Quantum Wasserstein "Metric" and Applications
Lecture 3

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Based on works with E. Caglioti, S. Jin, C. Mouhot, T. Paul

Outline of Lecture 3

This last lecture discusses various features of our extension of optimal transport to the quantum setting. In particular, the following topics will be studied

- Kantorovich-type duality for quantum optimal transport
- triangle inequality for the quantum pseudometric $\mathfrak{d}$ on $\mathfrak{D}$
- structure of optimal couplings for the pseudometric $\mathfrak{d}$

RESTRICTED TRIANGLE INEQUALITY

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Restricted Triangle Inequality

Theorem 1 For all $\rho_1, \rho_2, \rho_3 \in \mathfrak{D} = \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d) \cup \mathcal{D}_2(\mathfrak{H})$, one has

$$\mathfrak{d}(\rho_1, \rho_3) \le \mathfrak{d}(\rho_1, \rho_2) + \mathfrak{d}(\rho_2, \rho_3)$$

provided that ρ_2 is a probability density in $\mathbf{R}^d \times \mathbf{R}^d$ or one of the ρ_js is a rank-1 density operator on $\mathfrak{H}$.

Recall that

$$c_\hbar(x, \xi; y, \hbar\nabla_y) = |x - y|^2 + |\xi + i\hbar\nabla_y|^2$$
$$C_\hbar(x, \hbar\nabla_x, y, \hbar\nabla_y) = |x - y|^2 - \hbar^2|\nabla_x - \nabla_y|^2$$

Lemma 2 For all $\alpha > 0$, one has

$$\begin{aligned}|x-z|^2+|\xi-\zeta|^2 \leq &(1+\alpha)c_\hbar(x,\xi;y,\hbar\nabla_y)\\&+(1+\tfrac{1}{\alpha})c_\hbar(z,\zeta;y,\hbar\nabla_y)\\ c_\hbar(x,\xi;z,\hbar\nabla_z)\leq&(1+\alpha)c_\hbar(x,\xi;y,\hbar\nabla_y)\\&+(1+\tfrac{1}{\alpha})C_\hbar(y,\hbar\nabla_y,z,\hbar\nabla_z)\\ C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z)\leq&(1+\alpha)C_\hbar(x,\hbar\nabla_x,y,\hbar\nabla_y)\\&+(1+\tfrac{1}{\alpha})C_\hbar(y,\hbar\nabla_y,z,\hbar\nabla_z)\end{aligned}$$

These operator inequalities mean that, for all $\phi \in \mathcal{S}(\mathbf{R}^{2d}_{x,\xi}\times\mathbf{R}^d_y\times\mathbf{R}^{2d}_{z,\zeta})$

$$\langle\phi|r.h.s. - l.h.s.|\phi\rangle \geq 0$$

Proof Write

$$\begin{aligned}C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z)=&|x-y+y-z|^2-\hbar^2|\nabla_x-\nabla_y+\nabla_y-\nabla_z|^2\\=&C_\hbar(x,\hbar\nabla_x,y,\hbar\nabla_y)+C_\hbar(y,\hbar\nabla_y,z,\hbar\nabla_z)\\&+2(x-y)\cdot(y-z)-2\hbar^2(\nabla_x-\nabla_y)\cdot(\nabla_y-\nabla_z)\end{aligned}$$

Use the Peter-Paul elementary inequality

$$2(x-y)\cdot(y-z) \leq \alpha|x-y|^2 + \tfrac{1}{\alpha}|y-z|^2$$

and, for operators A, B, the analogous inequality

$$A^*B + B^*A \leq \alpha|A|^2 + \tfrac{1}{\alpha}|B|^2$$

with $A = A^* = -i\hbar(\partial_{x_j} - \partial_{y_j})$ and $B = B^* = -i\hbar(\partial_{y_j} - \partial_{z_j})$ for all indices $j = 1, \ldots, d$. (Observe that these operators commute, which is inessential here). The operator inequality comes from expanding

$$0 \leq \left|\alpha^{\frac{1}{2}}A - \alpha^{-\frac{1}{2}}B\right|^2 = \alpha|A|^2 + \tfrac{1}{\alpha}|B|^2 - A^*B - B^*A$$

Hence

$$2(x-y)\cdot(y-z) - 2\hbar^2(\nabla_x - \nabla_y)\cdot(\nabla_y - \nabla_z)$$
$$\leq \alpha C_\hbar(x, \hbar\nabla_x, y, \hbar\nabla_y) + \tfrac{1}{\alpha}C_\hbar(y, \hbar\nabla_y, z, \hbar\nabla_z)$$

With the previous inequality involving $C_\hbar(x, \hbar\nabla_x, z, \hbar\nabla_z)$, we arrive at the 3rd inequality of Lemma 2. q.e.d.

Lemma 3 For all $\alpha > 0$, one has

$$c_\hbar(x,\xi;z,\hbar\nabla_z) \leq (1+\alpha)(|x-y|^2+|\xi-\eta|^2) + (1+\tfrac{1}{\alpha})c_\hbar(y,\eta;z,\hbar\nabla_z)$$

$$C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z) \leq (1+\alpha)c_\hbar(x,\hbar\nabla_x,y,\eta) + (1+\tfrac{1}{\alpha})c_\hbar(y,\eta,z,\hbar\nabla_z)$$

These operator inequalities mean that

$$\langle\phi|r.h.s.-l.h.s.|\phi\rangle \geq 0$$

for all $\phi \in \mathcal{S}(\mathbf{R}^{2d}_{x,\xi}\times\mathbf{R}^{d}_{y,\eta}\times\mathbf{R}^{2d}_{z,\zeta})$

Same method of proof as for Lemma 2.

Quiz 1

Write the proof of Lemma 3

Assume for example that ρ_1 and $\rho_2 \in \mathcal{D}_2(\mathfrak{H})$ while ρ_3 is a rank-1 density operator, and let $Q \in \mathcal{C}(\rho_1, \rho_2)$. Set

$$T := Q \otimes \rho_3 \,, \quad T_{13} = \operatorname{tr}_2 T \in \mathcal{C}(\rho_1, \rho_3)$$

Hence, by the 3rd inequality in Lemma 3

$$\begin{aligned}
\mathfrak{d}(\rho_1, \rho_3)^2 &\le \operatorname{tr}_{\mathfrak{H}^{\otimes 2}}(T_{13}^{\frac{1}{2}} C_\hbar(x, \hbar\nabla_x, z, \hbar\nabla_z) T_{13}^{\frac{1}{2}}) \\
&= \operatorname{tr}_{\mathfrak{H}^{\otimes 3}}(T^{\frac{1}{2}} C_\hbar(x, \hbar\nabla_x, z, \hbar\nabla_z) T^{\frac{1}{2}}) \\
&\le (1+\alpha) \operatorname{tr}_{\mathfrak{H}^{\otimes 3}}(T^{\frac{1}{2}} C_\hbar(x, \hbar\nabla_x, y, \hbar\nabla_y) T^{\frac{1}{2}}) \\
&\quad + (1+\tfrac{1}{\alpha}) \operatorname{tr}_{\mathfrak{H}^{\otimes 3}}(T^{\frac{1}{2}} C_\hbar(y, \hbar\nabla_y, z, \hbar\nabla_z) T^{\frac{1}{2}}) \\
&= (1+\alpha) \operatorname{tr}_{\mathfrak{H}^{\otimes 2}}(Q^{\frac{1}{2}} C_\hbar(x, \hbar\nabla_x, y, \hbar\nabla_y) Q^{\frac{1}{2}}) \\
&\quad + (1+\tfrac{1}{\alpha}) \underbrace{\operatorname{tr}_{\mathfrak{H}^{\otimes 2}}((\rho_2 \otimes \rho_3)^{\frac{1}{2}} C_\hbar(y, \hbar\nabla_y, z, \hbar\nabla_z) (\rho_2 \otimes \rho_3^{\frac{1}{2}})}_{=\mathfrak{d}(\rho_2, \rho_3)^2}
\end{aligned}$$

Minimizing the last r.h.s. in $Q \in \mathcal{C}(\rho_1, \rho_2)$ shows that

$$\mathfrak{d}(\rho_1, \rho_3)^2 \leq (1+\alpha)\mathfrak{d}(\rho_1, \rho_2)^2 + (1+\tfrac{1}{\alpha})\mathfrak{d}(\rho_2, \rho_3)^2$$

Minimizing the r.h.s. in $\alpha > 0$, i.e. setting

$$\alpha := \frac{\mathfrak{d}(\rho_2, \rho_3)}{\mathfrak{d}(\rho_1, \rho_2)} \quad \text{assuming } \mathfrak{d}(\rho_1, \rho_2) > 0$$

leads to

$$\mathfrak{d}(\rho_1, \rho_3)^2 \leq \mathfrak{d}(\rho_1, \rho_2)^2 + \mathfrak{d}(\rho_2, \rho_3)^2 + 2\mathfrak{d}(\rho_1, \rho_2)\mathfrak{d}(\rho_2, \rho_3)$$

Conclude by taking the square root of both sides of this inequality.

q.e.d.

Quiz 2

Complete the proof by justifying the equality

$$\operatorname{tr}_{\mathfrak{H}^{\otimes 2}}(T_{13}^{\frac{1}{2}} C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z) T_{13}^{\frac{1}{2}}) \\ = \operatorname{tr}_{\mathfrak{H}^{\otimes 3}}(T^{\frac{1}{2}} C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z) T^{\frac{1}{2}})$$

(1) Prove this identity when $C_\hbar$ is replaced with $(I_{\mathfrak{H}^{\otimes 2}} + \frac{1}{n} C_\hbar)^{-1} C_\hbar$

(2) Using the Fatou lemma for trace-class operators, prove that

$$\lim_{n\to\infty} \operatorname{tr}_{\mathfrak{H}^{\otimes 2}} \left(T_{13}^{\frac{1}{2}} \frac{C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z)}{I_{\mathfrak{H}^{\otimes 2}} + \frac{1}{n} C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z)} T_{13}^{\frac{1}{2}} \right) \\ = \operatorname{tr}_{\mathfrak{H}^{\otimes 2}} \left(T_{13}^{\frac{1}{2}} C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z) T_{13}^{\frac{1}{2}} \right)$$

$$\lim_{n\to\infty} \operatorname{tr}_{\mathfrak{H}^{\otimes 3}} \left(T^{\frac{1}{2}} \frac{C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z)}{I_{\mathfrak{H}^{\otimes 3}} + \frac{1}{n} C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z)} T^{\frac{1}{2}} \right) \\ = \operatorname{tr}_{\mathfrak{H}^{\otimes 3}} \left(T^{\frac{1}{2}} C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z) T^{\frac{1}{2}} \right)$$

Quiz 3

Complete the proof of Theorem 1 by treating the missing cases where one of the ρ_js is a rank-1 density operator.

Lemma 4 Let f be a probability density on $\mathbf{R}^d \times \mathbf{R}^d$, let $R \in \mathcal{D}(\mathfrak{H})$ and $Q \in \mathcal{C}(f, R)$. There exists a weakly measurable map

$$\mathbf{R}^d \times \mathbf{R}^d \ni (x, \xi) \mapsto Q_f(x, \xi) \in \mathcal{L}^1(\mathfrak{H})$$

defined a.e. so that

$$Q_f(x, \xi) = Q_f(x, \xi)^* \geq 0\,, \quad \mathrm{tr}(Q(x, \xi)) = 1$$

and

$$Q(x, \xi) = f(x, \xi) Q_f(x, \xi) \quad \text{a.e. in } (x, \xi) \in \mathbf{R}^d \times \mathbf{R}^d$$

Proof First replace f with a Borel representative, and consider the set $\mathcal{N} := f^{-1}(\{0\})$ which is Borel measurable. Pick $u \in \mathfrak{H}$ such that $\|u\|_{\mathfrak{H}} = 1$, and set

$$Q_f(x, \xi) := \frac{Q(x, \xi) + \mathbf{1}_{\mathcal{N}}(x, \xi)|u\rangle\langle u|}{f(x, \xi) + \mathbf{1}_{\mathcal{N}}(x, \xi)} \in \mathcal{L}(\mathfrak{H})$$

Obviously

$$Q(x,\xi)=Q(x,\xi)^*\geq 0 \ \&\ f(x,\xi)\geq 0 \implies Q_f(x,\xi)=Q_f(x,\xi)^*\geq 0$$

Moreover

$$\mathrm{tr}_{\mathfrak{H}}(Q(x,\xi)+\mathbf{1}_{\mathcal{N}}(x,\xi)|u\rangle\langle u|)=f(x,\xi)+\mathbf{1}_{\mathcal{N}}(x,\xi)$$

so that

$$\mathrm{tr}_{\mathfrak{H}}(Q_f(x,\xi))=1$$

Finally

$$f(x,\xi)Q_f(x,\xi)=\frac{f(x,\xi)Q(x,\xi)}{f(x,\xi)+\mathbf{1}_{\mathcal{N}}(x,\xi)}=Q(x,\xi)$$

Indeed, since $Q(x,\xi)=Q(x,\xi)^*\geq 0$ and $\mathrm{tr}_{\mathfrak{H}}(Q(x,\xi)=f(x,\xi)$, then $f(x,\xi)=0 \implies Q(x,\xi)=0$. q.e.d.

Proof of Triangle Inequality with Classical Mid-Point

Consider for example the case where both ρ_1 and $\rho_3 \in \mathcal{D}_2(\mathfrak{H})$, and assume that $\rho_2 = f(y,\eta)dyd\eta \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$. Choose couplings $Q^1 \in \mathcal{C}(\rho_1, f)$ while $Q^3 \in \mathcal{C}(f, \rho_3)$. Call Q^3_f the disintegration of Q^3 w.r.t. f as in Lemma 4. Set

$$T(y,\eta) := Q^1(y,\eta) \otimes Q^3_f(y,\eta)\,.$$

By construction

$$T(y,\eta) = T(y,\eta)^* \geq 0$$

and

$$\begin{aligned}\mathrm{tr}_1(T(y,\eta)) =& f(y,\eta)Q^3_f(y,\eta) = Q^3(y,\eta)\\ \mathrm{tr}_3(T(y,\eta)) =& Q^1(y,\eta)\,\mathrm{tr}_{\mathfrak{H}}(Q^3_f(y,\eta)) = Q^1(y,\eta)\end{aligned}$$

In particular

$$\int_{\mathbf{R}^{2d}} T(y,\eta)dyd\eta =: \mathcal{Q} \in \mathcal{C}(\rho_1, \rho_3)$$

By the 2nd inequality in Lemma 3

$$
\begin{aligned}
\mathfrak{d}(\rho_1,\rho_3)^2 &\le \mathrm{tr}_{\mathfrak{H}^{\otimes 2}}(\mathcal{Q}^{\frac12} C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z)\mathcal{Q}^{\frac12}) \\
&= \int_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}^{\otimes 2}}(T(y,\eta)^{\frac12} C_\hbar(x,\hbar\nabla_x,z,\hbar\nabla_z)T(y,\eta)^{\frac12})dyd\eta \\
&\le (1+\alpha)\int_{\mathbf{R}^{2d}} \mathrm{tr}_1\left(\mathrm{tr}_3(T(y,\eta)^{\frac12} c_\hbar(x,\hbar\nabla_x,y,\eta)T(y,\eta)^{\frac12})\right)dyd\eta \\
&+(1+\tfrac{1}{\alpha})\int_{\mathbf{R}^{2d}} \mathrm{tr}_3\left(\mathrm{tr}_1(T(y,\eta)^{\frac12} c_\hbar(x,\hbar\nabla_x,y,\eta)T(y,\eta)^{\frac12})\right)dyd\eta \\
&\le (1+\alpha)\int_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}(Q^1(y,\eta)^{\frac12} c_\hbar(x,\hbar\nabla_x,y,\eta)Q^1(y,\eta)^{\frac12})dyd\eta \\
&+(1+\tfrac{1}{\alpha})\int_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}\left(Q^3_f(y,\eta)^{\frac12} c_\hbar(x,\hbar\nabla_x,y,\eta)Q^3_f(y,\eta)^{\frac12}\right)f(y,\eta)dyd\eta
\end{aligned}
$$

Minimizing the last r.h.s. in $Q^1 \in \mathcal{C}(\rho_1,\rho_2)$ and in $Q^3 \in \mathcal{C}(\rho_2,\rho_3)$

$$
\mathfrak{d}(\rho_1,\rho_3)^2 \le (1+\alpha)\mathfrak{d}(\rho_1,\rho_2)^2 + (1+\tfrac{1}{\alpha})\mathfrak{d}(\rho_2,\rho_3)^2
$$

and we conclude as in the rank-1 case. q.e.d.

Quiz 4

(1) Complete the missing details in the proof of Theorem 1 in the case where $\rho_1, \rho_3 \in \mathcal{D}_2(\mathfrak{H})$ and $\rho_2 = f(y,\eta)dyd\eta$. In particular, prove the identity

$$\begin{aligned} &\operatorname{tr}_{\mathfrak{H}^{\otimes 2}}(\mathcal{Q}^{\frac{1}{2}} C_\hbar(x, \hbar\nabla_x, z, \hbar\nabla_z)\mathcal{Q}^{\frac{1}{2}}) \\ &= \int_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}^{\otimes 2}}(T(y,\eta)^{\frac{1}{2}} C_\hbar(x, \hbar\nabla_x, z, \hbar\nabla_z) T(y,\eta)^{\frac{1}{2}}) dy d\eta \end{aligned}$$

(2) Write the proof of Theorem 1 in the missing cases.

APPLICATIONS OF RESTRICTED TRIANGLE INEQUALITY

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Definition of $\mathfrak{d}$ on $\mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d) \times \mathcal{D}_2(\mathfrak{H})$

So far we have defined $\mathfrak{d}(\mu, R) = \mathfrak{d}(R, \mu)$ for $\mu \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ and $R \in \mathcal{D}_2(\mathfrak{H})$ only when $\mu = f(x,\xi)dxd\xi$ — i.e. only when $\mu \ll dxd\xi$.

Theorem 5

For each $R \in \mathcal{D}_2(\mathfrak{H})$, the map $f \mapsto \mathfrak{d}(f, R)$, defined for all f such that $f(x,\xi)dxd\xi \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ has a unique extension to $\mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ satisfying

$$|\mathfrak{d}(\mu, R) - \mathfrak{d}(\nu, R)| \le \mathcal{W}_2(f, g)\,, \qquad \mu, \nu \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$$

Proof For all f, g probability densities with finite 2nd order moments on $\mathbf{R}^d \times \mathbf{R}^d$, one has the triangle inequality

$$\mathfrak{d}(f, R) \le \mathfrak{d}(f, g) + \mathfrak{d}(g, R)$$

so that

$$\mathfrak{d}(f, R) - \mathfrak{d}(g, R) \le \mathfrak{d}(f, g) = \mathcal{W}_2(f, g)$$

Exchanging f and g in the inequality above implies that

$$|\mathfrak{d}(f, R) - \mathfrak{d}(g, R)| \le \mathcal{W}_2(f, g)$$

The function $f \mapsto \mathfrak{d}(f, R)$ is Lipschitz-continuous for the metric $\mathcal{W}_2$. It has a unique Lipschitz-continuous extension to $\mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ by the following density argument. q.e.d.

Lemma 6

Let $\mu \in \mathcal{P}_2(\mathbf{R}^n)$ and let $\chi_\epsilon(x) = \chi(x/\epsilon)/\epsilon^n$ be an even C^∞ mollifier with support in $B_\epsilon(0)$. Then $f_\epsilon := \chi_\epsilon \star \mu$ is a C^∞ probability density on $\mathbf{R}^n$ and

$$\mathcal{W}_2(f_\epsilon, \mu) \to 0 \quad \text{as } \epsilon \to 0$$

Proof For all $\phi \in C_0(\mathbf{R}^n)$, one has $\|\phi - \phi \star \chi_\epsilon\|_{L^\infty(\mathbf{R}^n)} \to 0$ as $\epsilon \to 0$. Hence $f_\epsilon \to \mu$ weakly in $\mathcal{P}(\mathbf{R}^n)$.

It remains to establish the tightness property. Assuming χ is even

$$\int_{\mathbf{R}^n} \mathbf{1}_{|x|>R} |x|^2 \chi_\epsilon \star \mu(x) dx = \int_{\mathbf{R}^n} \chi_\epsilon \star (\mathbf{1}_{|x|>R} |x|^2) \mu(dx)$$

On the other hand, for all $\epsilon \in (0,1)$

$$\chi_\epsilon \star (\mathbf{1}_{|x|>R}|x|^2) \leq \mathbf{1}_{|x|+1\geq R} \int_{\mathbf{R}^n} |x-\epsilon y|^2 \chi(y)dy$$

$$\leq 2\mathbf{1}_{|x|+1\geq R} \left(|x|^2 + \epsilon^2 \underbrace{\int_{\mathbf{R}^n} |y|^2 \chi(y)dy}_{\leq 1} \right)$$

Hence

$$\sup_{0<\epsilon<1} \int_{\mathbf{R}^n} \mathbf{1}_{|x|>R}|x|^2 \chi_\epsilon \star \mu(x)dx \leq 2\int_{\mathbf{R}^n} \mathbf{1}_{|x|+1>R}(|x|^2+1)\mu(dx) \to 0$$

as $R \to \infty$, by dominated convergence.

Therefore

$$\mathcal{W}_2(\chi_\epsilon \star \mu, \mu) \to 0 \qquad \text{as } \epsilon \to 0$$

q.e.d.

$\mathcal{W}_2$ is the Classical Limit of $\mathfrak{d}$

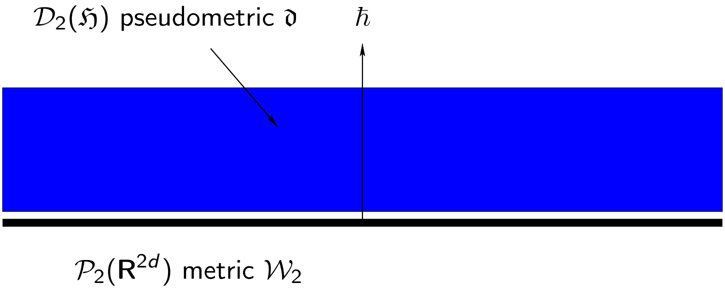
Theorem 7

Let $R_\hbar, S_\hbar \in \mathcal{D}_2(\mathfrak{H})$ and $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$. Assume that μ, ν are the classical limits of $R_\hbar, S_\hbar$ respectively, i.e.

$$\mathfrak{d}(\mu, R_\hbar) + \mathfrak{d}(\nu, S_\hbar) \to 0 \quad \text{as } \hbar \to 0$$

Then

$$\lim_{\hbar \to 0} \mathfrak{d}(R_\hbar, S_\hbar) = \mathfrak{d}(\mu, \nu)$$



Proof By the restricted triangle inequality

$$\mathfrak{d}(R_\hbar, S_\hbar) \leq \mathfrak{d}(R_\hbar, \mu) + \mathfrak{d}(\mu, \nu) + \mathfrak{d}(\nu, S_\hbar)$$

so that

$$\overline{\lim_{\hbar \to 0}} \, \mathfrak{d}(R_\hbar, S_\hbar) \leq \mathfrak{d}(\mu, \nu) = \mathcal{W}_2(\mu, \nu)$$

On the other hand, by Theorem 1 (2) of Lecture 1

$$\mathfrak{d}(R_\hbar, \mu)^2 \geq \mathcal{W}_2(\mathcal{H}[R_\hbar], \mu)^2 - d\hbar \implies \lim_{\hbar \to 0} \mathcal{W}_2(\mathcal{H}[R_\hbar], \mu) = 0$$

$$\mathfrak{d}(S_\hbar, \nu)^2 \geq \mathcal{W}_2(\mathcal{H}[S_\hbar], \nu)^2 - d\hbar \implies \lim_{\hbar \to 0} \mathcal{W}_2(\mathcal{H}[S_\hbar], \nu) = 0$$

Hence

$$\mathfrak{d}(R_\hbar, S_\hbar)^2 \geq \mathcal{W}_2(\mathcal{H}[R_\hbar], \mathcal{H}[S_\hbar])^2 - 2d\hbar$$

implies that

$$\underline{\lim}_{\hbar\to 0} \mathfrak{d}(R_\hbar, S_\hbar) \geq \lim_{\hbar\to 0} \mathcal{W}_2(\mathcal{H}[R_\hbar], \mathcal{H}[S_\hbar]) = \mathcal{W}_2(\mu, \nu)$$

Summarizing

$$\mathcal{W}_2(\mu, \nu) \leq \underline{\lim}_{\hbar\to 0} \mathfrak{d}(R_\hbar, S_\hbar) \leq \overline{\lim}_{\hbar\to 0} \mathfrak{d}(R_\hbar, S_\hbar) \leq \mathcal{W}_2(\mu, \nu)$$

q.e.d.

QUANTUM KANTOROVICH DUALITY

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E. Caglioti, F.G., T. Paul: arXiv: 2101.03256 [math-ph], to appear in Ann. Sc. Norm. Super. Pisa Cl. Sci. (5)

First we consider the case of $\mathfrak{d}(f,R)$ where f is a probability density on $\mathbf{R}^d\times\mathbf{R}^d$ with finite 2nd order moments and $R\in\mathcal{D}_2(\mathfrak{H})$.

Define the set $\mathfrak{k}$ of test Kantorovich potentials as follows

$$\mathfrak{k}:=\{(a,B)\;:\;a\in C_b(\mathbf{R}^d\times\mathbf{R}^d)\text{ and }B=B^*\in\mathcal{L}(\mathfrak{H})\\ \text{s.t. }\;a(x,\xi)I_{\mathfrak{H}}+B\le c_\hbar(x,\xi)\}$$

The operator inequality means that for all $\phi\in H^1(\mathbf{R}^d)\cap L^2(\mathbf{R}^d;|y|^2dy)$

$$a(x,\xi)\|\phi\|^2_{\mathfrak{H}}+\langle\phi|B|\phi\rangle\le\langle\phi|c_\hbar(x,\xi)|\phi\rangle\,,\qquad x,\xi\in\mathbf{R}^d$$

Theorem 8 Under the above conditions on f and R

$$\mathfrak{d}(f,R)^2=\min_{Q\in\mathcal{C}(f,R)}\int_{\mathbf{R}^{2d}}\operatorname{tr}_{\mathfrak{H}}\left(Q(x,\xi)^{\frac12}c_\hbar(x,\xi)Q(x,\xi)^{\frac12}\right)dxd\xi$$
$$=\sup_{(a,B)\in\mathfrak{k}}\left(\int_{\mathbf{R}^{2d}}a(x,\xi)f(x,\xi)dxd\xi+\operatorname{tr}_{\mathfrak{H}}(BR)\right)$$

Set $\mathcal{E} := C_b(\mathbf{R}^{2d}; \mathcal{L}(\mathfrak{H}))$ with $\|T\|_E := \sup_{x,\xi\in\mathbf{R}^d} \|T(x,\xi)\|_{\mathcal{L}(\mathfrak{H})}$,

$$G(T) := \begin{cases} 0 & \text{if } T(x,\xi) = T(x,\xi)^* \geq -c_\hbar(x,\xi) \\ +\infty & \text{otherwise} \end{cases}$$

and

$$H(T) := \begin{cases} \int_{\mathbf{R}^{2d}} af(x,\xi)dxd\xi + \operatorname{tr}_{\mathfrak{H}}(BR) & \text{if } \begin{cases} T(x,\xi) = T(x,\xi)^* \\ = a(x,\xi)I_{\mathfrak{H}} + B \end{cases} \\ +\infty & \text{otherwise} \end{cases}$$

Theorem 8 follows from the Fenchel-Rockafellar duality formula

$$\inf_{T\in E}(G(T)+H(T)) = \max_{\Lambda\in E'}(-G^*(-\Lambda) - H^*(\Lambda))$$

Next we consider the case of $\mathfrak{d}(R, S)$ where $R, S \in \mathcal{D}_2(\mathfrak{H})$.

Define the set $\mathfrak{K}$ of test Kantorovich potentials as follows

$$\begin{aligned}\mathfrak{K} := \{(A, B) \,:\, A = A^* \text{ and } B = B^* \in \mathcal{L}(\mathfrak{H}) \\ \text{s.t. } A \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes B \le C_\hbar\}\end{aligned}$$

The operator inequality means that for all $\Phi \equiv \Phi(x, y) \in \mathfrak{H} \otimes \mathfrak{H}$ s.t. $(\nabla_x - \nabla_y)\Phi \in L^2(\mathbf{R}^d \times \mathbf{R}^d)$ and $\Phi \in L^2(\mathbf{R}^d; |x-y|^2 dxdy)$

$$\langle \Phi | A \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes B | \Phi \rangle \le \langle \Phi | C_\hbar | \Phi \rangle$$

Theorem 9 For all $R, S \in \mathcal{D}_2(\mathfrak{H})$, one has

$$\mathfrak{d}(R, S)^2 = \min_{T \in \mathcal{C}(R,S)} \mathrm{tr}_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac{1}{2}} C_\hbar T^{\frac{1}{2}}) = \sup_{(A,B)\in\mathfrak{K}} \mathrm{tr}_{\mathfrak{H}}(AR + BS)$$

GENERALIZED TRIANGLE INEQUALITY

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In general, we do not know how to disintegrate $Q_{12} \in \mathcal{C}(R_1, R_2)$ w.r.t. R_2 for $R_1, R_2 \in \mathcal{D}_2(\mathfrak{H})$, and we do not know how to glue along R_2 couplings $Q_{12} \in \mathcal{C}(R_1, R_2)$ and $Q_{23} \in \mathcal{C}(R_2, R_3)$. Therefore, the proof of the triangle inequality for $\mathcal{W}_2$ does not seem to have an analogue for $\mathfrak{d}$ when the mid-point is a density operator of rank > 1.

Theorem 10

For all $\rho_1, \rho_2, \rho_3 \in \mathfrak{D}$, one has

$$\mathfrak{d}(\rho_1, \rho_3) < \mathfrak{d}(\rho_1, \rho_2) + \mathfrak{d}(\rho_2, \rho_3) + \sqrt{d\hbar}$$

In particular

$$\mathfrak{d}(\rho_1, \rho_3) < \mathfrak{d}(\rho_1, \rho_2) + \mathfrak{d}(\rho_2, \rho_3) + \frac{1}{\sqrt{2}}\mathfrak{d}(\rho_2, \rho_2)$$

Remark Compare this result with the De Palma-Trevisan triangle inequality for their distance [Ann. H. Poincaré 2021]

Lemma 11 For each $R, S \in \mathcal{D}_2(\mathfrak{H})$, one has

$$\mathfrak{d}(R,S)^2 \geq \mathfrak{d}(R,\mathcal{H}[S])^2 - d\hbar$$

Proof of Thm 10 Using $\mathcal{H}[\rho_2]$ as mid-point, the restricted triangle inequality implies that

$$\mathfrak{d}(\rho_1,\rho_3) \leq \mathfrak{d}(\rho_1,\mathcal{H}[\rho_2]) + \mathfrak{d}(\mathcal{H}[\rho_2],\rho_3)$$

Lemma 11 implies that

$$\mathfrak{d}(\rho_1,\mathcal{H}[\rho_2]) \leq \sqrt{\mathfrak{d}(\rho_1,\rho_2)^2 + d\hbar} < \mathfrak{d}(\rho_1,\rho_2) + \tfrac{1}{2}\sqrt{d\hbar}$$
$$\mathfrak{d}(\mathcal{H}[\rho_2],\rho_3) \leq \sqrt{\mathfrak{d}(\rho_2,\rho_3)^2 + d\hbar} < \mathfrak{d}(\rho_2,\rho_3) + \tfrac{1}{2}\sqrt{d\hbar}$$

The second inequalities above result from the following elementary observation

$$X > Y > 0 \implies \sqrt{X^2 + Y^2} \leq X + \tfrac{1}{2}Y$$

With the restricted triangle inequality above, this implies the first generalized triangle inequality.
To get the second inequality, observe that

$$\rho_2 \in \mathcal{D}_2(\mathfrak{H}) \implies \mathfrak{d}(\rho_2, \rho_2) \geq \sqrt{2d\hbar}$$

q.e.d.

Remark in fact, we have proved the more precise inequality

$$\mathfrak{d}(\rho_1, \rho_3) \leq \sqrt{\mathfrak{d}(\rho_1, \rho_2)^2 + d\hbar} + \sqrt{\mathfrak{d}(\rho_2, \rho_3)^2 + d\hbar}$$

For all $a \in C_b(\mathbf{R}^d \times \mathbf{R}^d)$ and $B = B^* \in \mathcal{L}(\mathfrak{H})$ satisfying

$$a(x,\xi)I_{\mathfrak{H}} + B \le c_\hbar(x,\xi)$$

one applies the Toeplitz map to the variables x, ξ, to find

$$\begin{aligned}\mathcal{T}[a] \otimes I_{\mathfrak{H}} + (2\pi\hbar)^d I_{\mathfrak{H}} \otimes B \le& (2\pi\hbar)^d \int |q,p\rangle\langle q,p| c_\hbar(q,p)dqdp \\ \le& (2\pi\hbar)^d \left(C_\hbar + d\hbar I_{\mathfrak{H}\otimes\mathfrak{H}}\right)\end{aligned}$$

(see the formula of Lecture 1 for the image of quadratic functions by the Toeplitz map). Thus, for all $T \in \mathcal{C}(R,S)$, one has

$$\begin{aligned}&(2\pi\hbar)^d \left(Tr_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac{1}{2}} C_\hbar T^{\frac{1}{2}}) + d\hbar \right) \\ \ge& \operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}} \left(T^{\frac{1}{2}} (\mathcal{T}[a] \otimes I_{\mathfrak{H}} + (2\pi\hbar)^d I_{\mathfrak{H}} \otimes B \right) T^{\frac{1}{2}}) \\ =& \operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}} \left(T(\mathcal{T}[a] \otimes I_{\mathfrak{H}} + (2\pi\hbar)^d I_{\mathfrak{H}} \otimes B \right)) \\ =& \operatorname{tr}_{\mathfrak{H}}(R\mathcal{T}[a]) + (2\pi\hbar)^d \operatorname{tr}_{\mathfrak{H}}(SB)\end{aligned}$$

Transforming $\mathrm{tr}_{\mathfrak{H}}(R\mathcal{T}[a])$ into an integral involving the functions a and $\mathcal{H}[R]$, i.e. (see lecture 1, formula (4) on Husimi transforms)

$$\mathrm{tr}_{\mathfrak{H}}(R\mathcal{T}[a]) = (2\pi\hbar)^d \int_{\mathbf{R}^{2d}} \mathcal{H}[R](q,p)a(q,p)dqdp$$

we arrive at the formula

$$\begin{aligned} &(2\pi\hbar)^d \left(Tr_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac{1}{2}} C_\hbar T^{\frac{1}{2}}) + d\hbar \right) \\ \geq (2\pi\hbar)^d &\left(\int_{\mathbf{R}^{2d}} \mathcal{H}[R](q,p)a(q,p)dqdp + \mathrm{tr}_{\mathfrak{H}}(SB) \right) \end{aligned}$$

Maximizing the r.h.s. in $a \in C_b(\mathbf{R}^d \times \mathbf{R}^d)$ and $B = B^* \in \mathcal{L}(\mathfrak{H})$ s.t.

$$a(x,\xi)I_{\mathfrak{H}} + B \le c_\hbar(x,\xi)$$

and applying the duality formula shows that

$$(2\pi\hbar)^d \left(Tr_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac{1}{2}} C_\hbar T^{\frac{1}{2}}) + d\hbar \right) \ge (2\pi\hbar)^d \mathfrak{d}(\mathcal{H}[R], S)^2$$

i.e.

$$Tr_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac{1}{2}} C_\hbar T^{\frac{1}{2}}) \ge \mathfrak{d}(\mathcal{H}[R], S)^2 - d\hbar$$

Minimizing the l.h.s. in $T \in \mathcal{C}(R, S)$ leads to the desired inequality.

q.e.d.

Quiz 5

Use Lemma 11 to recover the following result (already proved in Lecture 1)

$$\mathfrak{d}(R,S)^2 \geq \mathfrak{d}(\mathcal{H}[R],\mathcal{H}[S])^2 - 2d\hbar$$

Remark If you include the proof of the duality formula, this is the longest and most difficult proof of the inequality above... On the other hand, Lemma 11 is a (much) stronger statement — it is the key to the generalized triangle inequality. That its proof is more involved is only natural.

Remarks

Summarizing, in order to prove the triangle inequality for $\mathfrak{d}$ when the intermediate point is not a classical density and none of the density operator involved is a rank-1 projection, you
(1) first use the exact triangle inequality

$$\mathfrak{d}(\rho_1, \rho_3) \leq \mathfrak{d}(\rho_1, \mathcal{H}[\rho_2]) + \mathfrak{d}(\mathcal{H}[\rho_2], \rho_3)$$

(2) and then pay the price for replacing ρ_2 with its Husimi function

$$\mathfrak{d}(\rho_1, \rho_3) \leq \sqrt{\mathfrak{d}(\rho_1, \rho_2)^2 + d\hbar} + \sqrt{\mathfrak{d}(\rho_2, \rho_3)^2 + d\hbar}$$

by Kantorovich duality for the the classical-to-quantum distance. The end of the proof is Kindergarten analysis.

The reason for the detour through $\mathcal{H}[\rho_2]$ instead of ρ_2 is due to the fact that we do not know how to solve the following quiz — which is, up to our (=FG+TP) knowledge, a (partially) open question

Quiz 6

Before working on this exercise, it is a good idea to review the proofs of Theorem 7.3 (triangle inequality for $\mathcal{W}_p$) and Lemma 7.6 (disintegration+glueing of couplings) in [Villani: TOT, AMS 2003].
Pick $\rho_1, \rho_2, \rho_3 \in \mathcal{D}_2(\mathfrak{H})$, all of them or rank ≥ 2 — otherwise, there is nothing to prove. Pick R_{12} and R_{23} to be optimal couplings of ρ_1, ρ_2 and ρ_2, ρ_3 (recall briefly why such couplings exist...)

(1) Assume there exists $T \in \mathcal{D}(\mathfrak{H} \otimes \mathfrak{H} \otimes \mathfrak{H})$ such that

$$\mathrm{tr}_1(T) = R_{23} \quad \text{and} \quad \mathrm{tr}_3(T) = R_{12}$$

Prove that

$$\mathfrak{d}(\rho_1, \rho_3) \leq \mathfrak{d}(\rho_1, \rho_2) + \mathfrak{d}(\rho_2, \rho_3)$$

(Hint: observe that $\mathrm{tr}_2(T) \in \mathcal{C}(\rho_1, \rho_3)$.)

Therefore, proving the triangle inequality boils down to proving the existence of such a T. The classical analogue of this is precisely the content of Lemma 7.6 in Villani's book.

Let us consider this problem in finite dimension: $\mathfrak{H} = \mathbf{C}^2$ (2 is the first interesting dimension, because if one of the densities ρ_j for $j = 1, 2, 3$ has rank one, the triangle inequality is known).
(2) Let $R, R' \in M_2(\mathbf{C})$. Find a necessary and sufficient condition on R, R' such that there exists $A, B, C \in M_2(\mathbf{C})$ for which the block-wise matrix

$$T := \begin{pmatrix} A & B \\ B^* & C \end{pmatrix}, \qquad A = A^*, \; C = C^*$$

satisfies

$$\tau'(T) := A + C = R \quad \text{and} \quad \tau(T) := \begin{pmatrix} \operatorname{tr}(A) & \operatorname{tr}(B) \\ \operatorname{tr}(B^*) & \operatorname{tr}(C) \end{pmatrix} = R'$$

(3) Assume now that $R, R' \in M_2(M_2(\mathbf{C}))$. Find a necessary and sufficient condition on R, R' such that there exists $A, B, C \in M_2(M_2(\mathbf{C}))$ for which the block-wise matrix

$$T := \begin{pmatrix} A & B \\ B^* & C \end{pmatrix}, \qquad A = A^*, \ C = C^*$$

satisfies

$$\tau'(T) = A + C = R \quad \text{and} \quad \begin{pmatrix} \mathrm{tr}_{M_2(\mathbf{C})}(A) & \mathrm{tr}_{M_2(\mathbf{C})}(B) \\ \mathrm{tr}_{M_2(\mathbf{C})}(B^*) & \mathrm{tr}_{M_2(\mathbf{C})}(C) \end{pmatrix} = R'$$

The notations need being explained. An element of $B \in M_2(M_2(\mathbf{C}))$ is of the form

$$B = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix} \quad \text{with } B_{kl} \in M_2(\mathbf{C})$$

Then

$$B^* := \begin{pmatrix} \overline{B_{11}^T} & \overline{B_{21}^T} \\ \overline{B_{12}^T} & \overline{B_{22}^T} \end{pmatrix}$$

while

$$\mathrm{tr}_{M_2(\mathbf{C})}(B) := B_{11} + B_{22}$$

(4) Explain how (3) is related to the problem of finding T as in (1), in the case where $\rho_1, \rho_2, \rho_3 \in \mathcal{D}(\mathbf{C}^2)$.
(5) Assuming that $R, R' \in \mathcal{D}(\mathbf{C}^2)$, does (the) block-wise matrix (matrices) T obtained in (3) satisfy $T = T^* \geq 0$?

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Denote $z := (x, \xi) \in \mathbf{R}^d \times \mathbf{R}^d$ and $Z := (y, -i\hbar\nabla_y)$, with

$$z \cdot Z := x \cdot y - i\hbar\xi \cdot \nabla_y$$

Thus $c_\hbar(x, \xi) = |Z|^2 + |z|^2 I_{\mathfrak{H}} - 2z \cdot Z \geq d\hbar I_{\mathfrak{H}}$ and by Weyl's theorem

$$\tilde{B} \in \mathcal{L}(\mathfrak{H}) \implies c_\hbar(z)^{-1}\tilde{B} \in \mathcal{K}(\mathfrak{H}) \implies \text{ess-spec}(c_\hbar(z) - \tilde{B}) = \varnothing$$

Assume that $\tilde{B} = \tilde{B}^*$ is such that $c_\hbar(z) - \tilde{B}$ has nondegenerate ground state for each $z \in \mathbf{R}^{2d}$ — for instance choose for $\tilde{B}$ a bounded multiplication operator (see [Reed-Simon IV, Thm XIII.47]) — and define next

$$\tilde{a}(z) := \min \operatorname{spec}(c_\hbar(z) - \tilde{B}) = \inf_{\|\phi\|_{\mathfrak{H}}=1} \langle \phi | c_\hbar(z) - \tilde{B} | \phi \rangle$$

$$\implies c_\hbar(z) - \tilde{B} \geq \tilde{a}(z) I_{\mathfrak{H}}$$

Besides $z \mapsto \tilde{a}(z)$ is continuous (even real-analytic) by the Kato-Rellich theorem (cf. [Reed-Simon IV, Thm XII.8]), and

$$\tilde{a}(z) \le \langle z|c_\hbar(z) - \tilde{B}|z\rangle = d\hbar - \langle z|\tilde{B}|z\rangle \le d\hbar + \|\tilde{B}\|$$
$$\tilde{a}(z) \ge d\hbar + \inf_{\|\phi\|_{\mathfrak{H}}=1} \langle\phi| - \tilde{B}|\phi\rangle \ge d\hbar - \|\tilde{B}\|$$

Hence $\tilde{a} \in C_b(\mathbf{R}^d \times \mathbf{R}^d)$ and we have obtained in this way

$$(\tilde{a}, \tilde{B}) \in \mathfrak{k}$$

The Kato-Rellich theorem also implies the existence of a continuous (even real-analytic) map

$$\mathbf{R}^d \times \mathbf{R}^d \ni z \mapsto \psi_z \in \mathfrak{H} \quad \text{s.t.} \quad \begin{cases} (c_\hbar(z) - \tilde{B})\psi_z = \tilde{a}(z)\psi_z \\ \text{and } \|\psi_z\|_{\mathfrak{H}} = 1,\ z \in \mathbf{R}^{2d} \end{cases}$$

Theorem 12

Under the assumptions above, for each probability density f with finite 2nd order moments, the map $z \mapsto f(z)|\psi_z\rangle\langle\psi_z|$ is an optimal coupling for the pseudometric $\mathfrak{d}$ between f and the operator

$$\mathcal{T}^{\tilde{B}}[f] := \int_{\mathbf{R}^{2d}} f(z)|\psi_z\rangle\langle\psi_z|dz \in \mathcal{D}_2(\mathfrak{H}) .$$

Example Take for example $\tilde{B} = 0$; then, one easily checks that

$$\tilde{a}(z) = d\hbar \,, \quad \ker(c_\hbar(z) - d\hbar I_{\mathfrak{H}}) = \mathbf{C}|z\rangle$$

where $|z\rangle$ is the Schrödinger coherent state centered at z, so that $\mathcal{T}^0[f] = \mathcal{T}[f]$ is the Toeplitz operator of symbol f. We already knew from Theorem 1 (1) in lecture 1 that

$$\mathfrak{d}(f, \mathcal{T}[f]) = \sqrt{d\hbar} = \inf_{\mathcal{P}_2(\mathbf{R}^{2d}) \times \mathcal{D}_2(\mathfrak{H})} \mathfrak{d}$$

Proof of Theorem 12

Set $Q(z) := f(z)|\psi_z\rangle\langle\psi_z|$, so that $Q(z)^{\frac{1}{2}} = \sqrt{f(z)}|\psi_z\rangle\langle\psi_z|$, and

$$\int_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}\left(Q(z)^{\frac{1}{2}} c_\hbar(z) Q(z)^{\frac{1}{2}}\right) dz = \int_{\mathbf{R}^{2d}} \langle\psi_z|c_\hbar(z)|\psi_z\rangle f(z)dz$$
$$= \int_{\mathbf{R}^{2d}} (\tilde{a}(z)\langle\psi_z|\psi_z\rangle + \langle\psi_z|B|\psi_z\rangle)f(z)dz$$
$$= \int_{\mathbf{R}^{2d}} \tilde{a}(z)f(z)dz + \mathrm{tr}_{\mathfrak{H}}\left(\tilde{B}\mathcal{T}^{\tilde{B}}[f]\right)$$

Since $(\tilde{a}, \tilde{B}) \in \mathfrak{k}$ and $Q \in \mathcal{C}(f, \mathcal{T}^{\tilde{B}}[f])$, this implies that

$$\int_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}\left(Q(z)^{\frac{1}{2}} c_\hbar(z) Q(z)^{\frac{1}{2}}\right) dz$$
$$= \min_{T \in \mathcal{C}(f, \mathcal{T}^{\tilde{B}}[f])} \int_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}\left(T(z)^{\frac{1}{2}} c_\hbar(z) T(z)^{\frac{1}{2}}\right) dz = \mathfrak{d}\left(f, \mathcal{T}^{\tilde{B}}[f]\right)^2$$

This also implies that

$$\int_{\mathbf{R}^{2d}} \tilde{a}(z)f(z)dz + \mathrm{tr}_{\mathfrak{H}}\left(\tilde{B}\mathcal{T}^{\tilde{B}}[f]\right)$$
$$= \sup_{(a,B)\in\mathfrak{k}} \int_{\mathbf{R}^{2d}} a(z)f(z)dz + \mathrm{tr}_{\mathfrak{H}}\left(B\mathcal{T}^{\tilde{B}}[f]\right)$$

— so that in this case, the sup is attained in $\mathfrak{k}$ (not true in general).

q.e.d.

Remark Thus the optimal transport map for $\mathfrak{d}$ between $\mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$ and $\mathcal{D}_2(\mathfrak{H})$ can be thought of as a **deformation** of the Toeplitz quantization, at least when $\tilde{B}$ is such that $c_\hbar(z) - \tilde{B}$ has a ground state of geometric multiplicity 1.

Question In Brenier's theorem, the classical optimal transport map is the gradient of a convex function. Is there some analogous property in the quantum setting?

If $(\tilde{a}, \tilde{B}) \in \mathfrak{k}$, one has

$$\underbrace{|Z|^2 + |z|^2 I_{\mathfrak{H}} - 2z \cdot Z}_{=c_\hbar(z)} \geq \tilde{a}(z) I_{\mathfrak{H}} + \tilde{B} \iff a(z) + B \geq z \cdot Z$$

with

$$a(z) := \tfrac{1}{2}(|z|^2 - \tilde{a}(z)) , \qquad B = \tfrac{1}{2}(|Z|^2 - \tilde{B})$$

One has $\mathrm{Dom}(c_\hbar(z)) = \mathrm{Dom}(|Z|^2) = H^2(\mathbf{R}^d) \cap L^2(\mathbf{R}^d, |y|^4 dy) =: D$

Definition Let B satisfy $|Z|^2 - 2B \in \mathcal{L}(\mathfrak{H})$. The Legendre dual of B is the convex function (upper enveloppe of affine functions)

$$B^L(z) := \sup_{\substack{\phi \in D \\ \|\phi\|_{\mathfrak{H}} = 1}} (z \cdot \langle \phi | Z | \phi \rangle - \langle \phi | B | \phi \rangle)$$

Theorem 13

(1) Under the same assumptions as in Theorem 12, setting

$$a(z) := \tfrac{1}{2}(|z|^2 - \tilde{a}(z)), \qquad B := \tfrac{1}{2}(|Z|^2 - \tilde{B})$$

one has

$$a = B^L$$

(2) Besides

$$\nabla a(z) = z - \nabla \tilde{a}(z) = \langle \psi_z | Z | \psi_z \rangle$$

Proof (1) follows from the definition and the variational formula for the ground state. As for (2), differentiate in z the identity

$$B\psi_z - z \cdot Z\psi_z + a(z)\psi_z = 0$$

and take the inner product with ψ_z to get

$$\underbrace{\langle \psi_z | B - z \cdot Z + a(z) | \dot{\psi}_z \rangle}_{=0 \text{ since } B=B^*,\, Z=Z^*,\, a(z)\in\mathbf{R}} + \langle \psi_z | -Z + \nabla a(z) | \psi_z \rangle = 0$$

q.e.d.

Remarks

(1) In the Knott-Smith theorem, optimal couplings for $\mathcal{W}_2$ are supported in the graph of the subdifferential of a l.c.s. convex function, while, in the Brenier theorem, the optimal transport map is the gradient of a convex function — in both cases, the function is obtained from an optimal Kantorovich potential by the same transformation as $\tilde{a} \mapsto a$. Theorem 13 (2) is a partial analogue of this crucial piece of information, except that, in the quantum setting, density operators are not "functions of Z".

(2) In classical optimal transport, there exist an optimal pair (a, b) of Kantorovich potentials; they are l.c.s. proper convex functions and are Legendre duals of each other, so that $\nabla a \circ \nabla b = \mathrm{Id}$; besides $a \in L^1_\mu$ and $b \in L^1_\nu$. In the present case, how should one define a "quantum gradient" of B?

(2') The idea is to use the phase space symplectic structure. For a smooth function $\alpha \equiv \alpha(x, \xi)$ on $\mathbf{R}^d \times \mathbf{R}^d$, one has

$$\partial_{x_j}\alpha = \{\xi_j, \alpha\}\,, \quad \partial_{\xi_j}\alpha = -\{x_j, \alpha\}\,, \qquad j = 1, \ldots, d$$

This suggests to define

$$\partial^Q_{y_j} B := \tfrac{i}{\hbar}[-i\hbar\partial_{y_j}, B]\,, \quad \partial^Q_{\eta_j} B := -\tfrac{i}{\hbar}[y_j, B]$$

Since

$$B\psi_z = z \cdot Z\psi_z + a(z)\psi_z\,, \quad B = B^*\,, \quad Z = Z^* \text{ and } a(z) \in \mathbf{R}$$

one easily checks that

$$\begin{cases} x_j = \langle \psi_z | \partial^Q_{y_j} B | \psi_z \rangle \\ \xi_j = \langle \psi_z | \partial^Q_{\eta_j} B | \psi_z \rangle \end{cases} \qquad j = 1, \ldots, d$$

This formula can be viewed as the inverse transform of Thm 13 (2)

(3) Analogous ideas on a definition of an optimal transport "map" between elements of $\mathcal{D}_2(\mathfrak{H})$ can be found in Caglioti-F.G.-Paul [arXiv: 2101.03256 [math-ph], Ann. SNS Pisa, to appear]. Partial results analogous to Theorem 13 have been obtained, but much remains to be done.

The proof of Theorem 13 suggests viewing the operator

$$-\tfrac{1}{2}(|x|^2 - \hbar^2\Delta_x - A)$$

as the "smallest eigenvalue" of the operator

$$\tfrac{1}{2}(|y|^2 - \hbar^2\Delta_y - B) - x\cdot y + \hbar^2\nabla_x\cdot\nabla_y$$

viewed as a "matrix" whose entries are operators in the x-variables. New ideas on this problem are obviously needed.