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Emanuele Caglioti, François Golse, Thierry Paul

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EMANUELE CAGLIOTI, FRANÇOIS GOLSE, AND THIERRY PAUL

ABSTRACT. We compare bipartite (Euclidean) matching problems in classical and quantum mechanics. The quantum case is treated in terms of a quantum version of the Wasserstein distance introduced in [F. Golse, C. Mouhot, T. Paul, Commun. Math. Phys. **343** (2016), 165–205]. We show that the optimal quantum cost can be cheaper than the classical one. We treat in detail the case of two particles: the equal mass case leads to equal quantum and classical costs. Moreover, we show examples with different masses for which the quantum cost is strictly cheaper than the classical cost.

CONTENTS

1. INTRODUCTION

The paradigm of modern optimal transport theory uses extensively the 2-Wasserstein distance between two Borel probability measures μ, ν on $\mathbf{R}^n$, defined as

$$W_2(\mu,\nu) := \inf_{\Pi \text{ coupling of } \mu \text{ and } \nu} \int |x-y|^2 \Pi(dx,dy). \tag{1}$$

We have called coupling[1] of the two probabilities μ and ν any Borel probability measure $\Pi(dx,dy)$ on $\mathbf{R}^n \times \mathbf{R}^n$ whose marginals on the first and the second factors are μ and ν resp., i.e.

$$\int_{\mathbf{R}^n\times\mathbf{R}^n} a(x)\Pi(dx,dy) = \int_{\mathbf{R}^n} a(x)\mu(dx), \int_{\mathbf{R}^n\times\mathbf{R}^n} b(y)\Pi(dx,dy) = \int_{\mathbf{R}^n} b(y)\nu(dy) \tag{2}$$

for all continuous and bounded test functions a and b.

Restricting the definition of W_2 to couplings of the form

$$\Pi = \delta(y - T(x))\mu(dy) \qquad \text{where } \nu = T_\#\mu\,, \tag{3}$$

i.e. where T is a Borel transformation of $\mathbf{R}^d$ such that ν is the image[2] of ν by T, one sees that the minimization problem in the definition of $W_2(\mu,\nu)$ contains the (quadratic)

[1] In the literature on optimal transport, couplings are also referred to as transport plans.

[2] The image of μ by the transformation T is the Borel measure denoted $T_\#\mu$, defined by $T_\#\mu(B) := \mu(T^{-1}(B))$ for each Borel set in $\mathbf{R}^d$.

Monge problem:

$$M(\mu,\nu) := \inf_{T\#\mu=\nu} \int_{\mathbf{R}^n} (x - T(x))^2 \mu(dx). \tag{4}$$

There is a converse result due to Knott, Smith and Brenier: under certain restrictions on the regularity of μ, any optimal coupling for the minimization problem defined by (1) is of the form (3) for some transport map T (see Theorem 2.12 in [6] for an extensive study).

Associated to W_2 is the bipartite matching problem which can be described as follows. Let us consider M material points on the real line $\{x_i\}_{i=1,\dots,M}$ with $x_i < x_{i+1}$, and with masses $\{m_i\}_{i=1,\dots,M}$, and on the other hand N points $\{y_i\}_{i=1,\dots,N}$ with $y_j < y_{j+1}$, and with masses $\{n_i\}_{i=1,\dots,N}$. We normalize the total mass as follows:

$$\sum_{i=1}^{M} m_i = \sum_{j=1}^{N} n_j = 1.$$

The bipartite problem consists in finding a coupling matrix $(p_{i,j})|_{i=1,\dots,N, j=1,\dots M}$ satisfying

$$\sum_{j=1}^{N} p_{i,j} = m_i, \qquad \sum_{i=1}^{M} p_{i,j} = n_j\,, \qquad p_{i,j} \geq 0 \text{ for each } i,j$$

which minimizes the quantity

$$\sum_{i,j} p_{i,j} |x_i - y_j|^2\,.$$

That is to say, we define the cost as

$$C_c := \inf_{\substack{p_{i,j}\geq 0 \\ \sum_{j=1}^{M} p_{i,j}=m_i,\ \sum_{i=1}^{M} p_{i,j}=n_j}} \sum_{i,j} p_{i,j} |x_i - y_j|^2.$$

It is natural to associate to the sets $\{x_i\}_{i=1,\dots,M}$ and $\{m_i\}_{i=1,\dots,M}$, and to the sets $\{y_i\}_{i=1,\dots,N}$ and $\{n_i\}_{i=1,\dots,N}$ the following discrete (Borel) probability measures

$$\mu := \sum_{i=1}^{M} m_i \delta_{x_i}, \qquad \nu := \sum_{j=1}^{N} n_j \delta_{y_j}.$$

It is easy to see that any optimal coupling of μ, ν for W_2 takes the form

$$\Pi = \sum_{i,j} p_{i,j} \delta_{x_i} \otimes \delta_{y_j}\,,$$

so that

$$C_c = W_2(\mu,\nu).$$

A general review of the bipartite problem is out of the scope of the present paper, and the reader is referred to [1] for a lucid presentation of the mathematical theory pertaining to this problem. Let us describe the simplest case $M = N = 2$.

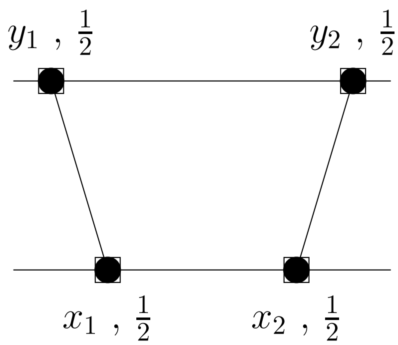

FIGURE 1. equal masses

In the case of equal masses, that is $m_1 = m_2 = n_1 = n_2 = \frac{1}{2}$, the optimal coupling is shown to be diagonal, in the sense that the mass $\frac{1}{2}$ is transported from the point x_1 to the point y_1, and likewise for x_2 and y_2. Thus

$$\Pi_{op} = \frac{1}{2}\delta_{x_1} \otimes \delta_{y_1} + \frac{1}{2}\delta_{x_2} \otimes \delta_{y_2},$$

or equivalently

$$\Pi_{op}(x,y) = \frac{1}{2}\delta(x - x_1)\delta(y - y_1) + \frac{1}{2}\delta(x - x_2)\delta(y - y_2),$$

and therefore the optimal transport cost is

$$C_c = \frac{1}{2}(x_1 - y_1)^2 + \frac{1}{2}(x_2 - y_2)^2 .$$

In the case of unequal masses, let us consider the example where $m_1 = \frac{1+\eta}{2}$ and $m_2 = \frac{1-\eta}{2}$ for some $0 < \eta < 1$, while $n_1 = n_2 = \frac{1}{2}$. In this case, one shows that the optimal transport moves the mass $\frac{1}{2}$ from x_1 to y_1, moves the remaining amount of the mass at x_1, i.e. $\frac{\eta}{2}$, from x_1 to y_2, and finally moves the mass $\frac{1-\eta}{2}$ from x_2 and y_2. The optimal coupling in this case is

$$\Pi_{op}(x,y) = \frac{1}{2}\delta(x - x_1)\delta(y - y_1) + \frac{\eta}{2}\delta(x - x_1)\delta(y - y_2) + \frac{1-\eta}{2}\delta(x - x_2)\delta(y - y_2),$$

so that the optimal transport cost is

$$C_c = \frac{1}{2}(x_1 - y_1)^2 + \frac{\eta}{2}(x_1 - y_2)^2 + \frac{1-\eta}{2}(x_2 - y_2)^2.$$

A quantum analogue to the Wasserstein distance has been recently introduced in [3] according to the general principle that, when passing from classical to quantum mechanics

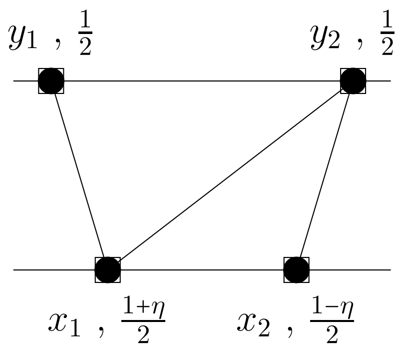

FIGURE 2. different masses

1. functions on phase-space should be replaced by operators on the Hilbert space of square integrable functions on the underlying configuration space, and
2. integration (over phase space) of classical functions should be replaced by the trace of the corresponding operators. Moreover,
3. coordinates q of the null section of the phase space should be replaced by the multiplication operator Q by the q variable, while coordinates p on the cotangent fibre should be replaced by the operator $P = -i\hbar\nabla$.

These considerations are consistent with the definition of quantum density matrices as self-adjoint positive operators of trace 1 on $\mathfrak{H} := L^2(\mathbf{R}^d)$. They are also consistent with the definition of couplings Π of two density matrices R and S as density matrices on $\mathfrak{H}\otimes\mathfrak{H}$ (identified with $L^2(\mathbf{R}^{2d})$) with marginals, i.e. partial traces on each factor of $\mathfrak{H}\otimes\mathfrak{H}$, equal to R and S. In other words

$$\text{trace}_{\mathfrak{H}\otimes\mathfrak{H}}((A\otimes I_{\mathfrak{H}})\Pi) = \text{trace}_{\mathfrak{H}}(AR), \quad \text{trace}_{\mathfrak{H}\otimes\mathfrak{H}}((I_{\mathfrak{H}}\otimes B)\Pi) = \text{trace}_{\mathfrak{H}}(BS) \tag{5}$$

for all bounded operators A, B on $\mathfrak{H}$, by analogy with (2).

Moreover they lead naturally to the following definition of the analogue of the Wasserstein distance between two quantum densities R and S. Consistently with (1) expressed on the phase-space $\mathbf{R}^{2d}$, therefore with $n = 2d$, we define

$$MK_2(R,S) := \inf_{\Pi \text{ coupling of } R \text{ and } S} \text{trace}\,(C\Pi), \tag{6}$$

with[3]

$$C := (P\otimes \mathrm{I} - I\otimes P)^2 + (Q\otimes I - I\otimes Q)^2 - 2d\hbar. \tag{7}$$

In other words, expressed as an operator on $L^2(\mathbf{R}^d, dx)\otimes L^2(\mathbf{R}^d, dy)$,

$$C = (x-y)^2 - \hbar^2(\nabla_x - \nabla_y)^2 - 2d\hbar = -4\hbar^2\nabla^2_{x-y} + (x-y)^2 - 2d\hbar. \tag{8}$$

The operator $C + 2d\hbar$ is the Hamiltonian of an harmonic oscillator in the variable $x-y$, and in particular $C \geq 0$. Thus $MK_2(R,S) \geq 0$ but MK_2 is not a distance (see [3] on p. 171).

[3]Note the unessential difference with the definition of the cost in [3, 4, 5] created by the shift $-2d\hbar$

Nevertheless, we established in [3] that, for any pair of density matrices R and S, the Husimi functions $\widetilde{W}[R]$ and $\widetilde{W}[S]$ of R and S satisfy

$$W_2(\widetilde{W}[R], \widetilde{W}[S])^2 \leq MK_2(R,S)^2 + 4d\hbar. \tag{9}$$

On the other hand, if R and S are Töplitz operators of symbols μ and ν,

$$MK_2(R,S)^2 \leq W_2(\mu,\nu)^2. \tag{10}$$

Let us recall that a Töplitz operator T (or positive quantization, or anti-Wick ordering quantization) of symbol a Borel probability measure τ on phase space is[4]

$$T := \int_{\mathbf{R}^{2d}} |q,p\rangle\langle q,p|\tau(dq,dp),$$

where $|q,p\rangle$ is a coherent state at point (q,p) i.e.

$$\langle x|q,p\rangle := (\pi\hbar)^{-d/4} e^{-(x-q)^2/2\hbar} e^{ipx/\hbar}. \tag{11}$$

We also recall the definition of the Husimi function of a density matrix R:

$$\widetilde{W}[R](q,p) := (2\pi\hbar)^{-d}\langle q,p|R|q,p\rangle.$$

The functional MK_2^2 (more precisely $MK_2^2 + 2d\hbar$ with the definition chosen in the present paper) has been systematically used and extended in [3, 4, 5] in order to study various problems, such as the validity of the mean-field limit uniformly in $\hbar$, the semiclassical approximation of quantum dynamics, and the problem of metrizing of the set of quantum densities in the semiclassical regime.

The quantum bipartite problem can be therefore stated as follows, in close analogy with the classical picture introduced earlier.

One considers two density matrices built in terms of the positions and masses already used for the classical bipartite problem, in the following way

$$R = \sum_{i=1}^{M} m_i |x_i, 0\rangle\langle x_i, 0|, \qquad S = \sum_{j=1}^{N} n_j |y_j, 0\rangle\langle y_j, 0|.$$

Indeed, it is natural to associate coherent states to material points, as they saturate the Heisenberg uncertainty inequalities. Moreover, one sees that R and S are precisely the Töplitz operators of symbols μ and ν respectively.

The quantum bipartite problem consists then in finding an optimal coupling of R and S for $MK_2(R,S)$ and the optimal quantum cost defined as

$$C_q := MK_2(R,S).$$

Since R and S are Töplitz operators, we know from (10) that

$$C_q \leq C_c.$$

[4] Here also, we use a different normalization than the one in [3, 4, 5], since we deal exclusively with density matrices. With the present normalization, one has trace $T = \int_{\mathbf{R}^{2d}} \tau(dq,dp)$.

The question we address in this paper is whether there exist pairs of density matrices for which

$$C_q < C_c.$$

In other words, we address the question of whether quantum optimal transportation can be cheaper than its classical analogue.

In this paper, we shall study the two cases introduced at the beginning of this section and described in Figures 1 and 2. For the sake of simplicity, we shall take $x_1 = -x_2 = -a, y_1 = -y_2 = -b$, with $a < b$ in the equal mass case, and $a = b$ in the unequal mass case.

In the equal mass case, studied in Section 2, both classical and quantum transport are achieved without splitting mass for each particle. As a result, the two costs are shown to be equal (see (22)), and an optimal quantum coupling is obtained by applying the Töplitz quantization to the optimal classical coupling.

In Section 3 we study the case where one of the density matrix involves different masses and construct a family of examples for which the optimal quantum cost is strictly cheaper than the classical one (see (32)).

We also show in Section 4 that the optimal quantum coupling cannot be the Töplitz quantization of any classical coupling: in particular the optimal quantum transport is different from the natural quantization of the underlying classical one. In fact the quantum optimal transport in the latter case does not correspond to the classical optimal transport and involves strictly quantum effects.

2. The equal mass case

For $a, b > 0$ we will transport a superposition of two density matrices which are pure sates associated to two coherent states of null momenta localized at $+a$ and $-a$ towards a similar density matrix associated to the points $(\pm b, 0)$ in phase space. In other words, we consider the coherent states denoted $|c\rangle$ for simplicity (instead of $|c, 0\rangle$ to be consistent with (11)), defined by the formula

$$\langle x|c\rangle := (\pi\hbar)^{-1/4} e^{-(x-c)^2/2\hbar}.$$

Set

$$R := \frac{1}{2}(|a\rangle\langle a| + |-a\rangle\langle -a|), \qquad S := \frac{1}{2}(|b\rangle\langle b| + |-b\rangle\langle -b|).$$

Define

$$\lambda := \langle a|{-a}\rangle = e^{-a^2/\hbar}, \qquad \mu := \langle b|{-b}\rangle = e^{-b^2/\hbar},$$

and consider the two pairs of orthogonal vectors

$$\phi_\pm := \frac{|a\rangle \pm |-a\rangle}{\sqrt{2(1 \pm \lambda)}}, \qquad \psi_\pm := \frac{|b\rangle \pm |-b\rangle}{\sqrt{2(1 \pm \mu)}}. \tag{12}$$

Hence

$$R = \alpha_+|\phi_+\rangle\langle\phi_+| + \alpha_-|\phi_-\rangle\langle\phi_-|, \qquad S = \beta_+|\psi_+\rangle\langle\psi_+| + \beta_-|\psi_-\rangle\langle\psi_-|,$$

with

$$\alpha_+ := \frac{1}{2}(1+\lambda), \qquad \alpha_- = \frac{1}{2}(1-\lambda), \qquad \beta_+ := \frac{1}{2}(1+\mu), \qquad \beta_- = \frac{1}{2}(1-\mu).$$

Every coupling of R and S belongs to the tensor product of the four-dimensional linear span of $\phi_\pm \otimes \psi_\pm$ with itself. Therefore, in order to compute trace(CQ) for such couplings, we need to project the cost operator C on the basis $\{\phi_+ \otimes \psi_+, \phi_+ \otimes \psi_-, \phi_- \otimes \psi_+, \phi_- \otimes \psi_-\}$. This is a tedious but straightforward computation which results in the following 4×4 matrix:

$$C = \begin{pmatrix} a^2\frac{1-\lambda}{1+\lambda} + b^2\frac{1-\mu}{1+\mu} & 0 & 0 & -2ab\frac{\lambda^2+\mu^2-\lambda^2\mu^2-\lambda\mu}{\sqrt{(1-\lambda^2)(1-\mu^2)}} \\ 0 & a^2\frac{1-\lambda}{1+\lambda} + b^2\frac{1+\mu}{1-\mu} & -2ab\frac{\lambda^2+\mu^2-\lambda^2\mu^2+\lambda\mu}{\sqrt{(1-\lambda^2)(1-\mu^2)}} & 0 \\ 0 & -2ab\frac{\lambda^2+\mu^2-\lambda^2\mu^2+\lambda\mu}{\sqrt{(1-\lambda^2)(1-\mu^2)}} & a^2\frac{1+\lambda}{1-\lambda} + b^2\frac{1-\mu}{1+\mu} & 0 \\ -2ab\frac{\lambda^2+\mu^2-\lambda^2\mu^2-\lambda\mu}{\sqrt{(1-\lambda^2)(1-\mu^2)}} & 0 & 0 & a^2\frac{1+\lambda}{1-\lambda} + b^2\frac{1+\mu}{1-\mu} \end{pmatrix}, \tag{13}$$

abbreviated for simplicity as

$$C = \begin{pmatrix} \mathcal{A} & 0 & 0 & \gamma \\ 0 & \mathcal{B} & \delta & 0 \\ 0 & \delta & \mathcal{C} & 0 \\ \gamma & 0 & 0 & \mathcal{D} \end{pmatrix}. \tag{14}$$

As a warm up in order to find an ansatz for the general case, we neglect the contributions of λ, μ, which are exponentially small in the Planck constant. In this case $\alpha_\pm = \beta_\pm = \frac{1}{2}$, and the cost is equal to

$$C_0 = \begin{pmatrix} a^2+b^2 & 0 & 0 & -2ab \\ 0 & a^2+b^2 & -2ab & 0 \\ 0 & -2ab & a^2+b^2 & 0 \\ -2ab & 0 & 0 & a^2+b^2 \end{pmatrix}.$$

On the other hand, one has

$$Q_0 := \begin{pmatrix} \frac{1}{4} & 0 & 0 & \frac{1}{4} \\ 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ 0 & \frac{1}{4} & \frac{1}{4} & 0 \\ \frac{1}{4} & 0 & 0 & \frac{1}{4} \end{pmatrix} \geq 0,$$

since the spectrum of Q_0 is easily shown to be $\{0, \frac{1}{2}\}$ by using the elementary formula

$$\det \begin{pmatrix} \bar{a} & 0 & 0 & \gamma \\ 0 & \bar{b} & \delta & 0 \\ 0 & \delta & \bar{c} & 0 \\ \gamma & 0 & 0 & \bar{d} \end{pmatrix} = (\bar{a}\bar{d} - \gamma^2)(\bar{b}\bar{c} - \delta^2) \text{ for all } \bar{a}, \bar{b}, \bar{c}, \bar{d}, \gamma, \delta \tag{15}$$

to compute the characteristic polynomial of Q_0. Moreover, one easily checks that $\text{trace}_2\, Q_0 = R$ and $\text{trace}_1\, Q_0 = S$ so that Q_0 is a coupling of R and S.

Another easy computation shows that

$$\operatorname{trace}(CQ_0) = (a-b)^2 .$$

Therefore

$$MK_2(R,S) \le (a-b)^2 = W_2(\tfrac{1}{2}(\delta_{-a}+\delta_a), \tfrac{1}{2}(\delta_{-b}+\delta_b)).$$

For the "true" case $\lambda\mu \neq 0$, we make the following ansatz on the coupling Q

$$Q = Q_0 + \frac{1}{4}\begin{pmatrix} p+\lambda+\mu & 0 & 0 & u \\ 0 & -p+\lambda-\mu & v & 0 \\ 0 & v & -p-\lambda+\mu & 0 \\ u & 0 & 0 & p-\lambda-\mu \end{pmatrix}, \; p,u,v \in \mathbf{R}.$$

Straightforward computations show that

$$\operatorname{trace} Q = \operatorname{trace} Q_0 = 1, \qquad \operatorname{trace}_2 Q = \operatorname{trace}_2 Q_0 = R, \qquad \operatorname{trace}_1 Q = \operatorname{trace}_1 Q_0 = S.$$

Using again (15) shows that

$$Q \ge 0 \Longleftrightarrow -1 + \sqrt{(\lambda+\mu)^2 + (1+u)^2} \le p \le 1 - \sqrt{(\lambda-\mu)^2 + (1+v)^2}.$$

Therefore, assuming that p,u,v satisfy this constaint, Q is a coupling of R and S.

Denoting $U := 1+u$ and $V := 1+v$, we compute $W := \operatorname{trace}(CQ)$ by using (13) and (14):

$$\begin{aligned} 4W &= 2\gamma U + 2\delta V + p(\mathcal{A}+\mathcal{B}-\mathcal{C}-\mathcal{D}) + \mathcal{A}+\mathcal{B}+\mathcal{C}+\mathcal{D} \\ &\quad +(\lambda+\mu)(\mathcal{A}-\mathcal{D}) + (\lambda-\mu)(\mathcal{B}-\mathcal{C}) \\ &= 2\gamma U + 2\delta V + p(\mathcal{A}-\mathcal{B}-\mathcal{C}+\mathcal{D}) + W' = 2\gamma U + 2\delta V + W', \end{aligned} \tag{16}$$

with

$$\begin{aligned} W' &:= \mathcal{A}+\mathcal{B}+\mathcal{C}+\mathcal{D} + \lambda(\mathcal{A}+\mathcal{B}-\mathcal{C}-\mathcal{D}) + \mu(\mathcal{A}-\mathcal{B}+\mathcal{C}-\mathcal{D}) \\ &= 4(a^2\frac{1+\lambda^2}{1-\lambda^2} + b^2\frac{1+\mu^2}{1-\mu^2}) - 8a^2\frac{\lambda^2}{1-\lambda^2} - 8b^2\frac{\mu^2}{1-\mu^2} \\ &= 4(a^2+b^2). \end{aligned} \tag{17}$$

Since W is linear in U,V, we minimize $\gamma U + \delta V$ by taking

$$U = \sqrt{(p+1)^2 - (\lambda+\mu)^2} \qquad \text{and} \qquad V = \sqrt{(p-1)^2 - (\lambda-\mu)^2},$$

and, since $\delta \le \gamma$, we conclude that

$$4W = 2T + W',$$

where

$$T = -\max_{-1+\lambda-\mu\leq p\leq 1-(\lambda-\mu)}\left(-\gamma\sqrt{(p+1)^2-(\lambda+\mu)^2}-\delta\sqrt{(p-1)^2-(\lambda-\mu)^2}\right)$$
$$=\frac{-2ab}{\sqrt{(1-\lambda^2)(1-\mu^2)}}\max_{-1+\lambda-\mu\leq p\leq 1-(\lambda-\mu)}\Big((1-\lambda\mu)\sqrt{(p+1)^2-(\lambda+\mu)^2}$$
$$+(1+\lambda\mu)\sqrt{(p-1)^2-(\lambda-\mu)^2}\Big).$$

One can check that the max is attained for $p=\lambda\mu\to 0$ as $\hbar\to 0$, and that

$$T=-\frac{4ab}{\sqrt{(1-\lambda^2)(1-\mu^2)}}\sqrt{1+\lambda^2\mu^2-\lambda^2-\mu^2}=-4ab.$$

Eventually, we arrive at the same result as in the semiclassical regime, viz.

$$MK_2(R,S)^2\leq(a-b)^2. \tag{18}$$

Since R and S are Töplitz operator, the inequality (18) was already known by using (10). Nevertheless we gave this explicit computation as we believe the result to be valid for more general density matrices than this Töplitz operators with discrete symbols.

In order to get a lower bound for $MK_2(R,S)$, we shall use a dual version of the definition of MK_2 proved in [2]. This alternative definition of MK_2 is obtained by applying theTöplitz quantization procedure to the Kantorovitch duality theorem for W_2 (see [6, 7]):

$$MK_2(R,S)=\sup_{\substack{A=A^*,\ B=B^* \text{ bounded operators on } \mathfrak{H}\\ \text{such that } A\otimes I+I\otimes B\leq C}}\operatorname{trace}(RA+SB). \tag{19}$$

We make the following diagonal ansatz on A and B:

$$A=\begin{pmatrix}\alpha_1 & 0\\ 0 & \alpha_2\end{pmatrix}\qquad B=\begin{pmatrix}\beta_1 & 0\\ 0 & \beta_2\end{pmatrix},$$

so that

$$A\otimes I=\begin{pmatrix}\alpha_1 & 0 & 0 & 0\\ 0 & \alpha_1 & 0 & 0\\ 0 & 0 & \alpha_2 & 0\\ 0 & 0 & 0 & \alpha_2\end{pmatrix}\quad\text{and}\quad I\otimes B=\begin{pmatrix}\beta_1 & 0 & 0 & 0\\ 0 & \beta_2 & 0 & 0\\ 0 & 0 & \beta_1 & 0\\ 0 & 0 & 0 & \beta_2\end{pmatrix}.$$

Hence

$$A\otimes I+I\otimes B-C:=\begin{pmatrix}a & 0 & 0 & -\gamma\\ 0 & b & -\delta & 0\\ 0 & -\delta & c & 0\\ -\gamma & 0 & 0 & d\end{pmatrix},$$

and, according to (14),

$$\bar a=\alpha_1+\beta_1-\mathcal{A},\quad \bar b=\alpha_1+\beta_2-\mathcal{B},\quad \bar c=\alpha_2+\beta_1-\mathcal{C},\quad \bar d=\alpha_2+\beta_2-\mathcal{D}.$$

Notice that

$$\bar a + \bar d = \bar b + \bar c.$$

Using (15) to compute the characteristic polynomial of $A\otimes I + I\otimes B - C$, we find that

$$A\otimes I + I\otimes B \le C \iff \bar a + \bar d \le -\sqrt{(\bar a - \bar d)^2 + 4\gamma^2} \text{ and } b + c \le -\sqrt{(\bar b - \bar c)^2 + 4\delta^2}. \tag{20}$$

Moreover,

$$\begin{aligned}\operatorname{trace}(AR+BS) &= \frac{1}{2}(\alpha_1+\alpha_2+\beta_1+\beta_2) + \frac{\lambda}{2}(\alpha_1-\alpha_2) + \frac{\mu}{2}(\beta_1-\beta_2)\\ &= \frac{1}{4}(\bar a + \bar b + \bar c + \bar d) + \frac{1}{4}(\bar a + \bar b - \bar c - \bar d)\lambda + \frac{1}{4}(\bar a - \bar b + \bar c - \bar d)\mu + a^2 + b^2.\end{aligned}$$

Let us denote

$$x := \bar a + \bar d = \bar b + \bar c,$$

so that

$$\operatorname{trace}(AR+BS) = \frac{1}{2}x + \frac{1}{4}(\lambda+\mu)(\bar a - \bar d) + \frac{1}{4}(\lambda-\mu)(\bar b - \bar c) + a^2 + b^2. \tag{21}$$

The constraints (20) are expressed as

$$\begin{aligned} x = \bar a + \bar d &\le -\sqrt{(\bar a - \bar d)^2 + 4\gamma^2}\,,\\ x = \bar b + \bar c &\le -\sqrt{(\bar b - \bar c)^2 + 4\delta^2}\,.\end{aligned}$$

Without loss of generality we assume that $\lambda \ge \mu$, that is to say $a < b$. Since the right hand side of (21) is linear in x, in $(\bar a - \bar d)$, and in $(\bar b - \bar c)$, one has to saturate the constraints to maximize $\operatorname{trace}(AR+BS)$. In other words, we must take

$$\bar a - \bar d = \sqrt{x^2 - 4\gamma^2}, \quad \text{and} \quad \bar b - \bar c = \sqrt{x^2 - 4\delta^2}.$$

Since $\delta \le \gamma \le 0$, this amounts to computing

$$\max_{x\le 2\delta} f(x), \qquad \text{with } f(x) := \frac{x}{2} + \frac{1}{4}(\lambda+\mu)\sqrt{x^2-4\gamma^2} + \frac{1}{4}(\lambda-\mu)\sqrt{x^2-4\delta^2}\,.$$

We check that $f'(x)$ is an increasing function of x^2, so that the maximum of $f(x)$ for $x \le 2\delta$ is attained at

$$f'(x) = 0 \iff x = -\frac{4ab(1-\lambda^2\mu^2)}{(1-\lambda^2)(1-\mu^2)}, \qquad \text{which implies } f(x) = -2ab.$$

We conclude from (21) that

$$MK_2(R,S)^2 \ge \operatorname{trace}(AR+BS) \ge a^2 + b^2 - 2ab = (a-b)^2\,.$$

Together with (18), this implies that

$$MK_2(R,S)^2 = (a-b)^2 = W_2(\tfrac12(\delta_{-a}+\delta_a), \tfrac12(\delta_{-b}+\delta_b))^2.$$

Therefore,

$$C_q = C_c, \tag{22}$$

so that the classical and the quantum optimal transport costs are equal in this case.

3. The unequal mass case

In this section, we construct a family of density matrices R and S for which the quantum cost of optimal transport is smaller than the classical analogous cost.

With the same notations as in previous section, we set

$$R := \tfrac{1+\eta}{2}|a\rangle\langle a| + \tfrac{1-\eta}{2}|-a\rangle\langle -a|, \qquad S := \tfrac{1}{2}|a\rangle\langle a| + \tfrac{1}{2}|-a\rangle\langle -a|, \qquad 0 < \eta < 1.$$

In other words, we consider the same situation as in the previous section with $a = b$, but with different masses for the quantum density matrix R.

In the orthonormal basis $\{\phi_+, \phi_-\}$, the density matrix R takes the form

$$R = \begin{pmatrix} \frac{1+\eta}{2} & \frac{\eta}{2}(1-\lambda^2) \\ \frac{\eta}{2}(1-\lambda^2) & \frac{1-\eta}{2} \end{pmatrix}, \tag{23}$$

while S is the same as before.

We define the "quantized classical" coupling as

$$Q_c := \tfrac{1}{2}|a;a\rangle\langle a;a| + \tfrac{1-\eta}{2}|-a;-a\rangle\langle -a;-a| + \tfrac{\eta}{2}|a;-a\rangle\langle a;-a|, \tag{24}$$

with the obvious notation

$$\langle a;b| := \langle a| \otimes \langle b|; \qquad |a;b\rangle := |a\rangle \otimes |b\rangle.$$

Obviously $Q_c \geq 0$ by construction, and

$$\text{trace}_2(Q_c) = \tfrac{1}{2}|a\rangle + \tfrac{\eta}{2}|a\rangle + \tfrac{1-\eta}{2}|-a\rangle\langle -a| = R, \quad \text{while } \text{trace}_1(Q_c) = S.$$

Viewed as a matrix in the basis $\{\phi_+ \otimes \psi_+, \phi_+ \otimes \psi_-, \phi_- \otimes \psi_+, \phi_- \otimes \psi_-\}$,

$$Q_c = \begin{pmatrix} \frac14(1+\lambda)^2 & 0 & \frac14\eta\sqrt{1-\lambda}(1+\lambda)^{\frac32} & \frac14(-1+\eta)(-1+\lambda^2) \\ 0 & \frac14(1-\lambda^2) & \frac14(-1+\eta)(-1+\lambda^2) & \frac14\eta(1-\lambda)^{\frac32}\sqrt{1+\lambda} \\ \frac14\eta\sqrt{1-\lambda}(1+\lambda)^{\frac32} & \frac14(-1+\eta)(-1+\lambda^2) & \frac14(1-\lambda^2) & 0 \\ \frac14(-1+\eta)(-1+\lambda^2) & \frac14\eta(1-\lambda)^{\frac32}\sqrt{1+\lambda} & 0 & \frac14(-1+\lambda)^2 \end{pmatrix}. \tag{25}$$

With (13), we easily compute

$$\text{trace}\,(CQ_c) = 2\eta a^2 = W_2(\tfrac{1+\eta}{2}\delta_a + \tfrac{1-\eta}{2}\delta_{-a}, \tfrac12\delta_a + \tfrac12\delta_{-a}). \tag{26}$$

Indeed, let us recall the classical optimal transport from R to S in this case: first, one "moves" the amount of mass $\frac12$ from a in R to a in S. The amount of mass $\frac{\eta}{2}$ remaining at a in R is transported to $-a$ in S, and the outstanding amount of mass $\frac{1-\eta}{2}$, located at $-a$ in R, is "transported" to $-a$ in S (see Figure 2).

For each $\epsilon > 0$, set

$$Q_\epsilon := Q_c + \epsilon Q_q, \tag{27}$$

with

$$Q_q := \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \tag{28}$$

One easily checks that

$$\operatorname{trace}_1(Q_q) = \operatorname{trace}_2(Q_q) = \operatorname{trace}(Q_q) = 0,$$

so that

$$\operatorname{trace}_1(Q_\epsilon) = S, \quad \text{and} \quad \operatorname{trace}_2(Q_\epsilon) = R, \quad \text{so that } \operatorname{trace}(Q_\epsilon) = 1. \tag{29}$$

The characteristic polynomial of Q_c is found to be of the form

$$\det(Q_c - tI) = tP_3(t),$$

where P_3 is a cubic polynomial satisfying

$$P_3(0) = -\tfrac{\eta}{8}(1-\eta)(1-\eta^2) < 0.$$

Therefore the spectrum of Q_c is $\{0, \lambda_1 > 0, \lambda_2 > 0, \lambda_3 > 0\}$ since $Q_c = Q^* \geq 0$. One can also check that

$$\det(Q_\epsilon - tI)|_{t=0} = \det Q_\epsilon = \epsilon\eta\lambda^2(1-\eta)(1-\lambda^4) + O(\epsilon^2) > 0 \quad \text{for } 0 < \epsilon \ll 1, \tag{30}$$

together with

$$\frac{d}{dt}\det(Q_c - tI)|_{t=0} := P_3(0) < 0.$$

Hence there exists C (independent of ϵ) such that

$$\frac{d}{dt}\det(Q_\epsilon - tI)|_{t=0} \leq C < 0 \qquad \text{for } 0 < \epsilon \ll 1. \tag{31}$$

Both (30) and (31) clearly imply that $\det(Q_\epsilon - tI)$ has a positive zero that is ϵ-close to 0, and three other roots which are ϵ-close to λ_1, λ_2 and $\lambda_3 > 0$ respectively. Therefore, $Q_\epsilon = Q_\epsilon^* > 0$ for $0 < \epsilon \ll 1$, and (29) implies that Q_ϵ is a coupling of R and S.

Another elementary computation shows that

$$\operatorname{trace}(CQ_q) = -\frac{8\eta^2\lambda^2}{1-\lambda^2},$$

so that

$$\begin{aligned} MK_2(R,S)^2 \leq \operatorname{trace}(CQ_\epsilon) &= \operatorname{trace}(CQ_c) - \epsilon\frac{8\eta^2\lambda^2}{1-\lambda^2} \\ &< W_2(\tfrac{1+\eta}{2}\delta_a + \tfrac{1-\eta}{2}\delta_{-a}, \tfrac{1}{2}\delta_a + \tfrac{1}{2}\delta_{-a}), \end{aligned}$$

for each ϵ satisfying $0 < \epsilon \ll 1$, according to formula (26). This shows that, in the present case

$$C_q < C_c, \tag{32}$$

which means that the quantum cost is (strictly) below the classical cost.

4. Concluding remarks on quantum optimal transport

The result of Section 2 shows that, in the equal mass case, an optimal coupling is given by the following matrix in the basis $\{\phi_+ \otimes \psi_+, \phi_+ \otimes \psi_-, \phi_- \otimes \psi_+, \phi_- \otimes \psi_-\}$:

$$Q = \frac{1}{4}\begin{pmatrix} 1+\lambda\mu+\lambda+\mu & 0 & 0 & \sqrt{(1+\lambda\mu)^2-(\lambda+\mu)^2} \\ 0 & 1-\lambda\mu+\lambda-\mu & \sqrt{(1-\lambda\mu)^2-(\lambda-\mu)^2} & 0 \\ 0 & \sqrt{(1-\lambda\mu)^2-(\lambda-\mu)^2} & 1-\lambda\mu-\lambda+\mu & 0 \\ \sqrt{(1+\lambda\mu)^2-(\lambda+\mu)^2} & 0 & 0 & 1+\lambda\mu-\lambda-\mu \end{pmatrix}.$$

In view of (12) and with the same notation as in (24), the optimal coupling Q is put in the form

$$Q = \frac{1}{2}\left(|a;b\rangle\langle a;b| + |-a;-b\rangle\langle -a;-b|\right). \tag{33}$$

In other words, Q is the Töplitz operator of symbol

$$\Pi(q,p;q',p') = \tfrac{1}{2}\delta_{(-a,0)}(q,p)\delta_{(-b,0)}(q',p') + \frac{1}{2}\delta_{(a,0)}(q,p)\delta_{(b,0)}(q',p').$$

Likewise R is the Töplitz operator of symbol

$$\mu(q,p) = \tfrac{1}{2}\big(\delta_{(-a,0)}(q,p) + \delta_{(a,0)}(q,p)\big), \tag{34}$$

while S is the Töplitz operator of symbol

$$\nu(q,p) = \tfrac{1}{2}\big(\delta_{(-b,0)}(q,p) + \delta_{(b,0)}(q,p)\big). \tag{35}$$

Equivalently

$$\begin{aligned} \Pi(q,p;q',p') &= \tfrac{1}{2}\Big(\big(\delta_{(-a,0)}(q,p) + \delta_{(a,0)}(q,p)\big)\delta((q',p') - \Phi(q,p))\Big) \\ &= \mu(q,p)\delta((q',p') - \Phi(q,p)), \end{aligned} \tag{36}$$

where Φ is any map satisfying $\Phi(a,0) = (b,0)$ and $\Phi(-a,0) = (-b,0)$.

The second equality in (36) is in agreement with the formula (4) in Section 1: in the equal mass case, an optimal quantum coupling Q is the Töplitz operator of symbol the classical optimal coupling associated to the optimal transport map

$$\big((-a,0),(a,0)\big) \mapsto \big((-b,0),(b,0)\big).$$

In the unequal mass case treated in Section 3, the coupling Q_c defined by (24) is also a Töplitz operator, with symbol

$$\begin{aligned} \Pi_c(q,p;q',p') &= \tfrac{1}{2}\delta_{(a,0)}(q,p)\delta_{(a,0)}(q',p') \\ &+ \tfrac{1-\eta}{2}\delta_{(-a,0)}(q,p)\delta_{(-a,0)}(q',p') + \tfrac{\eta}{2}\delta_{(a,0)}(q,p)\delta_{(-a,0)}(q',p'). \end{aligned}$$

This expression is easily interpreted as the optimal coupling associated to the "transport" introduced in Section 1, Figure 2, exactly as in the equal mass case. But, as explained in the previous section, Q_c cannot be an optimal coupling, since the coupling Q_ϵ defined by (27) leads to a strictly lower quantum cost.

We did not compute any optimal coupling in this situation. Observe however that Q_q is expressed in terms of the orthonormal systems (12) specialized to $a = b$ (so that $\lambda = \mu$), and takes the form

$$Q_q = \sum_{i,j,k,l=\pm 1} q_{i,j,k,l}|ia;ja\rangle\langle ka;la|.$$

The contribution of the "diagonal" terms $q_{i,j,i,j}$ defines a Töplitz operator, unlike the off-diagonal terms such as $q_{1,1,-1,1} = \frac{-4\lambda}{(1-\lambda^2)^2} \neq 0$ for instance.

In general, when R and S are Töplitz operators of symbols μ and ν satisfying $MK_2(R,S) < W_2(\mu,\nu)$, no optimal coupling Q_{op} of R and S can be a Töplitz operator. If such was the case, the Töplitz symbol of Q_{op} would be a coupling of μ and ν with classical transport cost $MK_2(R,S) < W_2(\mu,\nu)$, which is impossible. The presence of nonclassical off-diagonal terms in Q_{op}, such as $q_{1,1,-1,1} = \frac{-4\lambda}{(1-\lambda^2)^2} \neq 0$ in the example discussed above, are precisely the reason why quantum optimal transport is cheaper in this case than classical optimal transport.

Finally, observe that both $q_{1,1,-1,1}$ and $W_2(\frac{1+\eta}{2}\delta_a + \frac{1-\eta}{2}\delta_{-a}, \frac{1}{2}\delta_a + \frac{1}{2}\delta_{-a}) - \operatorname{trace}(CQ_\epsilon)$ are exponentially small as $\hbar \to 0$, but of course are not small for $\hbar = 1$.

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(E.C.) Sapienza Università di Roma, Dipartimento di Matematica, Piazzale Aldo Moro 5, 00185 Roma
E-mail address: `caglioti@mat.uniroma1.it`

(F.G.) CMLS, Ecole polytechnique, 91128 Palaiseau Cedex, France
E-mail address: `francois.golse@polytechnique.edu`

(T.P.) CMLS, CNRS, Ecole polytechnique, 91128 Palaiseau Cedex, France
E-mail address: `thierry.paul@polytechnique.edu`