\square$

3.2. Conclusion and remarks

Theorem 3.12. *The following duality holds*

$$\min_{\Pi(\rho)} \int_{\mathbb{R}^{Nd}} \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} \mathrm{d}P(x_1, \ldots, x_N)$$

$$= \sup \left\{ N \int u(x) \mathrm{d}\rho(x) \ : \ u \in L^1_\rho \ and \ u(x_1) + \ldots + u(x_n) \le c(x_1, \ldots, x_n) \right\}, \quad (3.11)$$

and the right-hand side of equation (3.11) *above admits a bounded maximizer.*

Proof. By Proposition 3.3

$$\min_{\Pi(\rho)} \int_{\mathbb{R}^{Nd}} \sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} \mathrm{d}P(x_1, \ldots, x_N) = \lim_{n \to \infty} \min K(c_n, P).$$

By Propositions 3.6, 3.7, 3.10 and 3.11

$$\min K(c_n, P) = \max D(c_n, u),$$

$$\sup \left\{ N \int u(x) \mathrm{d}\rho(x) \ \middle| \ \begin{array}{c} u \in L^1_\rho \ and \\ u(x_1) + \ldots + u(x_n) \le c(x_1, \ldots, x_n) \end{array} \right\} = \lim_{n \to \infty} \max D(c_n, u),$$

and there exists a sequence $\{u_n\}$ where u_n is a maximizer of $D(c_n, u)$ and where $|u_n|$ is uniformly bounded, thus weakly compact in L^1_ρ. $\qquad\square$

Corollary 3.13. *Assume that ρ does not have atoms then there exists $0 < \alpha$ such that for every minimizer P of $K(c, \cdot)$*

$$P(D_\alpha) = 0.$$

Proof. For every Kantorovich potential u exploiting the duality (or complementary slackness) relations we obtains that for every minimizer P of $K(c, \cdot)$

$$u(x_1) + \ldots + u(x_N) = c(x_1, \ldots, x_N) \quad P - \text{a.e.}$$

Since there exists a bounded Kantorovich potential we obtain the conclusion. $\qquad\square$

Remark 3.14. Driven by the interest in some application we have chosen to present the result in the case in the case of Coulomb cost. However fixing some constants and exponent (in particular in Lem. 3.4, Prop. 3.7 and Sect. 3.1) and the definition of *bad set* the same result may be proved for several costs which are lower semi-continuous and bounded from below. Among them

$$\sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|^s}.$$

The case of even less regular costs has been considered in [1] but in that case it is necessary to give a different interpretation of the problems.

In [17] Kellerer considered a duality theory for multimarginal problems for a very wide class of costs. However in order to have existence of maximizers for the dual problems (see Thm. 2.21 in [17]) it is required that the cost c be controlled by a direct sum of functions in L^1_ρ also from above. In the case of the Coulomb cost this would read

$$\sum_{1 \le i < j \le N} \frac{1}{|x_i - x_j|} \le u(x_1) + \ldots + u(x_N)$$

and this is not possible since the right-hand side allows for $x_1 = \ldots = x_n$.

References

[1] M. Beiglböck, Ch. Léonard and W. Schachermayer, A general duality theorem for the monge–kantorovich transport problem. *Stud. Math.* **209** (2012) 2.

[2] A. Braides, Gamma-convergence for Beginners. Vol. 22. Oxford University Press, Oxford (2002).

[3] G. Buttazzo, L. De Pascale and P. Gori-Giorgi, Optimal-transport formulation of electronic density-functional theory. *Phys. Rev. A* **85** (2012) 062502.

[4] G. Carlier, On a class of multidimensional optimal transportation problems. *J. Convex Anal.* **10** (2003) 517–530.

[5] G. Carlier and B. Nazaret, Optimal transportation for the determinant. *ESAIM: COCV* **14** (2008) 678–698.

[6] M. Colombo, L. De Pascale and S. Di Marino, Multimarginal optimal transport maps for 1-dimensional repulsive costs. *Canad. J. Math.* (2013).

[7] M. Colombo and S. Di Marino, Equality between monge and kantorovich multimarginal problems with coulomb cost. *Ann. Mat. Pura Appl.* (2013) 1–14.

[8] C. Cotar, G. Friesecke and C. Klüppelberg, Density functional theory and optimal transportation with coulomb cost. *Commun. Pure Appl. Math.* **66** (2013) 548–599.

[9] G. Dal Maso, An introduction to *Γ*-convergence. Springer (1993).

[10] G. Friesecke, Ch.B Mendl, B. Pass, C. Cotar and C. Klüppelberg, N-density representability and the optimal transport limit of the hohenberg−kohn functional. *J. Chem. Phys.* **139** (2013) 164–109.

[11] W. Gangbo and A. Swiech, Optimal maps for the multidimensional monge−kantorovich problem. *Comm. Pure Appl. Math.* **51** (1998) 23–45.

[12] N. Ghoussoub and A. Moameni, A self-dual polar factorization for vector fields. *Comm. Pure Appl. Math.* **66** (2013) 905–933.

[13] P. Gori-Giorgi and M. Seidl, Density functional theory for strongly-interacting electrons: perspectives for physics and chemistry. *Phys. Chem. Chem. Phys.* **12** (2010) 14405–14419.

[14] P. Gori-Giorgi, M. Seidl and G. Vignale, Density-functional theory for strongly interacting electrons. *Phys. Rev. Lett.* **103** (2009) 166402.

[15] H. Heinich, Problème de monge pour n probabilités. *C. R. Math.* **334** (2002) 793–795.

[16] P. Hohenberg and W. Kohn, Inhomogeneous electron gas. *Phys. Rev.* **136** (1964) B864.

[17] H.G. Kellerer, Duality theorems for marginal problems. *Probab. Theory Relat. Fields* **67** (1984) 399–432.

[18] Walter Kohn and Lu Jeu Sham, Self-consistent equations including exchange and correlation effects. *Phys. Rev.* **140** (1965) A1133.

[19] E.H. Lieb. Density functionals for coulomb systems. *Int J. Quantum Chem.* **24** (1983) 243–277.

[20] Ch.B Mendl and L. Lin, Kantorovich dual solution for strictly correlated electrons in atoms and molecules. *Phys. Rev. B* **87** (2013) 125106.

[21] B. Pass, Uniqueness and monge solutions in the multimarginal optimal transportation problem. *SIAM J. Math. Anal.* **43** (2011) 2758–2775.

[22] B. Pass, On the local structure of optimal measures in the multi-marginal optimal transportation problem. *Calc. Var. Partial Differ. Equ.* **43** (2012) 529–536.

[23] S.T. Rachev and L. Rüschendorf, Mass transportation problems. *Probab. Appl.* Springer-Verlag (1998), Vol. I.

[24] M. Seidl, Strong-interaction limit of density-functional theory. *Phys. Rev. A* **60** (1999) 4387.

[25] M. Seidl, P. Gori-Giorgi and A. Savin, Strictly correlated electrons in density-functional theory: A general formulation with applications to spherical densities. *Phys. Rev. A* **75** (2007) 042511.

[26] M. Seidl, J.P Perdew and M. Levy, Strictly correlated electrons in density-functional theory. *Phys. Rev. A* **59** (1999) 51.