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► **To cite this version:**

François Golse, Thierry Paul. Optimal transport pseudometrics for quantum and classical densities. Journal of Functional Analysis, 2022, 282 (9), pp.109417. 10.1016/j.jfa.2022.109417. hal-03671845

HAL Id: hal-03671845

<https://u-paris.hal.science/hal-03671845v1>

Submitted on 22 Jul 2024

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OPTIMAL TRANSPORT PSEUDOMETRICS FOR QUANTUM AND CLASSICAL DENSITIES

FRANÇOIS GOLSE AND THIERRY PAUL

ABSTRACT. This paper proves variants of the triangle inequality for the quantum analogues of the Wasserstein metric of exponent 2 introduced in [F. Golse, C. Mouhot, T. Paul: Commun. Math. Phys. **343** (2016), 165–205] to compare two density operators, and in [F. Golse, T. Paul: Arch. Rational Mech. Anal. **223** (2017), 57–94] to compare a phase space probability measure and a density operator. The argument differs noticeably from the classical proof of the triangle inequality for Wasserstein metrics, which is based on a disintegration theorem for probability measures, and uses in particular an analogue of the Kantorovich duality for the functional defined in [F. Golse, T. Paul: loc. cit.]. Finally, this duality theorem is used to define an analogue of the Brenier transport map for the functional defined in [F. Golse, T. Paul: loc. cit.] to compare a phase space probability measure and a density operator.

1. INTRODUCTION

Quantum mechanics is known to be well approximated by classical mechanics in situations where high frequency oscillations in the wave functions are involved, by analogy with the approximation of “wave optics” by geometrical optics (as explicitly mentioned by Landau and Lifshitz at the beginning of §46 in [17]).

However, there is no true analogue of the wave function (defined on the configuration space) in classical mechanics which is formulated on the phase space of the system. The classical limit of quantum mechanics can be expressed in terms of the convergence of functions or distributions (the Wigner, or the Husimi functions) on phase space associated to the orthogonal projections on the line spanned by the wave functions (in the case of pure quantum states), or more generally with the density operators (in the case of quantum mixed states) of the particles considered [18, 12]. The high frequency oscillations mentioned above are captured by the momentum dependence of the values of these functions on phase space, which remains present after passing to the limit in the sense of distributions. These are the appropriate notions of convergence used in the mathematical description of the classical limit: see for instance Theorems III.1 and III.2 in [18], or section 1 in [12].

On the other hand, the weak convergence of Borel probability measures in Euclidean spaces is known to be metrized by a class of distances originating from generalizations of the Monge problem of optimal transport. These distances are associated with various names, and referred to as either Monge-Kantorovich, or

Date: February 1, 2022.

1991 Mathematics Subject Classification. 49Q22, 81Q20 (81Q05).

Key words and phrases. Quantum Wasserstein metric, Triangle inequality, Kantorovich duality, Classical limit, Optimal transport.

Kantorovich-Rubinstein, or Wasserstein distances: see chapter 7 of [22] for a complete description, and especially Theorem 7.12 in that chapter for the topological properties of these distances. See also [5] for a fast and yet rather detailed description of the case of discrete measures.

This suggests the idea of comparing a quantum state and its classical limit by measuring the Monge-Kantorovich-Rubinstein-Wasserstein distance between its Husimi function and its weak limit. Similarly, one could compare two quantum states by measuring the Monge-Kantorovich-Rubinstein-Wasserstein distance between their Husimi functions: this is the approach followed by Życzkowski and Słomczyński in [23]. This approach has the advantage of involving only well known objects (the notion of Husimi function, defined in formula (25) of [18], and the Monge-Kantorovich-Rubinstein-Wasserstein distances defined in chapter 7 of [22]). Unfortunately, the evolution of the Husimi function of quantum states following the quantum dynamics described by the Schrödinger, or Heisenberg, or von Neumann equations is rather complicated [3] (even for polynomial potentials of high degree: see equations (6)-(8) in [2]).

To avoid the difficulties incurred in translating the quantum dynamics in terms of classical objects, another approach to the same problem was proposed in [13]. The new idea in [13] was to work directly on quantum objects, using the well known formal analogy between (quantum) density operators on $L^2(\mathbf{R}^d)$ and (Borel) probability measures on the phase space \mathbf{R}^{2d} of classical mechanics, between the trace of trace-class operators on $L^2(\mathbf{R}^d)$ and the Lebesgue integral for functions of $L^1(\mathbf{R}^{2d})$, and between the commutator for operators on $L^2(\mathbf{R}^d)$ and the Poisson bracket on \mathbf{R}^{2d} . This idea was extended in [14] to compare directly (quantum) density operators on $L^2(\mathbf{R}^d)$ and (classical) probability measures on \mathbf{R}^{2d} — which are obviously very different objects — by means of a functional denoted E_{\hbar} in [14]. Other quantum analogues of Wasserstein distances have been proposed and studied by various authors: see for instance [7, 8, 9, 10, 16, 23].

The present paper achieves several different goals. First, the functional constructed in [13] to compare density operators on $L^2(\mathbf{R}^d)$, and in [14] to compare (quantum) density operators on $L^2(\mathbf{R}^d)$ and probability measures on the (classical) phase space \mathbf{R}^{2d} are unified into a single functional \mathfrak{d} , a deformation of the Monge-Kantorovich-Wasserstein distance of exponent 2 denoted $\text{dist}_{\text{MK},2}$, defined on $\mathfrak{D}_2 \times \mathfrak{D}_2$, where \mathfrak{D}_2 is the (disjoint) union of the set $\mathcal{P}_2(\mathbf{R}^{2d})$ of phase-space probability measures with finite second moment, and of the set $\mathcal{D}_2(L^2(\mathbf{R}^d))$ of density operators (positive operators of trace 1, see (1) below) with finite energy for the harmonic oscillator.

The complete technical definition of \mathfrak{d} and its main properties will require some material exposed in Sections 2 and 3 below. Let us nevertheless give immediately the definition of \mathfrak{d} : for $\mu, \nu, f dx d\xi \in \mathcal{P}_2(\mathbf{R}^{2d})$ and $R, S \in \mathcal{D}_2(L^2(\mathbf{R}^d))$

$$\left\{ \begin{array}{l} \mathfrak{d}(\mu, \nu) := \text{dist}_{\text{MK},2}(\mu, \nu), \\ \mathfrak{d}(f, R) := \left(\inf_{Q \in \mathcal{C}(f, R)} \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2} c_{\hbar}(x, \xi) Q(x, \xi)^{1/2}) dx d\xi \right)^{1/2}, \\ \mathfrak{d}(R, S) := \left(\inf_{T \in \mathcal{C}(R, S)} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(T^{1/2} C_{\hbar} T^{1/2}) \right)^{1/2}. \end{array} \right.$$

Here $\mathcal{C}(f, R)$ is the set of couplings of f and R , namely the operator-valued measurable functions $Q(x, \xi)$ such that $Q(x, \xi) = Q(x, \xi)^* \geq 0$ and $\text{trace}_{\mathfrak{H}} Q(x, \xi) = f(x, \xi)$ for a.e. $(x, \xi) \in \mathbf{R}^{2d}$ while $\int_{\mathbf{R}^{2d}} Q(x, \xi) dx d\xi = R$, and the cost operator-valued function $c_{\hbar}(x, \xi) = |x - y|^2 + |\xi + i\hbar \nabla_y|^2$ defined as a self-adjoint operator on $L^2(\mathbf{R}_y^d)$.

Meanwhile, $\mathcal{C}(R, S)$ is the set of couplings of R and S , namely the density operators on $L^2(\mathbf{R}^d) \otimes L^2(\mathbf{R}^d)$ whose two marginals with respects to the two tensorial factors are equal to R and S (once again see Section 2 for precise definition when f is Lebesgue absolutely continuous and Theorem 3.1 for the extension to the general case $f \in \mathcal{P}_2(\mathbf{R}^{2d})$).

It was observed already in [13] that the restriction of \mathfrak{d} to the set of density operators, denoted MK_2^{\hbar} in [13], is not a bona fide metric, since $\mathfrak{d}(R, R) \geq \sqrt{2d\hbar}$ for all $R \in \mathcal{D}_2(L^2(\mathbf{R}^d))$ (see Theorem 2.3 in [13]). Nevertheless, it is important for applications to check whether \mathfrak{d} satisfies the other properties of metrics. That the restriction of \mathfrak{d} to $\mathcal{D}_2(\mathfrak{H})$ is symmetric is obvious. But, on the other hand, there seem to be very serious difficulties with the triangle inequality for the deformed “pseudometric” \mathfrak{d} . In particular, at variance with most other properties of the pseudo-metric \mathfrak{d} , the question of the triangle inequality for \mathfrak{d} seems to require arguments which significantly differ from those used in the proof of the triangle inequality for the Monge-Kantorovich-Wasserstein metric $\text{dist}_{\text{MK},2}$.

Our first main result in the present paper bears on a variant of the triangle inequality for \mathfrak{d} .

Theorem A. (Triangle inequality) *For all $\rho_1, \rho_2, \rho_3 \in \mathfrak{D}_2$, the deformation \mathfrak{d} of the Monge-Kantorovich-Wasserstein distance $\text{dist}_{\text{MK},2}$ satisfies*

(a) the restricted triangle inequality if ρ_2 is a Borel probability measure on \mathbf{R}^{2d} , or if there exists $j \in \{1, 2, 3\}$ such that ρ_j is a rank-one density operator:

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

(b) the approximate triangle inequality in all other cases

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

It is worth mentioning at this point that DePalma and Trevisan [10] recently introduced another “pseudometric” on the set of quantum density operators, different from \mathfrak{d} , but for which they have obtained another variant of the triangle inequality, of the form

$$d(R_1, R_3) \leq d(R_1, R_2) + d(R_2, R_3) + d(R_2, R_2).$$

This modified triangle inequality, or its analogue in Theorem A (b) of the present paper can be understood as follows. At variance with the classical setting, in the quantum setting, transporting a density operator on itself has a *positive* cost, and this is the reason for the appearance of $d(R_2, R_2)$ on the right hand side of the inequality above. The same is true of \mathfrak{d} — except that the additional term $\sqrt{d\hbar}$ on the right hand side of the inequality in Theorem A (b) does not depend on R_1 or R_2 . Of course, the general lower bound $\mathfrak{d}(R_1, R_2) \geq \sqrt{2d\hbar}$ (see Theorem 2.3 in [13]) implies the inequality

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

which is of the same type as the DePalma-Trevisan inequality (with however a better coefficient $\frac{1}{\sqrt{2}}$ multiplying the additional term).

In the case where ρ_1, ρ_2 are probability densities, the exact, but restricted triangle inequality in Theorem A (a) had already been proved, and applied in [15] to produce semiclassical upper bounds for \mathfrak{d} in situations more general than those considered in either [13] or [14], which obtained such upper bounds in the only case of Töplitz density operators (see Theorems 2.3 (1) in [13] and 2.4 (1) in [14]).

If the intermediate point ρ_2 is a density operator, the proof of the triangle inequality for the Monge-Kantorovich-Wasserstein distances on the set of probability measures on \mathbf{R}^{2d} makes use of mathematical objects or results which do not seem to have analogues for density operators on $L^2(\mathbf{R}^d)$. Statement (b) in Theorem A is proved by a completely different method, based on the following Kantorovich duality formula for the pseudometric defined in [14], which is our second main result in this paper.

Theorem B. (Kantorovich duality) *For each probability density f on \mathbf{R}^{2d} with finite second moments, and each density operator R on $L^2(\mathbf{R}^d)$ with finite energy for the harmonic oscillator, one has*

$$\mathfrak{d}(f, R)^2 = \sup_{\substack{a \in C_b(\mathbf{R}^{2d}, \mathbf{R}), B = B^* \in \mathcal{L}(L^2(\mathbf{R}^d)) \\ a(x, \xi) \in L^2(\mathbf{R}^d_y) + B \leq |x-y|^2 + |\xi + i\hbar \nabla_y|^2}} \left(\int_{\mathbf{R}^{2d}} a(x, \xi) f(x, \xi) dx d\xi + \text{trace}(BR) \right)$$

As a consequence of the various properties of \mathfrak{d} listed above, one can prove first that the ‘‘pseudometric’’ \mathfrak{d} is indeed a deformation of the Monge-Kantorovich-Wasserstein metric $\text{dist}_{\text{MK},2}$ in the following sense.

Theorem C. (Classical limit) *Let R_{\hbar}, S_{\hbar} be families of finite energy density operators on $L^2(\mathbf{R}^d)$, and let μ, ν be Borel probability measures on \mathbf{R}^{2d} such that $\mathfrak{d}(R_{\hbar}, \mu)$ and $\mathfrak{d}(\nu, S_{\hbar})$ satisfy*

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

Then

$$\text{dist}_{\text{MK},2}(\mu, \nu) = \lim_{\hbar \rightarrow 0^+} \mathfrak{d}(R_{\hbar}, S_{\hbar}).$$

Another rather important consequence of the so-called restricted triangle inequality (Theorem A (a)) is the extension by continuity of $\mathfrak{d}(\rho_1, \rho_2)$ to pairs ρ_1, ρ_2 where ρ_1 or ρ_2 is a (Borel) probability measure with finite second moments that is not absolutely continuous with respect to the Lebesgue measure on phase-space, and therefore not given by a probability density as in the original definition in [14].

The duality theorem above (Theorem B) has other consequences for the pseudometric \mathfrak{d} than the approximate triangle inequality in Theorem A (b).

In the last section of the paper, we focus on $\mathfrak{d}(r, S)$ for $r \in \mathcal{P}_2(\mathbf{R}^{2d})$ and $S \in \mathcal{D}_2(\mathbf{R}^d)$.

We investigate a (semi)quantum analogue of the Knott-Smith-Brenier Theorem and a (semi)quantum analogue of the Legendre transform in the case where the supremum in the Kantorovich duality is attained by two optimal potentials $\tilde{a} \in C_b(\mathcal{R}^{2d})$ and $\tilde{B} \in \mathcal{L}(L^2(\mathcal{R}^d, dy))$:

$$\mathfrak{d}(r, S)^2 = \int_{\mathbf{R}^{2d}} \tilde{a}(x, \xi) f(x, \xi) dx d\xi + \text{trace}_{L^2(\mathbf{R}^d)} \tilde{B}R.$$

In particular, we state a gradient aspect of our (semi)quantum Brenier Theorem in the form of the two equalities (13), the analogue of the gradient structure in the classical setting, and we show moreover that

$$a(x, \xi) := \frac{1}{2}(\xi^2 + x^2 - \tilde{a}(x, \xi))$$

is the semiquantum-Legendre transform of

$$B := \frac{1}{2}(-\nabla_y^2 + y^2 - \tilde{B}),$$

in the sense that

$$a(x, \xi) = \sup_{\substack{\phi \in \text{Dom}(B) \\ \|\phi\|=1}} (x \cdot \langle \phi | y | \phi \rangle + \xi \cdot \langle \phi | -i\hbar \nabla_y | \phi \rangle - \langle \phi | B | \phi \rangle).$$

The outline of this paper is as follows: the definition of \mathfrak{d} on \mathfrak{D}_2 is recalled in detail in section 2. The “restricted” triangle inequality Theorem A (a) (see Theorem 3.1 below) is proved in section 3, along with the extension of \mathfrak{d} to Borel probability measures on the classical phase space that are not absolutely continuous with respect to the Lebesgue measure, by a density argument stated as Lemma 3.2. We conclude section 3 with a detailed discussion of the difficulties in extending the proof of Theorem A (a) to the case where the intermediate point ρ_2 is a density operator of rank larger than one.

The Kantorovich duality theorem (Theorem B) is proved in section 4 (see Theorem 4.1).

With the duality theorem, one proves in section 5 an important inequality stated as Theorem 5.4, which generalizes both Theorem 2.3 (2) in [13] and Theorem 2.4 (2) from [14]. Theorem A (b) then follows from Theorem A (a) and Theorem 5.4 by an elementary inequality (see Theorem 5.1).

The deformation theorem (Theorem C) is proved in section 5 as a consequence of Theorem A (see Theorem 5.5). (Notice however, that Theorem C only uses part (a) in Theorem A).

2. EXTENDING THE MONGE-KANTOROVICH-WASSERSTEIN DISTANCE OF EXPONENT 2 TO QUANTUM DENSITY OPERATORS

Henceforth we denote by $\mathcal{P}(\mathbf{R}^n)$ the set of Borel probability measures on \mathbf{R}^n , and set

$$\mathcal{P}_2(\mathbf{R}^n) := \{ \mu \in \mathcal{P}(\mathbf{R}^n) \text{ s.t. } \int_{\mathbf{R}^n} |x|^2 \mu(dx) < \infty \}.$$

We also denote by $\mathcal{P}^{ac}(\mathbf{R}^n)$ the set of probability densities on \mathbf{R}^n , identified with Borel probability measures on \mathbf{R}^n that are absolutely continuous with respect to the Lebesgue measure, and set $\mathcal{P}_2^{ac}(\mathbf{R}^n) = \mathcal{P}_2(\mathbf{R}^n) \cap \mathcal{P}^{ac}(\mathbf{R}^n)$.

With $\mathfrak{H} := L^2(\mathbf{R}^d)$, the sets of density operators, and of finite-energy density operators on \mathfrak{H} , are defined respectively as follows:

$$\begin{aligned} \mathcal{D}(\mathfrak{H}) &:= \{ T \in \mathcal{L}(\mathfrak{H}) \text{ s.t. } T = T^* \geq 0 \text{ and } \text{trace}_{\mathfrak{H}}(T) = 1 \}, \\ \mathcal{D}_2(\mathfrak{H}) &:= \{ T \in \mathcal{D}(\mathfrak{H}) \text{ s.t. } \text{trace}_{\mathfrak{H}}(T^{1/2} H T^{1/2}) < \infty \}, \end{aligned}$$

where

$$H = H(x, \hbar \nabla_x) = -\frac{1}{2} \hbar^2 \Delta_x + \frac{1}{2} |x|^2.$$

In the sequel, we seek to extend the Monge-Kantorovich(-Wasserstein) distance $\text{dist}_{\text{MK},2}$ to the set¹

$$(1) \quad \mathfrak{D}_2 := \mathcal{D}_2(\mathfrak{H}) \cup \mathcal{P}_2(\mathbf{R}^{2d}).$$

The set of couplings, or transference plans, between two elements μ, ν of $\mathcal{P}(\mathbf{R}^n)$ is

$$\begin{aligned} \mathcal{C}(\mu, \nu) := & \{ \rho \in \mathcal{P}(\mathbf{R}^n \times \mathbf{R}^n) \text{ s.t. for all } \phi, \psi \in C_b(\mathbf{R}^n) \\ & \iint_{\mathbf{R}^n \times \mathbf{R}^n} (\phi(x) + \psi(y)) \rho(dx dy) = \int_{\mathbf{R}^n} \phi(x) \mu(dx) + \int_{\mathbf{R}^n} \psi(y) \nu(dy) \}. \end{aligned}$$

(See formula (1.2) in chapter 1 of [22]). Notice that $\mu \otimes \nu \in \mathcal{C}(\mu, \nu)$, which is therefore nonempty.

We recall the definition of the Monge-Kantorovich distance of exponent 2 between two probability measures $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^n)$:

$$\text{dist}_{\text{MK},2}(\mu, \nu) := \min_{\rho \in \mathcal{C}(\mu, \nu)} \left(\iint_{\mathbf{R}^n \times \mathbf{R}^n} |x - y|^2 \rho(dx dy) \right)^{1/2}.$$

(See Definitions 7.1.1 and Theorem 7.3 in chapter 7 in [22]. That the inf is indeed a min is explained in the last paragraph of Theorem 1.3 in chapter 1, and in Proposition 2.1 in chapter 2 of [22].)

Obviously, extending $\text{dist}_{\text{MK},2}$ to \mathfrak{D}_2 requires first defining the notion of coupling between two arbitrary elements of \mathfrak{D}_2 . The notion of coupling between two elements of \mathfrak{D}_2 is defined by analogy with the case of two elements of $\mathcal{P}(\mathbf{R}^n)$. For each pair of density operators $R, S \in \mathcal{D}(\mathfrak{H})$, one sets

$$\mathcal{C}(R, S) := \{ T \in \mathcal{D}(\mathfrak{H} \otimes \mathfrak{H}) \text{ s.t. } \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(T(A \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes B)) = \text{trace}_{\mathfrak{H}}(RA + SB) \}.$$

(This is Definition 2.1 in [13].) Here again, $R \otimes S \in \mathcal{C}(R, S)$, so that $\mathcal{C}(R, S) \neq \emptyset$.

For each probability density on phase space $f \in \mathcal{P}^{ac}(\mathbf{R}^{2d})$ and each density operator $R \in \mathcal{D}(\mathfrak{H})$, a coupling of f and R is an operator-valued measurable function

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

such that

$$Q(x, \xi) = Q(x, \xi)^* \geq 0 \quad \text{and} \quad \text{trace}_{\mathfrak{H}}(Q(x, \xi)) = f(x, \xi) \quad \text{for a.e. } (x, \xi) \in \mathbf{R}^{2d},$$

while

$$\int_{\mathbf{R}^{2d}} Q(x, \xi) dx d\xi = R.$$

The set of couplings of f and R is denoted $\mathcal{C}(f, R) = \mathcal{C}(R, f)$.

Observe that $Q(x, \xi) \in \mathcal{L}^1(\mathfrak{H})$ which is separable for a.e. $(x, \xi) \in \mathbf{R}^{2d}$, since f is a probability density, and therefore is finite for a.e. $(x, \xi) \in \mathbf{R}^{2d}$. (See Definition 2.1 in [14].) The map $f \otimes R : (x, \xi) \mapsto f(x, \xi)R$ always belongs to $\mathcal{C}(f, R)$, so that $\mathcal{C}(f, R) \neq \emptyset$.

Next we define the transport cost. The (quantum-to-quantum) transport cost between two quantum states corresponding with the position “variables” (operators) x and y , and the momentum “variables” (operators) $-i\hbar\nabla_x$ and $-i\hbar\nabla_y$

¹Note that the index n refers to the dimension of spaces on which classical densities are defined. Since the classical space underlying quantum mechanics is the phase-space of the classical system, $n = 2d$ where d is the dimension on which the quantum wave function lives.

is

$$C_{\hbar} = C(x, y, -i\hbar\nabla_x, -i\hbar\nabla_y) := \sum_{j=1}^d \left((x_j - y_j)^2 - \hbar^2 (\partial_{x_j} - \partial_{y_j})^2 \right).$$

Similarly, the (classical-to-quantum) transport cost between a classical state with phase space variables (x, ξ) and quantum states corresponding with the position “variable” (operator) y , and the momentum “variable” (operator) $-i\hbar\nabla_y$ is

$$c_{\hbar}(x, \xi) = c(x, \xi, y, -i\hbar\nabla_y) := \sum_{j=1}^d \left((x_j - y_j)^2 + (\xi_j + i\hbar\partial_{y_j})^2 \right).$$

Then, we define the extension \mathfrak{d} of $\text{dist}_{\text{MK},2}$ to \mathfrak{D}_2 . For all $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^{2d})$, each $f \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ and each $R, S \in \mathcal{D}_2(\mathfrak{H})$, set

$$(2) \quad \mathfrak{d}(\mu, \nu) := \text{dist}_{\text{MK},2}(\mu, \nu) \in [0, +\infty)$$

and

$$(3) \quad \mathfrak{d}(f, R) = \mathfrak{d}(R, f) := \left(\inf_{Q \in \mathcal{C}(f, R)} \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2} c_{\hbar}(x, \xi) Q(x, \xi)^{1/2}) dx d\xi \right)^{1/2},$$

(see Definition 2.2 in [14], with a slight change in the normalization of the transport cost operator $c_{\hbar}(x, \xi)$), while

$$(4) \quad \mathfrak{d}(R, S) := \left(\inf_{T \in \mathcal{C}(R, S)} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(T^{1/2} C_{\hbar} T^{1/2}) \right)^{1/2}$$

(as in Definition 2.2 of [13]). Observe that we have not yet defined $\mathfrak{d}(\mu, R)$ for $\mu \in \mathcal{P}_2(\mathbf{R}^{2d}) \setminus \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$. This will be done later by a density argument.

We begin our discussion of the properties of \mathfrak{d} with the following observations.

Lemma 2.1. *For each $f \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ and each $R, S \in \mathcal{D}_2(\mathfrak{H})$, one has*

$$\mathfrak{d}(f, R) \in [\sqrt{d\hbar}, +\infty) \quad \text{and} \quad \mathfrak{d}(R, S) \in [\sqrt{2d\hbar}, +\infty).$$

Proof. The lower bounds appear in Theorems 2.3 of [13] and Theorem 2.4 of [14]. They are consequences of the operator inequalities

$$c_{\hbar}(x, \xi) \geq d\hbar I_{\mathfrak{H}} \quad \text{for all } x, \xi \in \mathbf{R}^d, \quad \text{and} \quad C_{\hbar} \geq 2d\hbar I_{\mathfrak{H} \otimes \mathfrak{H}}$$

(see [13] on p. 183 and section 3.1 of [14] on p. 71).

For each $Q \in \mathcal{C}(f, R)$, one has

$$\int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}} \left(Q(x, \xi)^{\frac{1}{2}} (|x|^2 + |\xi|^2) Q(x, \xi)^{\frac{1}{2}} \right) dx d\xi = \int_{\mathbf{R}^{2d}} (|x|^2 + |\xi|^2) f(x, \xi) dx d\xi < \infty$$

while, for each $n \geq 1$,

$$\begin{aligned} & \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}} \left(\left(I + \frac{1}{n} H(y, \hbar\nabla_y) \right)^{-1} H(y, \hbar\nabla_y) Q(x, \xi) \right) dx d\xi \\ &= \text{trace}_{\mathfrak{H}} \left(\left(I + \frac{1}{n} H(y, \hbar\nabla_y) \right)^{-1} H(y, \hbar\nabla_y) \int_{\mathbf{R}^{2d}} Q(x, \xi) dx d\xi \right) \\ &= \text{trace}_{\mathfrak{H}} \left(\left(I + \frac{1}{n} H(y, \hbar\nabla_y) \right)^{-1} H(y, \hbar\nabla_y) R \right). \end{aligned}$$

By Proposition A.3 in [15]

$$\begin{aligned} \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}} \left(Q(x, \xi)^{\frac{1}{2}} \left(I + \frac{1}{n} H(y, \hbar \nabla_y) \right)^{-1} H(y, \hbar \nabla_y) Q(x, \xi)^{\frac{1}{2}} \right) dx d\xi \\ \rightarrow \text{trace}_{\mathfrak{H}} \left(R^{\frac{1}{2}} H(y, \hbar \nabla_y) R^{\frac{1}{2}} \right) < \infty, \end{aligned}$$

and, for a.e. $(x, \xi) \in \mathbf{R}^{2d}$,

$$\begin{aligned} \text{trace}_{\mathfrak{H}} \left(\left(I + \frac{1}{n} H(y, \hbar \nabla_y) \right)^{-1} H(y, \hbar \nabla_y) Q(x, \xi) \right) \\ \rightarrow \text{trace}_{\mathfrak{H}} \left(Q(x, \xi)^{\frac{1}{2}} H(y, \hbar \nabla_y) Q(x, \xi)^{\frac{1}{2}} \right). \end{aligned}$$

Thus, by monotone convergence,

$$\begin{aligned} \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}} \left(Q(x, \xi)^{\frac{1}{2}} H(y, \hbar \nabla_y) Q(x, \xi)^{\frac{1}{2}} \right) dx d\xi \\ = \text{trace}_{\mathfrak{H}} \left(R^{\frac{1}{2}} H(y, \hbar \nabla_y) R^{\frac{1}{2}} \right) < \infty. \end{aligned}$$

For a.e. $(x, \xi) \in \mathbf{R}^{2d}$, the operator $Q(x, \xi) \in \mathcal{L}^1(\mathfrak{H})$ is a nonnegative self-adjoint operator, and has a spectral decomposition of the form

$$Q(x, \xi) = \sum_{k \geq 1} \lambda_k(x, \xi) |e_k(x, \xi)\rangle \langle e_k(x, \xi)|$$

where λ_k is a measurable real-valued function and e_k a measurable \mathfrak{H} -valued function for each $k \geq 1$ such that

$$\lambda_k(x, \xi) \geq 0 \text{ for a.e. } (x, \xi) \in \mathbf{R}^{2d}, \quad \sum_{k \geq 1} \lambda_k(x, \xi) = f(x, \xi),$$

while

$$(e_k(x, \xi))_{k \geq 1} \text{ is a complete orthonormal system in } \mathfrak{H} \text{ for a.e. } (x, \xi) \in \mathbf{R}^{2d}.$$

Thus

$$\begin{aligned} \sum_{k \geq 1} \int_{\mathbf{R}^{2d}} \lambda_k(x, \xi) \langle e_k(x, \xi) | H(y, \hbar \nabla_y) | e_k(x, \xi) \rangle dx d\xi \\ = \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}} \left(Q(x, \xi)^{\frac{1}{2}} H(y, \hbar \nabla_y) Q(x, \xi)^{\frac{1}{2}} \right) dx d\xi < \infty \end{aligned}$$

so that

$$\lambda_k(x, \xi) > 0 \implies e_k(x, \xi) \in L^2(\mathbf{R}^d; |y|^2 dy) \cap H^1(\mathbf{R}^d).$$

Now, one has the elementary pointwise inequalities

$$(x_j - y_j)^2 \leq 2(x_j^2 + y_j^2),$$

and its analogue for operators

$$(\xi_j + i\hbar \partial_{y_j})^2 \leq 2(\xi_j^2 - \hbar^2 \partial_{y_j}^2),$$

meaning that

$$\langle \psi | (\xi_j + i\hbar \partial_{y_j})^2 | \psi \rangle \leq 2\xi_j^2 \|\psi\|_{\mathfrak{H}}^2 + 2\|\hbar \partial_{y_j} \psi\|_{\mathfrak{H}}^2 = 2\langle \psi | \xi_j^2 - \hbar^2 \partial_{y_j}^2 | \psi \rangle$$

for all $j = 1, \dots, d$. Hence

$$\begin{aligned} & \sum_{k \geq 1} \sum_{j=1}^d \int_{\mathbf{R}^{2d}} \lambda_k(x, \xi) \langle e_k(x, \xi) | (x_j - y_j)^2 + (\xi_j + i\hbar \partial_{y_j})^2 | e_k(x, \xi) \rangle dx d\xi \\ &= \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{\frac{1}{2}} c(x, \xi, y, \hbar \nabla_y) Q(x, \xi)^{\frac{1}{2}}) dx d\xi \\ &= \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{\frac{1}{2}} (|x|^2 + |\xi|^2 + H(y, \hbar \nabla_y)) Q(x, \xi)^{\frac{1}{2}}) dx d\xi < \infty \end{aligned}$$

for each $Q \in \mathcal{C}(f, R)$ with $f \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ and each $R \in \mathcal{D}_2(\mathfrak{H})$. Since we have seen that $\mathcal{C}(f, R) \neq \emptyset$, this implies in particular that $\mathfrak{d}(f, R) < \infty$.

If $T \in \mathcal{C}(R, S)$ with $R, S \in \mathcal{D}_2(\mathfrak{H})$, applying Proposition A.3 in [15] shows that

$$\begin{aligned} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(((I + \frac{1}{n}H)^{-1}H) \otimes I_{\mathfrak{H}})T) &= \text{trace}_{\mathfrak{H}}(((I + \frac{1}{n}H)^{-1}H)R) \\ &\rightarrow \text{trace}_{\mathfrak{H}}\left(R^{\frac{1}{2}}HR^{\frac{1}{2}}\right) < \infty, \end{aligned}$$

while

$$\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(((I + \frac{1}{n}H)^{-1}H) \otimes I_{\mathfrak{H}})T) \rightarrow \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}\left(T^{\frac{1}{2}}(H \otimes I_{\mathfrak{H}})T^{\frac{1}{2}}\right).$$

Thus

$$\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}\left(T^{\frac{1}{2}}(H \otimes I_{\mathfrak{H}})T^{\frac{1}{2}}\right) = \text{trace}_{\mathfrak{H}}\left(R^{\frac{1}{2}}HR^{\frac{1}{2}}\right) < \infty,$$

and similarly

$$\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}\left(T^{\frac{1}{2}}(I_{\mathfrak{H}} \otimes H)T^{\frac{1}{2}}\right) = \text{trace}_{\mathfrak{H}}\left(S^{\frac{1}{2}}HS^{\frac{1}{2}}\right) < \infty.$$

Write the spectral decomposition of T as

$$T = \sum_{k \geq 1} \tau_k |\Phi_k\rangle \langle \Phi_k|$$

where $(\Phi_k)_{k \geq 1}$ is a complete orthonormal system in $\mathfrak{H} \otimes \mathfrak{H}$, while

$$\tau_k \geq 0 \text{ for all } k \geq 1 \quad \text{and} \quad \sum_{k \geq 1} \tau_k = 1.$$

Hence

$$\sum_{k \geq 1} \sum_{j=1}^d \tau_j \iint_{\mathbf{R}^d \times \mathbf{R}^d} (x_j^2 \Phi_k(x, y)^2 + (\hbar \partial_{x_j} \Phi_k(x, y))^2) dx dy = \text{trace}_{\mathfrak{H}}\left(R^{\frac{1}{2}}HR^{\frac{1}{2}}\right) < \infty$$

$$\sum_{k \geq 1} \sum_{j=1}^d \tau_j \iint_{\mathbf{R}^d \times \mathbf{R}^d} (y_j^2 \Phi_k(x, y)^2 + (\hbar \partial_{y_j} \Phi_k(x, y))^2) dx dy = \text{trace}_{\mathfrak{H}}\left(S^{\frac{1}{2}}HS^{\frac{1}{2}}\right) < \infty$$

so that

$$\begin{aligned} \tau_j > 0 \implies \Phi_j &\equiv \Phi_j(x, y) \in L^2(\mathbf{R}_y^d; L^2(\mathbf{R}^d; |x|^2 dx) \cap H^1(\mathbf{R}_x^d)) \\ &\quad \cap L^2(\mathbf{R}_x^d; L^2(\mathbf{R}^d; |y|^2 dy) \cap H^1(\mathbf{R}_y^d)). \end{aligned}$$

We use the operator inequality

$$(-i\hbar \partial_{x_j} + i\hbar \partial_{y_j})^2 \leq -2\hbar^2(\partial_{x_j}^2 + \partial_{y_j}^2),$$

meaning that, for all $\psi \equiv \psi(x, y) \in L^2(\mathbf{R}_x^d; H^1(\mathbf{R}_y^d)) \cap L^2(\mathbf{R}_y^d; H^1(\mathbf{R}_x^d))$, one has

$$\langle \psi | (-i\hbar \partial_{x_j} + i\hbar \partial_{y_j})^2 | \psi \rangle \leq 2\|\hbar \partial_{x_j} \psi\|_{L^2}^2 + 2\|\hbar \partial_{y_j} \psi\|_{L^2}^2 = \langle \psi | -2\hbar^2(\partial_{x_j}^2 + \partial_{y_j}^2) | \psi \rangle.$$

Thus, for each $k \geq 1$ such that $\tau_k > 0$, one has

$$\langle \Phi_k | (x_j - y_j)^2 - \hbar^2 (\partial_{x_j} - \partial_{y_j})^2 | \Phi_k \rangle \leq 2 \langle \Phi_k | x_j^2 - \hbar^2 \partial_{x_j}^2 | \Phi_k \rangle + 2 \langle \Phi_k | y_j^2 - \hbar^2 \partial_{y_j}^2 | \Phi_k \rangle,$$

so that, for each $T \in \mathcal{C}(R, S)$ with $R, S \in \mathcal{D}_2(\mathfrak{H})$,

$$\begin{aligned} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(T^{\frac{1}{2}} C_{\hbar} T^{\frac{1}{2}} \right) &= \sum_{k \geq 1} \tau_k \sum_{j=1}^d \langle \Phi_k | (x_j - y_j)^2 - \hbar^2 (\partial_{x_j} - \partial_{y_j})^2 | \Phi_k \rangle \\ &\leq 2 \sum_{k \geq 1} \tau_k \sum_{j=1}^d (\langle \Phi_k | x_j^2 - \hbar^2 \partial_{x_j}^2 | \Phi_k \rangle + \langle \Phi_k | y_j^2 - \hbar^2 \partial_{y_j}^2 | \Phi_k \rangle) \\ &= 2 \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(T^{\frac{1}{2}} (H \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes H) T^{\frac{1}{2}} \right) \\ &= 2 \text{trace}_{\mathfrak{H}} \left(R^{\frac{1}{2}} H R^{\frac{1}{2}} + S^{\frac{1}{2}} H S^{\frac{1}{2}} \right) < \infty. \end{aligned}$$

Since we have seen that $\mathcal{C}(R, S) \neq \emptyset$, this implies in particular that $\mathfrak{d}(R, S) < \infty$ for each $R, S \in \mathcal{D}_2(\mathfrak{H})$. \square

3. RESTRICTED TRIANGLE INEQUALITY

The main result in this section is the following theorem. Let us recall that, so far, we have defined $\mathfrak{d}(\mu, R) = \mathfrak{d}(R, \mu)$ for all $R \in \mathcal{D}_2(\mathfrak{H})$ only in the case where $\mu \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$, and not for all $\mu \in \mathcal{P}_2(\mathbf{R}^{2d})$.

Theorem 3.1. *There is a unique extension of \mathfrak{d} defining a map $\mathfrak{D}_2 \times \mathfrak{D}_2 \rightarrow [0, +\infty)$ still denoted \mathfrak{d} , satisfying the triangle inequality for each $\rho_1, \rho_2, \rho_3 \in \mathfrak{D}_2$:*

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

if $\rho_2 \in \mathcal{P}_2(\mathbf{R}^{2d})$, or if $\rho_j \in \{R \in \mathcal{D}_2(\mathfrak{H}) \text{ s.t. } R^2 = R\}$ for some $j \in \{1, 2, 3\}$.

This theorem is an extension of Theorem 3.5 of [15], which proves the triangle inequality in the case where $\rho_1, \rho_2 \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ and $\rho_3 \in \mathcal{D}_2(\mathfrak{H})$.

Proof. The proof of this theorem is split in several steps.

Step 1: extension to \mathfrak{D}_2 . As a consequence of Theorem 3.5 of [15], one has

$$|\mathfrak{d}(\rho_1, \rho_3) - \mathfrak{d}(\rho_2, \rho_3)| \leq \mathfrak{d}(\rho_1, \rho_2) = \text{dist}_{\text{MK},2}(\rho_1, \rho_2)$$

for all $\rho_1, \rho_2 \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ and all $\rho_3 \in \mathcal{D}_2(\mathfrak{H})$.

Lemma 3.2. *The set $\mathcal{P}_2^{ac}(\mathbf{R}^n)$ is dense in $\mathcal{P}_2(\mathbf{R}^{2d})$ for the metric $\text{dist}_{\text{MK},2}$.*

The proof of this lemma is deferred until after the proof of Theorem 3.1.

Taking Lemma 3.2 for granted, we conclude that the Lipschitz continuous function \mathfrak{d} on $\mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ with values in the complete space $[0, +\infty)$ has a unique continuous extension to $\mathcal{P}_2(\mathbf{R}^{2d})$.

Step 2: triangle inequality when $\rho_2 \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$. The triangle inequality has already been proved in Theorem 3.5 of [15] for $\rho_1, \rho_2 \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ and $\rho_3 \in \mathcal{D}_2(\mathfrak{H})$. It remains only to treat the case where $\rho_1, \rho_3 \in \mathcal{D}_2(\mathfrak{H})$ while $\rho_2 \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$.

We first recall the disintegration result stated as Lemma A.4 in [15].

Lemma 3.3. *Let $f \in \mathcal{P}^{ac}(\mathbf{R}^{2d})$ and $R \in \mathcal{D}_2(\mathfrak{H})$, and let $Q \in \mathcal{C}(f, R)$. There exists a $\sigma(\mathcal{L}^1(\mathfrak{H}), \mathcal{L}(\mathfrak{H}))$ weakly measurable operator valued function $(x, \xi) \mapsto Q_f(x, \xi)$ defined a.e. on \mathbf{R}^{2d} such that*

$$Q_f(x, \xi) = Q_f(x, \xi)^* \geq 0, \quad \text{trace}_{\mathfrak{H}}(Q_f(x, \xi)) = 1, \quad \text{and } Q(x, \xi) = f(x, \xi)Q_f(x, \xi)$$

for a.e. $(x, \xi) \in \mathbf{R}^{2d}$.

Let us briefly recall the notion of weak measurability. Any continuous linear functional on $\mathcal{L}^1(\mathfrak{H})$ is of the form $T \mapsto \text{trace}_{\mathfrak{H}}(AT)$ for some $A \in \mathcal{L}(\mathfrak{H})$, so that the topological dual of $\mathcal{L}^1(\mathfrak{H})$ is $\mathcal{L}(\mathfrak{H})$. The $\sigma(\mathcal{L}^1(\mathfrak{H}), \mathcal{L}(\mathfrak{H}))$ weak topology on $\mathcal{L}^1(\mathfrak{H})$ is defined as in section 2 of chapter 3 in [4]. Then, the map Q_f is $\sigma(\mathcal{L}^1(\mathfrak{H}), \mathcal{L}(\mathfrak{H}))$ weakly measurable if $(x, \xi) \mapsto \text{trace}_{\mathfrak{H}}(AQ(x, \xi))$ is a complex-valued measurable function on \mathbf{R}^{2d} for all $A \in \mathcal{L}(\mathfrak{H})$.

For each $Q^1 \in \mathcal{C}(\rho_1, \rho_2)$ and each $Q^3 \in \mathcal{C}(\rho_2, \rho_3)$, set

$$Q^{13}(x, \xi) := Q^1(x, \xi) \otimes Q_{\rho_2}^3(x, \xi).$$

By construction,

$$Q^{13}(x, \xi) = Q^{13}(x, \xi)^* \geq 0,$$

and one has

$$\begin{aligned} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q^{13}(x, \xi)(A \otimes I)) &= \text{trace}_{\mathfrak{H}}(Q^1(x, \xi)A) \text{trace}_{\mathfrak{H}}(Q_{\rho_2}^3(x, \xi)) \\ &= \text{trace}_{\mathfrak{H}}(Q^1(x, \xi)A), \end{aligned}$$

while

$$\begin{aligned} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q^{13}(x, \xi)(I \otimes A)) &= \text{trace}_{\mathfrak{H}}(Q^1(x, \xi)) \text{trace}_{\mathfrak{H}}(Q_{\rho_2}^3(x, \xi)A) \\ &= \rho_2(x, \xi) \text{trace}_{\mathfrak{H}}(Q_{\rho_2}^3(x, \xi)A) = \text{trace}_{\mathfrak{H}}(Q^3(x, \xi)A). \end{aligned}$$

This immediately implies that

$$T_{13} = \int_{\mathbf{R}^{2d}} Q^{13}(x, \xi) dx d\xi \in \mathcal{C}(\rho_1, \rho_3).$$

Next we recall the ‘‘Peter-Paul inequality’’ for operators (Lemma A.1 in [15]).

Lemma 3.4. *Let L_1, L_2 be (unbounded) self-adjoint operators on $L^2(\mathbf{R}^n)$. For each $\alpha > 0$*

$$\langle \psi | L_1 L_2 + L_2 L_1 | \psi \rangle \leq \alpha \langle \psi | L_1^2 | \psi \rangle + \frac{1}{\alpha} \langle \psi | L_2^2 | \psi \rangle, \quad \psi \in \text{Dom}(L_1) \cap \text{Dom}(L_2).$$

With this lemma, we prove the following operator inequality.

Lemma 3.5. *For each $\alpha > 0$ and each $(y, \eta) \in \mathbf{R}^{2d}$, one has*

$$C(x, \hbar \nabla_x, z, \hbar \nabla_z) \leq (1 + \alpha) c(y, \eta, x, \hbar \nabla_x) \otimes I_{\mathfrak{H}} + (1 + \frac{1}{\alpha}) I_{\mathfrak{H}} \otimes c(y, \eta, z, \hbar \nabla_z).$$

In other words, for all $\alpha > 0$

$$\begin{aligned} \phi \equiv \phi(x, z) \in L^2(\mathbf{R}_x^d; L^2(\mathbf{R}_z^d, |z|^2 dz) \cap H^1(\mathbf{R}_z^d)) \cap L^2(\mathbf{R}_x^d, L^2(\mathbf{R}_z^d, |z|^2 dz) \cap H^1(\mathbf{R}_z^d)) \\ \implies \langle \phi | C(x, \hbar \nabla_x, z, \hbar \nabla_z) | \phi \rangle \leq (1 + \alpha) \int_{\mathbf{R}^d} \langle \phi(\cdot, z) | c_{\hbar}(y, \eta) | \phi(\cdot, z) \rangle dz \\ + (1 + \frac{1}{\alpha}) \int_{\mathbf{R}^d} \langle \phi(x, \cdot) | c_{\hbar}(y, \eta) | \phi(x, \cdot) \rangle dx. \end{aligned}$$

The proof of this lemma is postponed until after the proof of Theorem 3.1.

For a.e. $(y, \eta) \in \mathbf{R}^{2d}$, the operators $Q^1(y, \eta), Q^3(y, \eta) \in \mathcal{L}^1(\mathfrak{H})$ are nonnegative self-adjoint and have spectral decompositions of the form

$$\begin{aligned} Q^1(y, \eta) &= \sum_{k \geq 1} \lambda_k^1(y, \eta) |e_k^1(y, \eta)\rangle \langle e_k^1(y, \eta)|, \\ Q^3(y, \eta) &= \sum_{k \geq 1} \lambda_k^3(y, \eta) |e_k^3(y, \eta)\rangle \langle e_k^3(y, \eta)|, \end{aligned}$$

where λ_k^1, λ_k^3 are measurable real-valued functions, while e_k^1, e_k^3 are measurable \mathfrak{H} -valued functions for each $k \geq 1$ such that

$$\lambda_k^1(y, \eta), \lambda_k^3(y, \eta) \geq 0 \text{ for a.e. } (y, \eta) \in \mathbf{R}^{2d}, \quad \sum_{k \geq 1} \lambda_k^1(y, \eta) = \sum_{k \geq 1} \lambda_k^3(y, \eta) = \rho_2(y, \eta),$$

while, for a.e. $(y, \eta) \in \mathbf{R}^{2d}$,

$$(e_k^1(y, \eta))_{k \geq 1} \text{ and } (e_k^3(y, \eta))_{k \geq 1} \text{ are complete orthonormal systems in } \mathfrak{H}.$$

Hence

$$Q^{13}(y, \eta) = \sum_{k, l \geq 1} \lambda_{kl}^{13}(y, \eta) |e_k^1(y, \eta) \otimes e_l^3(y, \eta)\rangle \langle e_k^1(y, \eta) \otimes e_l^3(y, \eta)|$$

with λ_{kl}^{13} measurable on \mathbf{R}^{2d} such that

$$\lambda_{kl}^{13}(y, \eta) \geq 0, \quad \sum_{k \geq 1} \lambda_{kl}^{13}(y, \eta) = \lambda_l^3(y, \eta), \quad \sum_{l \geq 1} \lambda_{kl}^{13}(y, \eta) = \lambda_k^1(y, \eta)$$

for a.e. $(y, \eta) \in \mathbf{R}^{2d}$. In particular

$$\lambda_{kl}^{13}(y, \eta) \leq \max(\lambda_k^1(y, \eta), \lambda_l^3(y, \eta)).$$

Therefore, as explained in the proof of Lemma 2.1

$$\lambda_{kl}^{13}(y, \eta) > 0 \implies \begin{cases} e_k^1(y, \eta) \in L^2(\mathbf{R}^d; |y|^2 dy) \cap H^1(\mathbf{R}^d), \\ e_l^3(y, \eta) \in L^2(\mathbf{R}^d; |y|^2 dy) \cap H^1(\mathbf{R}^d), \end{cases}$$

so that

$$\begin{aligned} &\langle e_k^1(y, \eta) \otimes e_l^3(y, \eta) | C(x, \hbar \nabla_x, z, \hbar \nabla_z) | e_k^1(y, \eta) \otimes e_l^3(y, \eta) \rangle \\ &\leq (1 + \alpha) \langle e_k^1(y, \eta) \otimes e_l^3(y, \eta) | c_{\hbar}(y, \eta) \otimes I_{\mathfrak{H}} | e_k^1(y, \eta) \otimes e_l^3(y, \eta) \rangle \\ &+ (1 + \frac{1}{\alpha}) \langle e_k^1(y, \eta) \otimes e_l^3(y, \eta) | I_{\mathfrak{H}} \otimes c_{\hbar}(y, \eta) | e_k^1(y, \eta) \otimes e_l^3(y, \eta) \rangle \\ &= (1 + \alpha) \langle e_k^1(y, \eta) | c_{\hbar}(y, \eta) | e_k^1(y, \eta) \rangle \\ &+ (1 + \frac{1}{\alpha}) \langle e_l^3(y, \eta) | c_{\hbar}(y, \eta) | e_l^3(y, \eta) \rangle. \end{aligned}$$

By monotone convergence

$$\begin{aligned}
& \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(Q^{13}(y, \eta)^{\frac{1}{2}} C_{\hbar} Q^{13}(y, \eta)^{\frac{1}{2}} \right) dy d\eta \\
&= \sum_{k, l \geq 1} \int_{\mathbf{R}^{2d}} \lambda_{kl}^{13}(y, \eta) \langle e_k^1(y, \eta) \otimes e_l^3(y, \eta) | C_{\hbar} | e_k^1(y, \eta) \otimes e_l^3(y, \eta) \rangle dy d\eta \\
&\leq (1 + \alpha) \sum_{k, l \geq 1} \int_{\mathbf{R}^{2d}} \lambda_{kl}^{13}(y, \eta) \langle e_k^1(y, \eta) | c_{\hbar}(y, \eta) | e_k^1(y, \eta) \rangle dy d\eta \\
&\quad + (1 + \frac{1}{\alpha}) \sum_{k, l \geq 1} \int_{\mathbf{R}^{2d}} \lambda_{kl}^{13}(y, \eta) \langle e_l^3(y, \eta) | c_{\hbar}(y, \eta) | e_l^3(y, \eta) \rangle dy d\eta \\
&= (1 + \alpha) \sum_{k \geq 1} \int_{\mathbf{R}^{2d}} \lambda_k^1(y, \eta) \langle e_k^1(y, \eta) | c_{\hbar}(y, \eta) | e_k^1(y, \eta) \rangle dy d\eta \\
&\quad + (1 + \frac{1}{\alpha}) \sum_{l \geq 1} \int_{\mathbf{R}^{2d}} \lambda_l^3(y, \eta) \langle e_l^3(y, \eta) | c_{\hbar}(y, \eta) | e_l^3(y, \eta) \rangle dy d\eta \\
&= (1 + \alpha) \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}} \left(Q^1(y, \eta)^{\frac{1}{2}} c_{\hbar}(y, \eta) Q^1(y, \eta)^{\frac{1}{2}} \right) dy d\eta \\
&\quad + (1 + \frac{1}{\alpha}) \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}} \left(Q^3(y, \eta)^{\frac{1}{2}} c_{\hbar}(y, \eta) Q^3(y, \eta)^{\frac{1}{2}} \right) dy d\eta.
\end{aligned}$$

Using Proposition A.3 in [15] and the monotone convergence theorem shows that

$$\begin{aligned}
& \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left((I + \frac{1}{n} C_{\hbar})^{-1} C_{\hbar} T_{13} \right) \\
&= \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left((I + \frac{1}{n} C_{\hbar})^{-1} C_{\hbar} Q^{13}(y, \eta) \right) dy d\eta \\
&\rightarrow \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(Q^{13}(y, \eta)^{\frac{1}{2}} C_{\hbar} Q^{13}(y, \eta)^{\frac{1}{2}} \right) dy d\eta \\
&= \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(T_{13}^{\frac{1}{2}} C_{\hbar} T_{13}^{\frac{1}{2}} \right).
\end{aligned}$$

Since we already know that $T_{13} \in \mathcal{C}(\rho_1, \rho_3)$, we have proved that

$$\begin{aligned}
& \mathfrak{d}(\rho_1, \rho_3)^2 \leq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(T_{13}^{\frac{1}{2}} C_{\hbar} T_{13}^{\frac{1}{2}} \right) \\
&\leq (1 + \alpha) \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}} \left(Q^1(y, \eta)^{\frac{1}{2}} c_{\hbar}(y, \eta) Q^1(y, \eta)^{\frac{1}{2}} \right) dy d\eta \\
&\quad + (1 + \frac{1}{\alpha}) \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}} \left(Q^3(y, \eta)^{\frac{1}{2}} c_{\hbar}(y, \eta) Q^3(y, \eta)^{\frac{1}{2}} \right) dy d\eta.
\end{aligned}$$

Minimizing the last right hand side in $Q^1 \in \mathcal{C}(\rho_2, \rho_1)$ and in $Q^3 \in \mathcal{C}(\rho_2, \rho_3)$ shows that

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

and minimizing the right hand side of this inequality in $\alpha > 0$ leads to the desired triangle inequality.

Step 3: triangle inequality when at least one ρ_j is a rank-one projection.

In the case where $R = |\psi\rangle\langle\psi|$ for some $\psi \in \mathfrak{H}$ such that $\|\psi\|_{\mathfrak{H}} = 1$, the structure of couplings of an element of $\mathcal{D}_2(\mathfrak{H})$ or of $\mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ with R is very simple.

Lemma 3.6. *If $R = |\psi\rangle\langle\psi|$ for some $\psi \in \mathfrak{H}$ such that $\|\psi\|_{\mathfrak{H}} = 1$, one has*

$$\mathcal{C}(f, R) = \mathcal{C}(R, f) = \{f \otimes R\} \quad \text{and} \quad \mathcal{C}(R, S) = \{R \otimes S\}$$

for each $f \in \mathcal{P}^{ac}(\mathbf{R}^{2d})$ and each $S \in \mathcal{D}_2(\mathfrak{H})$.

We postpone the proof of this lemma until after the proof of Theorem 3.1.

On the other hand, using Lemma 3.4 leads to the following operator inequalities.

Lemma 3.7. *For each $\alpha > 0$*

$$\begin{aligned} |x - z|^2 + |\xi - \zeta|^2 &\leq (1 + \alpha)c(x, \xi, y, \hbar\nabla_y) + (1 + \frac{1}{\alpha})c(z, \zeta, y, \hbar\nabla_y), \\ c(x, \xi, z, \hbar\nabla_z) &\leq (1 + \alpha)c(x, \xi, y, \hbar\nabla_y) + (1 + \frac{1}{\alpha})C(y, \hbar\nabla_y, z, \hbar\nabla_z), \\ C(x, \hbar\nabla_x, z, \hbar\nabla_z) &\leq (1 + \alpha)C(x, \hbar\nabla_x, y, \hbar\nabla_y) + (1 + \frac{1}{\alpha})C(y, \hbar\nabla_y, z, \hbar\nabla_z). \end{aligned}$$

In other words, for each $\psi \equiv \psi(y) \in H^1(\mathbf{R}^d) \cap L^2(\mathbf{R}^d; |y|^2 dy)$

$$(|x - z|^2 + |\xi - \zeta|^2)\|\psi\|_{\mathfrak{H}}^2 \leq (1 + \alpha)\langle\psi|c_{\hbar}(x, \xi)|\psi\rangle + (1 + \frac{1}{\alpha})\langle\psi|c_{\hbar}(z, \zeta)|\psi\rangle,$$

while, for each $\phi \equiv \phi(z) \in H^1(\mathbf{R}^d) \cap L^2(\mathbf{R}^d; |z|^2 dz)$

$$\langle\phi|c_{\hbar}(x, \xi)|\phi\rangle\|\psi\|_{\mathfrak{H}}^2 \leq (1 + \alpha)\langle\psi|c_{\hbar}(x, \xi)|\psi\rangle\|\phi\|_{\mathfrak{H}}^2 + (1 + \frac{1}{\alpha})\langle\psi \otimes \phi|C_{\hbar}|\psi \otimes \phi\rangle.$$

Similarly, for each $\phi_1 \equiv \phi_1(w)$ and $\phi_3 \equiv \phi_3(w) \in L^2(\mathbf{R}^d; |w|^2 dw) \cap H^1(\mathbf{R}^d)$, one has

$$\begin{aligned} \langle\phi_1 \otimes \phi_3|C_{\hbar}|\phi_1 \otimes \phi_3\rangle\|\psi\|_{\mathfrak{H}}^2 &\leq (1 + \alpha) \int_{\mathbf{R}^d} \langle\phi_1 \otimes \psi|C_{\hbar}|\phi_1 \otimes \psi\rangle|\phi_3(z)|^2 dz \\ &\quad + (1 + \frac{1}{\alpha}) \int_{\mathbf{R}^d} \langle\psi \otimes \phi_3|C_{\hbar}|\psi \otimes \phi_3\rangle|\phi_1(x)|^2 dx. \end{aligned}$$

We shall give the proof of these inequalities at the end of the present section.

Thus, for each $f, g \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$, pick Φ convex on \mathbf{R}^{2d} such that an optimal coupling of f and g for $\text{dist}_{\text{MK}, 2}$ is $f(x, \xi)\delta((z, \zeta) - \nabla\Phi(x, \xi))$ (such a Φ exists by Theorem 2.12 in chapter 2 of [22]),

$$Q(x, \xi, z, \zeta) := f(x, \xi)\delta((z, \zeta) - \nabla\Phi(x, \xi))|\psi\rangle\langle\psi|,$$

where $R = |\psi\rangle\langle\psi|$ with $\psi \in L^2(\mathbf{R}^d; |y|^2 dy) \cap H^1(\mathbf{R}^d)$ and $\|\psi\|_{\mathfrak{H}} = 1$. The first inequality in Lemma 3.7 implies that

$$\begin{aligned} (|x - \nabla_x\Phi(x, \xi)|^2 + |\xi - \nabla_{\xi}\Phi(x, \xi)|^2)f(x, \xi) &\leq (1 + \alpha)f(x, \xi)\langle\psi|c_{\hbar}(x, \xi)|\psi\rangle \\ &\quad + (1 + \frac{1}{\alpha})f(x, \xi)\langle\psi|c_{\hbar}(\nabla\Phi(x, \xi))|\psi\rangle. \end{aligned}$$

Integrating both sides of this inequality leads to

$$\begin{aligned} \mathfrak{d}(f, g)^2 &= \int_{\mathbf{R}^{2d}} (|x - \nabla_x\Phi(x, \xi)|^2 + |\xi - \nabla_{\xi}\Phi(x, \xi)|^2)f(x, \xi) dx d\xi \\ &\leq (1 + \alpha) \int_{\mathbf{R}^{2d}} f(x, \xi)\langle\psi|c_{\hbar}(x, \xi)|\psi\rangle dx d\xi \\ &\quad + (1 + \frac{1}{\alpha}) \int_{\mathbf{R}^{2d}} f(x, \xi)\langle\psi|c_{\hbar}(\nabla\Phi(x, \xi))|\psi\rangle dx d\xi \\ &\leq (1 + \alpha) \int_{\mathbf{R}^{2d}} f(x, \xi)\langle\psi|c_{\hbar}(x, \xi)|\psi\rangle dx d\xi \\ &\quad + (1 + \frac{1}{\alpha}) \int_{\mathbf{R}^{2d}} g(z, \zeta)\langle\psi|c_{\hbar}(z, \zeta)|\psi\rangle dz d\zeta \\ &\leq (1 + \alpha)\mathfrak{d}(f, R)^2 + (1 + \frac{1}{\alpha})\mathfrak{d}(R, g)^2 \end{aligned}$$

since $\mathcal{C}(f, R) = \{f \otimes R\}$ and $\mathcal{C}(g, R) = \{g \otimes R\}$ by Lemma 3.6. Minimizing in $\alpha > 0$ implies that

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

For all $f \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ and each $S \in \mathcal{D}_2(\mathfrak{H})$, write the spectral decomposition of S

$$S = \sum_{k \geq 1} \sigma_k |e_k\rangle \langle e_k|, \quad \text{with } \sigma_k \geq 0 \text{ and } \sum_{k \geq 1} \sigma_k = 1$$

where $e_k \in L^2(\mathbf{R}^d, |z|^2 dz) \cap H^1(\mathbf{R}^d)$ for each $k \geq 1$ with $\sigma_k > 0$ is such that $(e_k)_{k \geq 1}$ is a complete orthonormal system in \mathfrak{H} . Similarly, let $(x, \xi) \mapsto Q(x, \xi)$ be a coupling of f and R , with spectral decomposition

$$Q(x, \xi) = \sum_{j \geq 1} \chi_j(x, \xi) |\psi_j^{x, \xi}\rangle \langle \psi_j^{x, \xi}|, \quad \text{with } \chi_j(x, \xi) \geq 0 \text{ and } \sum_{j \geq 1} \chi_j(x, \xi) = f(x, \xi)$$

for a.e. $(x, \xi) \in \mathbf{R}^{2d}$. Here again $\psi_j^{x, \xi} \in L^2(\mathbf{R}^d, |y|^2 dy) \cap H^1(\mathbf{R}^d)$ for each $j \geq 1$ with $\chi_j(x, \xi) > 0$ is such that $(\psi_j^{x, \xi})_{j \geq 1}$ is a complete orthonormal system in \mathfrak{H} .

In the case considered here, either S is a rank-one operator, in which case $\sigma_1 = 1$ and $\sigma_k = 0$ for all $k \geq 2$, or $R = |\psi\rangle \langle \psi|$ with $\|\psi\|_{\mathfrak{H}} = 1$, in which case the only coupling of f and R is $Q(x, \xi) = f(x, \xi)R$ by Lemma 3.6. In this latter case, one can take $\psi_1^{x, \xi} = \psi$, and $\chi_1(x, \xi) = f(x, \xi)$ with $\chi_j(x, \xi) = 0$ for all $j \geq 2$.

The second inequality in Lemma 3.7 implies that

$$\begin{aligned} \langle e_k | c_{\bar{h}}(x, \xi) | e_k \rangle &= \langle \psi_j^{x, \xi} | \psi_j^{x, \xi} \rangle \langle e_k | c_{\bar{h}}(x, \xi) | e_k \rangle \\ &\leq (1 + \alpha) \langle \psi_j^{x, \xi} | c_{\bar{h}}(x, \xi) | \psi_j^{x, \xi} \rangle \langle e_k | e_k \rangle + (1 + \frac{1}{\alpha}) \langle \psi_j^{x, \xi} \otimes e_k | C_{\bar{h}} | \psi_j^{x, \xi} \otimes e_k \rangle \\ &\leq (1 + \alpha) \langle \psi_j^{x, \xi} | c_{\bar{h}}(x, \xi) | \psi_j^{x, \xi} \rangle + (1 + \frac{1}{\alpha}) \langle \psi_j^{x, \xi} \otimes e_k | C_{\bar{h}} | \psi_j^{x, \xi} \otimes e_k \rangle \end{aligned}$$

for all $j, k \geq 1$ and a.e. $(x, \xi) \in \mathbf{R}^{2d}$ such that $\chi_j(x, \xi) > 0$.

Multiplying both sides of this inequality by $\chi_j(x, \xi)\sigma_k$, summing in $j, k \geq 1$ and integrating in (x, ξ) shows that

$$\begin{aligned} \mathfrak{d}(f, S)^2 &\leq \int_{\mathbf{R}^{2d}} f(x, \xi) \text{trace}_{\mathfrak{H}} \left(S^{\frac{1}{2}} c_{\bar{h}}(x, \xi) S^{\frac{1}{2}} \right) dx d\xi \\ &= \int_{\mathbf{R}^{2d}} \sum_{j, k \geq 1} \chi_j(x, \xi) \sigma_k \langle e_k | c_{\bar{h}}(x, \xi) | e_k \rangle dx d\xi \\ &\leq (1 + \alpha) \int_{\mathbf{R}^{2d}} \sum_{j \geq 1} \chi_j(x, \xi) \langle \psi_j^{x, \xi} | c_{\bar{h}}(x, \xi) | \psi_j^{x, \xi} \rangle dx d\xi \text{trace}_{\mathfrak{H}}(S) \\ &\quad + (1 + \frac{1}{\alpha}) \int_{\mathbf{R}^{2d}} \sum_{j, k \geq 1} \chi_j(x, \xi) \sigma_k \langle \psi_j^{x, \xi} \otimes e_k | C_{\bar{h}} | \psi_j^{x, \xi} \otimes e_k \rangle \\ &= (1 + \alpha) \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{\frac{1}{2}} c_{\bar{h}}(x, \xi) Q(x, \xi)^{\frac{1}{2}}) dx d\xi \\ &\quad + (1 + \frac{1}{\alpha}) \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((Q(x, \xi) \otimes S)^{\frac{1}{2}} C_{\bar{h}}(Q(x, \xi) \otimes S)^{\frac{1}{2}}) dx d\xi. \end{aligned}$$

Arguing as in the proof of Lemma 2.1 by monotone convergence, using Proposition A.3 in [15], one has

$$\begin{aligned}
& \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((Q(x, \xi) \otimes S)^{\frac{1}{2}} C_{\hbar}(Q(x, \xi) \otimes S)^{\frac{1}{2}}) dx d\xi \\
&= \lim_{n \rightarrow \infty} \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((Q(x, \xi) \otimes S)^{\frac{1}{2}} (I + \frac{1}{n} C_{\hbar})^{-1} C_{\hbar}(Q(x, \xi) \otimes S)^{\frac{1}{2}}) dx d\xi \\
&= \lim_{n \rightarrow \infty} \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((Q(x, \xi) \otimes S)(I + \frac{1}{n} C_{\hbar})^{-1} C_{\hbar}) dx d\xi \\
&= \lim_{n \rightarrow \infty} \text{trace}_{\mathfrak{H}}((R \otimes S)(I + \frac{1}{n} C_{\hbar})^{-1} C_{\hbar}) \\
&= \lim_{n \rightarrow \infty} \text{trace}_{\mathfrak{H}}((R \otimes S)^{\frac{1}{2}} (I + \frac{1}{n} C_{\hbar})^{-1} C_{\hbar} (R \otimes S)^{\frac{1}{2}}) \\
&= \text{trace}_{\mathfrak{H}}((R \otimes S)^{\frac{1}{2}} C_{\hbar} (R \otimes S)^{\frac{1}{2}}) = \mathfrak{d}(R, S)^2
\end{aligned}$$

since $\mathcal{C}(R, S) = \{R \otimes S\}$ by Lemma 3.6 because R or S is a rank-one projection. Thus

$$\begin{aligned}
\mathfrak{d}(f, S)^2 &\leq (1 + \alpha) \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{\frac{1}{2}} c_{\hbar}(x, \xi) Q(x, \xi)^{\frac{1}{2}}) dx d\xi \\
&\quad + (1 + \frac{1}{\alpha}) \mathfrak{d}(R, S)^2.
\end{aligned}$$

Minimizing in $Q \in \mathcal{C}(f, R)$ leads to

$$\mathfrak{d}(f, S)^2 \leq (1 + \alpha) \mathfrak{d}(f, R)^2 + (1 + \frac{1}{\alpha}) \mathfrak{d}(R, S)^2,$$

and minimizing in $\alpha > 0$ the right hand side of this inequality gives

$$\mathfrak{d}(f, S) \leq \mathfrak{d}(f, R) + \mathfrak{d}(R, S).$$

Finally, let $R, S, T \in \mathcal{D}_2(\mathfrak{H})$, and let $P \in \mathcal{C}(R, S)$. Write the spectral decompositions of P and T as

$$\begin{aligned}
P &= \sum_{k \geq 1} \varpi_k |\phi_k\rangle \langle \phi_k|, & \text{with } \varpi_k \geq 0 & \quad \text{and } \sum_{k \geq 1} \varpi_k = 1, \\
T &= \sum_{l \geq 1} \tau_l |f_l\rangle \langle f_l|, & \text{with } \tau_l \geq 0 & \quad \text{and } \sum_{l \geq 1} \tau_l = 1,
\end{aligned}$$

where $\phi_k \equiv \phi_k(x, y)$ lies in the form domain of C_{\hbar} for each $k \geq 1$ such that $\varpi_k > 0$, while $f_l \in L^2(\mathbf{R}^d, |w|^2 dw) \cap H^1(\mathbf{R}^d)$ for each $l \geq 1$ with $\tau_l > 0$, and are such that $(\phi_k)_{k \geq 1}$ and $(f_l)_{l \geq 1}$ are complete orthonormal systems in $\mathfrak{H} \otimes \mathfrak{H}$ and \mathfrak{H} respectively.

Assume that S or T is a rank-one projection. If the rank of S is one, then $\mathcal{C}(R, S) = \{R \otimes S\}$ by Lemma 3.6, so that $P = R \otimes S$. Otherwise, T has rank one, in which case $\tau_1 = 1$, and $\tau_j = 0$ for all $j \geq 2$, so that $T = |f_1\rangle \langle f_1|$.

The third inequality in Lemma 3.7 implies that

$$\begin{aligned}
\int_{\mathbf{R}^d} \langle \phi_k(\cdot, y) \otimes f_l | C_{\hbar} | \phi_k(\cdot, y) \otimes f_l \rangle dy &\leq (1 + \alpha) \langle \phi_k | C_{\hbar} | \phi_k \rangle \langle f_l | f_l \rangle \\
&\quad + (1 + \frac{1}{\alpha}) \int_{\mathbf{R}^d} \langle \phi_k(x, \cdot) \otimes f_l | C_{\hbar} | \phi_k(x, \cdot) \otimes f_l \rangle dx.
\end{aligned}$$

Multiplying both sides of this inequality by $\varpi_k \tau_l$ and summing in k, l shows that

$$\begin{aligned} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((R \otimes T)^{\frac{1}{2}}(I + \frac{1}{n}C_{\hbar})^{-1}C_{\hbar}(R \otimes T)^{\frac{1}{2}}) &= \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((R \otimes T)(I + \frac{1}{n}C_{\hbar})^{-1}C_{\hbar}) \\ &= \sum_{k, l \geq 1} \varpi_k \tau_l \int_{\mathbf{R}^d} \langle \phi_k(\cdot, y) \otimes f_l | (I + \frac{1}{n}C_{\hbar})^{-1}C_{\hbar} | \phi_k(\cdot, y) \otimes f_l \rangle dy \\ &\leq \sum_{k, l \geq 1} \varpi_k \tau_l \int_{\mathbf{R}^d} \langle \phi_k(\cdot, y) \otimes f_l | C_{\hbar} | \phi_k(\cdot, y) \otimes f_l \rangle dy \\ &\leq (1 + \alpha) \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(P^{\frac{1}{2}}C_{\hbar}P^{\frac{1}{2}}) \text{trace}_{\mathfrak{H}}(S) \\ &\quad + (1 + \frac{1}{\alpha}) \sum_{k, l \geq 1} \varpi_k \tau_l \int_{\mathbf{R}^d} \langle \phi_k(x, \cdot) \otimes f_l | C_{\hbar} | \phi_k(x, \cdot) \otimes f_l \rangle dx. \end{aligned}$$

Using again monotone convergence and Proposition A.3 on [15] as in the proof of Lemma 2.1 shows that

$$\begin{aligned} \mathfrak{d}(R, T)^2 &\leq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((R \otimes T)^{\frac{1}{2}}C_{\hbar}(R \otimes T)^{\frac{1}{2}}) \\ &= \lim_{n \rightarrow \infty} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((R \otimes T)^{\frac{1}{2}}(I + \frac{1}{n}C_{\hbar})^{-1}C_{\hbar}(R \otimes T)^{\frac{1}{2}}), \end{aligned}$$

and similarly

$$\begin{aligned} &\sum_{k, l \geq 1} \varpi_k \tau_l \int_{\mathbf{R}^d} \langle \phi_k(x, \cdot) \otimes f_l | C_{\hbar} | \phi_k(x, \cdot) \otimes f_l \rangle dx \\ &= \lim_{n \rightarrow \infty} \sum_{k, l \geq 1} \varpi_k \tau_l \int_{\mathbf{R}^d} \langle \phi_k(x, \cdot) \otimes f_l | (I + \frac{1}{n}C_{\hbar})^{-1}C_{\hbar} | \phi_k(x, \cdot) \otimes f_l \rangle dx \\ &= \lim_{n \rightarrow \infty} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H} \otimes \mathfrak{H}}((P \otimes T)(I \otimes (I + \frac{1}{n}C_{\hbar})^{-1}C_{\hbar})) \\ &= \lim_{n \rightarrow \infty} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((S \otimes T)(I + \frac{1}{n}C_{\hbar})^{-1}C_{\hbar}) \\ &= \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((S \otimes T)^{\frac{1}{2}}C_{\hbar}(S \otimes T)^{\frac{1}{2}}) = \mathfrak{d}(S, T)^2, \end{aligned}$$

since $\mathcal{C}(S, T) = \{S \otimes T\}$ by Lemma 3.6 because S or T is a rank-one orthogonal projection. Thus

$$\mathfrak{d}(R, T)^2 \leq (1 + \alpha)\mathfrak{d}(R, S)^2 + (1 + \frac{1}{\alpha})\mathfrak{d}(S, T)^2,$$

and minimizing in $\alpha > 0$ implies that

$$\mathfrak{d}(R, T) \leq \mathfrak{d}(R, S) + \mathfrak{d}(S, T).$$

Step 4: remaining cases. After Step 2, we know that the triangle inequality

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

holds for $\rho_1, \rho_3 \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d}) \cup \mathcal{D}_2(\mathfrak{H})$ and all $\rho_2 \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$. By the density argument of Step 1 and the continuity of \mathfrak{d} on $\mathcal{P}_2(\mathbf{R}^{2d})$ in each of its argument, this inequality must hold for all $\rho_1, \rho_3 \in \mathfrak{D}_2$ and all $\rho_2 \in \mathcal{P}_2(\mathbf{R}^{2d})$. \square

Finally, we prove the lemmas taken for granted in the proof of Theorem 3.1. We begin with the density of $\mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ in $\mathcal{P}_2(\mathbf{R}^{2d})$ for the metric $\text{dist}_{\text{MK}, 2}$.

Proof of Lemma 3.2. Let $\mu \in \mathcal{P}_2^{ac}(\mathbf{R}^n)$, and let $\chi_\epsilon(x) = \frac{1}{\epsilon^n} \chi(\frac{x}{\epsilon})$ be an even mollifier. For each $\phi \in C_0(\mathbf{R}^n)$, one has $\|\phi - \chi_\epsilon \star \phi\|_{L^\infty} \rightarrow 0$ as $\epsilon \rightarrow 0$, so that

$$\left| \int_{\mathbf{R}^n} \phi(x) \mu(dx) - \int_{\mathbf{R}^n} \phi(x) (\chi_\epsilon \star \mu)(x) dx \right| \leq \int_{\mathbf{R}^n} |\phi - \chi_\epsilon \star \phi|(x) \mu(dx) \rightarrow 0$$

as $\epsilon \rightarrow 0$. Hence $\chi_\epsilon \star \mu \rightarrow \mu$ weakly as $\epsilon \rightarrow 0$. On the other hand

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

and, assuming without loss of generality that $\text{supp}(\chi) \subset B(0, 1)$ and $0 < \epsilon < 1$, one has

$$\begin{aligned} \chi_\epsilon \star (\mathbf{1}_{|x| \geq R} |x|^2) &= \int_{\mathbf{R}^n} \mathbf{1}_{|x - \epsilon y| \geq R} |x - \epsilon y|^2 \chi(y) dy \\ &\leq \mathbf{1}_{|x| + 1 \geq R} \int_{\mathbf{R}^n} |x - \epsilon y|^2 \chi(y) dy \\ &\leq 2 \mathbf{1}_{|x| + 1 \geq R} \left(|x|^2 + \epsilon^2 \int_{\mathbf{R}^n} |y|^2 \chi(y) dy \right) \leq 2 \mathbf{1}_{|x| + 1 \geq R} (|x|^2 + 1) \end{aligned}$$

Hence

$$\sup_{0 < \epsilon < 1} \int_{|x| \geq R} |x|^2 (\chi_\epsilon \star \mu)(x) dx \leq 2 \int_{|x| > R-1} (|x|^2 + 1) \mu(dx) \rightarrow 0$$

by dominated convergence. By Theorem 7.12 of [22],

$$\text{dist}_{\text{MK},2}(\mu, \mu \star \chi_\epsilon) \rightarrow 0 \quad \text{as } \epsilon \rightarrow 0.$$

□

Next we prove that the set of couplings of a density operator, or of a probability density with a rank-one orthogonal projection is trivial.

Proof of Lemma 3.6. The case of $\mathcal{C}(R, S)$ is Lemma 7.1 of [6]. Next assume that $R = |\psi\rangle\langle\psi|$ with $\|\psi\|_{\mathfrak{H}} = 1$. Then, for each $Q \in \mathcal{C}(f, R)$, one has

$$\int_{\mathbf{R}^{2d}} \langle \phi | Q(x, \xi) | \phi \rangle dx d\xi = \langle \phi | R | \phi \rangle = 0 \quad \text{for each } \phi \in (\mathbf{C}\psi)^\perp.$$

Since $Q(x, \xi) = Q(x, \xi)^* \geq 0$ for a.e. $(x, \xi) \in \mathbf{R}^{2d}$, this implies that

$$Q(x, \xi) \phi = 0 \quad \text{for all } \phi \in (\mathbf{C}\psi)^\perp, \quad \text{for a.e. } (x, \xi) \in \mathbf{R}^{2d},$$

so that

$$Q(x, \xi) \mathbf{C}\psi \subset \mathbf{C}\psi, \quad \text{for a.e. } (x, \xi) \in \mathbf{R}^{2d}.$$

In other words, there exists $\lambda(x, \xi) \in \mathbf{C}$ such that

$$Q(x, \xi) \psi = \lambda(x, \xi) \psi, \quad \text{for a.e. } (x, \xi) \in \mathbf{R}^{2d}.$$

Choose a complete orthonormal system $(e_j)_{j \geq 1}$ in $(\mathbf{C}\psi)^\perp$; setting $e_0 = \psi$, the system $(e_j)_{j \geq 0}$ is orthonormal and complete in \mathfrak{H} , so that

$$\lambda(x, \xi) = \langle \psi | Q(x, \xi) | \psi \rangle = \sum_{j \geq 0} \langle e_j | Q(x, \xi) | e_j \rangle = \text{trace}_{\mathfrak{H}}(Q(x, \xi)) = f(x, \xi)$$

for a.e. $(x, \xi) \in \mathbf{R}^{2d}$. Thus

$$Q(x, \xi) \psi = f(x, \xi) \psi, \quad Q(x, \xi) \phi = 0 \quad \text{for all } \phi \in (\mathbf{C}\psi)^\perp,$$

which means that

$$Q(x, \xi) = f(x, \xi)R, \quad \text{for a.e. } (x, \xi) \in \mathbf{R}^{2d}.$$

In other words, $\mathcal{C}(f, R) = \{f \otimes R\}$. \square

Finally we prove the operator inequalities used in the proof of Theorem 3.1

Proof of Lemma 3.5. Observe that

$$C(x, \hbar\nabla_x, z, \hbar\nabla_z) = \sum_{j=1}^d ((x_j - y_j + y_j - z_d)^2 + (-i\hbar\partial_{x_j} + i\hbar\partial_{y_j} - i\hbar\partial_{y_j} + i\hbar\partial_{z_j})^2)$$

so that, expanding each square in the sum leads to

$$\begin{aligned} C(x, \hbar\nabla_x, z, \hbar\nabla_z) &= c(x, \hbar\nabla_x, y, \eta) + c(y, \eta, z, \hbar\nabla_z) \\ &+ 2 \sum_{j=1}^d ((x_j - y_j)(y_j - z_d) + (-i\hbar\partial_{x_j} + i\hbar\partial_{y_j})(-i\hbar\partial_{y_j} + i\hbar\partial_{z_j})). \end{aligned}$$

Now we apply Lemma 3.4, first with $L_1 = (x_j - y_j)$ and $L_2 = (y_j - z_j)$, then with $L_1 = -i\hbar\partial_{x_j} + i\hbar\partial_{y_j}$ and $L_2 = -i\hbar\partial_{y_j} + i\hbar\partial_{z_j}$, so that

$$\begin{aligned} &2(x_j - y_j)(y_j - z_d) + 2(-i\hbar\partial_{x_j} + i\hbar\partial_{y_j})(-i\hbar\partial_{y_j} + i\hbar\partial_{z_j}) \\ &\leq \alpha(x_j - y_j)^2 + \frac{1}{\alpha}(y_j - z_d)^2 + \alpha(-i\hbar\partial_{x_j} + i\hbar\partial_{y_j})^2 + \frac{1}{\alpha}(-i\hbar\partial_{y_j} + i\hbar\partial_{z_j})^2, \end{aligned}$$

meaning that

$$\begin{aligned} \phi &\equiv \phi(x, z) \in L^2(\mathbf{R}_x^d; L^2(\mathbf{R}_z^d, |z|^2 dz) \cap H^1(\mathbf{R}_z^d)) \cap L^2(\mathbf{R}_x^d; L^2(\mathbf{R}_z^d, |z|^2 dz) \cap H^1(\mathbf{R}_z^d)) \\ &\implies 2\langle \phi | (x_j - y_j)(y_j - z_d) + (-i\hbar\partial_{x_j} + i\hbar\partial_{y_j})(-i\hbar\partial_{y_j} + i\hbar\partial_{z_j}) | \phi \rangle \\ &\leq \alpha \langle \phi | (x_j - y_j)^2 + (-i\hbar\partial_{x_j} + i\hbar\partial_{y_j})^2 | \phi \rangle \\ &\quad + \frac{1}{\alpha} \langle \phi | (y_j - z_d)^2 + (-i\hbar\partial_{y_j} + i\hbar\partial_{z_j})^2 | \phi \rangle \end{aligned}$$

for $j = 1, \dots, d$. Therefore

$$\begin{aligned} \phi &\equiv \phi(x, z) \in L^2(\mathbf{R}_x^d; L^2(\mathbf{R}_z^d, |z|^2 dz) \cap H^1(\mathbf{R}_z^d)) \cap L^2(\mathbf{R}_x^d; L^2(\mathbf{R}_z^d, |z|^2 dz) \cap H^1(\mathbf{R}_z^d)) \\ &\implies \langle \phi | C(x, \hbar\nabla_x, z, \hbar\nabla_z) | \phi \rangle \leq (1 + \alpha) \langle \phi | c(y, \eta, x, \hbar\nabla_x) | \phi \rangle \\ &\quad + (1 + \frac{1}{\alpha}) \langle \phi | c(y, \eta, z, \hbar\nabla_z) | \phi \rangle \end{aligned}$$

for each $(y, \eta) \in \mathbf{R}^{2d}$, which is the operator inequality in Lemma 3.5. \square

Proof of Lemma 3.7. Write

$$|x - z|^2 = |x - y + y - z|^2 = \sum_{j=1}^d ((x_j - y_j)^2 + (y_j - z_j)^2 + 2(x_j - y_j)(y_j - z_j)).$$

Since

$$2(x_j - y_j)(y_j - z_j) \leq \alpha(x_j - y_j)^2 + \frac{1}{\alpha}(y_j - z_j)^2$$

by Lemma 3.4, we conclude that

$$\begin{aligned} (5) \quad |x - z|^2 &\leq \sum_{j=1}^d ((1 + \alpha)(x_j - y_j)^2 + (1 + \frac{1}{\alpha})(y_j - z_j)^2) \\ &= (1 + \alpha)|x - y|^2 + (1 + \frac{1}{\alpha})|y - z|^2. \end{aligned}$$

Then

$$\begin{aligned} |\xi - \zeta|^2 &= \sum_{j=1}^d (\xi_j + i\hbar\partial_{y_j} - i\hbar\partial_{y_j} - \zeta_j)^2 \\ &= \sum_{j=1}^d ((\xi_j + i\hbar\partial_{y_j})^2 + (-i\hbar\partial_{y_j} - \zeta_j)^2 + 2(\xi_j + i\hbar\partial_{y_j})(-i\hbar\partial_{y_j} - \zeta_j)). \end{aligned}$$

Applying Lemma 3.4 with $L_1 = \xi_j + i\hbar\partial_{y_j}$ and $L_2 = -i\hbar\partial_{y_j} - \zeta_j$ shows that

$$\begin{aligned} &2\langle\psi|(\xi_j + i\hbar\partial_{y_j})(-i\hbar\partial_{y_j} - \zeta_j)|\psi\rangle \\ &\leq \alpha\langle\psi|(\xi_j + i\hbar\partial_{y_j})^2|\psi\rangle + \frac{1}{\alpha}\langle\psi|(-i\hbar\partial_{y_j} - \zeta_j)^2|\psi\rangle \end{aligned}$$

for all $\psi \in H^1(\mathbf{R}^d)$ and all $\xi, \zeta \in \mathbf{R}^d$, so that

$$(6) \quad |\xi - \zeta|^2 \|\psi\|_{\mathfrak{H}}^2 \leq (1 + \alpha)\langle\psi|\xi + i\hbar\nabla_y|^2|\psi\rangle + (1 + \frac{1}{\alpha})\langle\psi| -i\hbar\nabla_y - \zeta|^2|\psi\rangle.$$

Therefore

$$\begin{aligned} (|x - z|^2 + |\xi - \zeta|^2)\|\psi\|_{\mathfrak{H}}^2 &\leq (1 + \alpha)\langle\psi|c(x, \xi, y, \hbar\nabla_y)|\psi\rangle \\ &\quad + (1 + \frac{1}{\alpha})\langle\psi|c(z, \zeta, y, i\hbar\nabla_y)|\psi\rangle \end{aligned}$$

for all $\alpha > 0$, all $x, \xi, z, \zeta \in \mathbf{R}^d$ and all $\phi \in H^1(\mathbf{R}^d)$, which is the first inequality in Lemma 3.7.

Next

$$\begin{aligned} |\xi + i\hbar\nabla_z|^2 &= \sum_{j=1}^d (\xi_j + i\hbar\partial_{y_j} - i\hbar\partial_{y_j} + i\hbar\partial_{z_j})^2 \\ &= \sum_{j=1}^d ((\xi_j + i\hbar\partial_{y_j})^2 + (-i\hbar\partial_{y_j} + i\hbar\partial_{z_j})^2 + 2(\xi_j + i\hbar\partial_{y_j})(-i\hbar\partial_{y_j} + i\hbar\partial_{z_j})). \end{aligned}$$

Applying Lemma 3.4 with $L_1 = \xi_j + i\hbar\partial_{y_j}$ and $L_2 = -i\hbar\partial_{y_j} + i\hbar\partial_{z_j}$ shows that

$$\begin{aligned} &2\langle\psi \otimes \phi|(\xi_j + i\hbar\partial_{y_j})(-i\hbar\partial_{y_j} + i\hbar\partial_{z_j})|\psi \otimes \phi\rangle \\ &\leq \alpha\langle\psi|(\xi_j + i\hbar\partial_{y_j})^2|\psi\rangle\|\phi\|_{\mathfrak{H}}^2 + \frac{1}{\alpha}\langle\psi \otimes \phi|(-i\hbar\partial_{y_j} + i\hbar\partial_{z_j})^2|\psi \otimes \phi\rangle \end{aligned}$$

for all $\phi, \psi \in H^1(\mathbf{R}^d)$, so that

$$(7) \quad \begin{aligned} \langle\phi|\xi + i\hbar\nabla_z|^2|\phi\rangle\|\psi\|_{\mathfrak{H}}^2 &\leq \langle\psi|\xi + i\hbar\nabla_y|^2|\psi\rangle\|\phi\|_{\mathfrak{H}}^2 \\ &\quad + \frac{1}{\alpha}\langle\psi \otimes \phi| -i\hbar\nabla_y + i\hbar\nabla_z|^2|\psi \otimes \phi\rangle. \end{aligned}$$

With (5), this implies that

$$\begin{aligned} \langle\phi|c(x, \xi, z, \hbar\nabla_z)|\phi\rangle\|\psi\|_{\mathfrak{H}}^2 &\leq (1 + \alpha)\langle\psi|c(x, \xi, y, \hbar\nabla_y)|\psi\rangle\|\phi\|_{\mathfrak{H}}^2 \\ &\quad + (1 + \frac{1}{\alpha})\langle\psi \otimes \phi|C(y, \hbar\nabla_y, z, \hbar\nabla_z)|\psi \otimes \phi\rangle_{\mathfrak{H}}, \end{aligned}$$

which is the second inequality in Lemma 3.7.

Finally

$$\begin{aligned} | -i\hbar\nabla_x + i\hbar\nabla_z|^2 &= \sum_{j=1}^d (-i\hbar\partial_{x_j} + i\hbar\partial_{y_j} - i\hbar\partial_{y_j} + i\hbar\partial_{z_j})^2 \\ &= | -i\hbar\nabla_x + i\hbar\nabla_y|^2 + | -i\hbar\nabla_y + i\hbar\nabla_z|^2 + 2\sum_{j=1}^d (-i\hbar\partial_{x_j} + i\hbar\partial_{y_j})(-i\hbar\partial_{y_j} + i\hbar\partial_{z_j}), \end{aligned}$$

and Lemma 3.4 implies that

$$\begin{aligned} & 2\langle \phi_1 \otimes \phi_3 | (-i\hbar\partial_{x_j} + i\hbar\partial_{y_j})(-i\hbar\partial_{y_j} + i\hbar\partial_{z_j}) | \phi_1 \otimes \phi_3 \rangle \|\psi\|_{\mathfrak{H}}^2 \\ & \leq \alpha \langle \phi_1 \otimes \psi | (-i\hbar\partial_{x_j} + i\hbar\partial_{y_j})^2 | \phi_1 \otimes \psi \rangle \|\phi_3\|_{\mathfrak{H}}^2 \\ & \quad + \frac{1}{\alpha} \langle \psi \otimes \phi_3 | (-i\hbar\partial_{y_j} + i\hbar\partial_{z_j})^2 | \psi \otimes \phi_3 \rangle \|\phi_1\|_{\mathfrak{H}}^2 \end{aligned}$$

for each $\phi_1, \phi_3, \psi \in H^1(\mathbf{R}^d)$. Thus

$$\begin{aligned} & \langle \phi_1 \otimes \phi_3 | -i\hbar\nabla_x + i\hbar\nabla_z |^2 | \phi_1 \otimes \phi_3 \rangle \|\psi\|_{\mathfrak{H}}^2 \\ (8) \quad & \leq (1 + \alpha) \langle \phi_1 \otimes \psi | -i\hbar\nabla_x + i\hbar\nabla_y |^2 | \phi_1 \otimes \psi \rangle \|\phi_3\|_{\mathfrak{H}}^2 \\ & \quad + (1 + \frac{1}{\alpha}) \langle \psi \otimes \phi_3 | -i\hbar\nabla_x + i\hbar\nabla_y |^2 | \psi \otimes \phi_3 \rangle \|\phi_1\|_{\mathfrak{H}}^2. \end{aligned}$$

With (5), this implies that

$$\begin{aligned} & \langle \phi_1 \otimes \phi_3 | C(x, \hbar\nabla_x, z, \hbar\nabla_z) | \phi_1 \otimes \phi_3 \rangle \|\psi\|_{\mathfrak{H}}^2 \\ & \leq (1 + \alpha) \langle \phi_1 \otimes \psi | C(x, \hbar\nabla_x, y, \hbar\nabla_y) | \phi_1 \otimes \psi \rangle \|\phi_3\|_{\mathfrak{H}}^2 \\ & \quad + (1 + \frac{1}{\alpha}) \langle \psi \otimes \phi_3 | C(y, \hbar\nabla_y, z, \hbar\nabla_z) | \psi \otimes \phi_3 \rangle \|\phi_1\|_{\mathfrak{H}}^2 \end{aligned}$$

which is precisely the last inequality in Lemma 3.7. \square

We conclude this section with a comment on the “restricted” triangle inequality established in Theorem 3.1, and in particular on the restriction to the cases where $\rho_2 \in \mathcal{P}_2(\mathbf{R}^{2d})$, or ρ_2 is a rank-one orthogonal projection.

The proof of Theorem 3.1 is based on the following pattern:

(a) Given ρ_1, ρ_2, ρ_3 of \mathfrak{D}_2 , and for *all* $T_{12} \in \mathcal{C}(\rho_1, \rho_2)$ and all $T_{23} \in \mathcal{C}(\rho_2, \rho_3)$, one constructs T_{123} satisfying the following conditions

$$T_{123} = T_{123}^* \geq 0$$

and

$$\text{proj}_1 T_{123} = T_{23}, \quad \text{proj}_3 T_{123} = T_{12},$$

where proj_k is the partial trace, or the integral in the k -th variable in T_{123} , for $k = 1, 2, 3$.

(b) For each $\alpha > 0$, one proves the following inequality between cost functions or operators:

$$C_{13} \leq (1 + \alpha)C_{12} + (1 + \frac{1}{\alpha})C_{23},$$

where C_{jk} is the transport cost from the j th to the k th “variable”.

(c) Then

$$T_{123}^{\frac{1}{2}} C_{13} T_{123}^{\frac{1}{2}} \leq (1 + \alpha) T_{123}^{\frac{1}{2}} C_{12} T_{123}^{\frac{1}{2}} + (1 + \frac{1}{\alpha}) T_{123}^{\frac{1}{2}} C_{23} T_{123}^{\frac{1}{2}}$$

and one “averages in all variables” both sides of this inequality. Observing that $T_{13} = \text{proj}_2 T_{123} \in \mathcal{C}(\rho_1, \rho_3)$, one finds that

$$\begin{aligned} \mathfrak{D}(\rho_1, \rho_3)^2 & \leq \text{proj}_1 \text{proj}_3 (T_{13}^{\frac{1}{2}} C_{13} T_{13}^{\frac{1}{2}}) = \text{proj}_1 \text{proj}_3 \text{proj}_2 (T_{123}^{\frac{1}{2}} C_{13} T_{123}^{\frac{1}{2}}) \\ & \leq (1 + \alpha) \text{proj}_1 \text{proj}_2 \text{proj}_3 (T_{123}^{\frac{1}{2}} C_{12} T_{123}^{\frac{1}{2}}) \\ & \quad + (1 + \frac{1}{\alpha}) \text{proj}_2 \text{proj}_3 \text{proj}_1 (T_{123}^{\frac{1}{2}} C_{23} T_{123}^{\frac{1}{2}}) \\ & \leq (1 + \alpha) \text{proj}_1 \text{proj}_2 (T_{12}^{\frac{1}{2}} C_{12} T_{12}^{\frac{1}{2}}) \\ & \quad + (1 + \frac{1}{\alpha}) \text{proj}_2 \text{proj}_3 (T_{23}^{\frac{1}{2}} C_{23} T_{23}^{\frac{1}{2}}). \end{aligned}$$

Minimizing the right hand side in T_{12} and T_{23} leads to the inequality

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

and one concludes by further minimizing the right hand side in $\alpha > 0$.

This argument closely follows the proof of the triangle inequality for $\text{dist}_{\text{MK},2}$ in chapter 7 of [22], except that, for a general exponent $p \neq 2$, step (b) is replaced with the triangle inequality for the Euclidean distance, and step (c) involves the Minkowski inequality in L^p . The reader can check that, for $p = 2$, Villani's argument can be replaced with steps (b)-(c) above.

Step (a) corresponds to the “glueing lemma”, Lemma 7.6 in chapter 7 of [22] — see also Remark 5.3.3 in chapter 5 of [1]. A first step in the proof of Lemma 7.6 is based on the disintegration of measure theorem (formula (7.2) in chapter 7 of [22]), or Theorem 5.3.1 in [1]). Lemma 2.3 (or Lemma A.4 in [15]) is the analogue of the disintegration of measure theorem for couplings between a probability density on phase space and an arbitrary element of \mathfrak{D}_2 . In truth, Lemma 2.3 treats only the case of a coupling of a probability density with an element of $\mathcal{D}(\mathfrak{H})$, but the case of a coupling of a probability density with an element of $\mathcal{P}(\mathbf{R}^{2d})$ is already known from formula (7.2) in chapter 7 of [22].

We do not know whether there exists an analogous disintegration formula for a coupling of $\mathcal{C}(R, S)$, where $R, S \in \mathcal{D}(\mathfrak{H})$, and even in the affirmative, it is unclear how this would help us achieving Step (a) in general in the case where $\rho_2 \in \mathcal{D}(\mathfrak{H})$. Of course, if ρ_2 is a rank one projection, $\mathcal{C}(\rho_2, \rho_1) = \{\rho_2 \otimes \rho_1\}$ and $\mathcal{C}(\rho_2, \rho_3) = \{\rho_2 \otimes \rho_3\}$, and one chooses $T_{123} = T_{12} \otimes \rho_3$.

One can also forget about the disintegration of measure theorem (formula (7.2) in chapter 7 of [22]), or Theorem 5.3.1 in [1]) and its analogue Lemma 2.3 above, and consider the problem posed in Step (a) in the case where $\rho_2 \in \mathcal{D}(\mathfrak{H})$ is not rank-one. If ρ_1, ρ_2, ρ_3 are rank-two density operators, T_{123} is to be sought in the set of linear maps on $\text{Ran}(\rho_1) \otimes \text{Ran}(\rho_2) \otimes \text{Ran}(\rho_3)$. That T_{123} exists is possible only if the compatibility condition $\text{proj}_1 \text{proj}_3 T_{123} = \text{proj}_3 \text{proj}_1 T_{123}$ holds, which is the case since $T_{12} \in \mathcal{C}(\rho_1, \rho_2)$ and $T_{23} \in \mathcal{C}(\rho_2, \rho_3)$, so that

$$\text{proj}_1 \text{proj}_3 T_{123} = \rho_2 = \text{proj}_3 \text{proj}_1 T_{123}.$$

The set of linear maps $T_{123} = T_{123}^*$ on $\text{Ran}(\rho_1) \otimes \text{Ran}(\rho_2) \otimes \text{Ran}(\rho_3)$, which is a 8-dimensional space, has dimension 36; the linear constraints $\text{proj}_1 T_{123} = T_{23}$ and $\text{proj}_3 T_{123} = T_{12}$ each involve 10 scalar linear equations, which are not independent since the second marginal of T_{12} and the first marginal of T_{23} are equal. Even with the 16 remaining degrees of freedom, it is not clear to us that the positivity constraint $T_{123} \geq 0$ in Step (a) can be satisfied.

Summarizing, we have not been able to prove the existence of T_{123} satisfying the conditions stated in Step (a) for all $\rho_1, \rho_2, \rho_3 \in \mathfrak{D}_2$, which is left to the reader as an open problem. Whenever $\rho_1, \rho_2, \rho_3 \in \mathfrak{D}_2$ are such that Step (a) can be achieved, one has

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

The restricted triangle inequality reported in Theorem 3.1 holds because Step (a) can be achieved for $\rho_2 \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ or for $\rho_2 = |\psi\rangle\langle\psi|$ with $\psi \in \mathfrak{H}$ and $\|\psi\|_{\mathfrak{H}} = 1$.

If $\rho_2 \in \mathcal{D}_2(\mathfrak{H})$ has rank at least 2, we do not know whether Step (a) can be achieved, and the triangle inequality with ρ_2 as intermediate point cannot be studied following the pattern above. However, we shall prove an “approximate” triangle

inequality of the form

$$\mathfrak{d}(\rho_1, \rho_3) \leq \mathfrak{d}(\rho_1, \rho_2) + \mathfrak{d}(\rho_2, \rho_3) + O\left(\sqrt{\hbar}\right).$$

We shall see below that the proof of this ‘‘approximate’’ triangle inequality is completely different from the pattern involving Steps (a)-(c).

4. KANTOROVICH DUALITY

The Kantorovich duality theorem is a fundamental result in the theory of optimal transport. In the case of the metric $\text{dist}_{\text{MK},2}$, it can be stated as follows (Theorem 1.3 or Proposition 1.22 in chapter 1 of [22], or Theorem 6.1.1 on chapter 6 of [1]).

Kantorovich Duality Theorem Let $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^n)$. Then

$$\begin{aligned} \text{dist}_{\text{MK},2}(\mu, \nu)^2 &= \min_{\rho \in \mathcal{C}(\mu, \nu)} \iint_{\mathbf{R}^{2n}} |x - y|^2 \rho(dx dy) \\ &= \sup_{\substack{a, b \in C_b(\mathbf{R}^n; \mathbf{R}) \\ a(x) + b(y) \leq |x - y|^2}} \left(\int_{\mathbf{R}^n} a(x) \mu(dx) + \int_{\mathbf{R}^n} b(x) \nu(dx) \right). \end{aligned}$$

In [6], we have proved the following analogue of the Kantorovich duality theorem for density operators.

Kantorovich Duality Theorem for Density Operators. Let $R, S \in \mathcal{D}_2(\mathfrak{H})$. Then

$$\mathfrak{d}(R, S)^2 = \min_{T \in \mathcal{C}(R, S)} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(T^{\frac{1}{2}} C_{\hbar} T^{\frac{1}{2}} \right) = \sup_{\substack{A=A^*, B=B^* \in \mathcal{L}(\mathfrak{H}) \\ A \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes B \leq C_{\hbar}}} \text{trace}_{\mathfrak{H}}(RA + SB).$$

The inequality constraint

$$A \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes B \leq C_{\hbar}$$

is to be understood as

$$\langle \Phi | C_{\hbar} - A \otimes I_{\mathfrak{H}} - I_{\mathfrak{H}} \otimes B | \Phi \rangle \geq 0$$

for all $\Phi \in \text{Form-Dom}(C_{\hbar})$, i.e. for all $\Phi \equiv \Phi(x, y) \in L^2(\mathbf{R}^{2d}; (1 + |x - y|^2) dx dy)$ such that

$$(\partial_{x_j} - \partial_{y_j}) \Phi \in L^2(\mathbf{R}^{2d}), \quad j = 1, \dots, d.$$

In the present section, we complete the extension of the Kantorovich duality to the set \mathfrak{D}_2 for the ‘‘pseudometric’’ \mathfrak{d} .

Theorem 4.1. *Let $p \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$ and $S \in \mathcal{D}_2(\mathfrak{H})$. Then*

$$\begin{aligned} \mathfrak{d}(p, S)^2 &= \min_{Q \in \mathcal{C}(p, S)} \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2} c_{\hbar}(x, \xi) Q(x, \xi)^{1/2}) dx d\xi \\ &= \sup_{\substack{a \in C_b(\mathbf{R}^{2d}; \mathbf{R}), B=B^* \in \mathcal{L}(\mathfrak{H}) \\ a(x, \xi) I_{\mathfrak{H}} + B \leq c_{\hbar}(x, \xi)}} \left(\int_{\mathbf{R}^{2d}} a(x, \xi) p(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}(BS) \right). \end{aligned}$$

Notice that the duality theorem implies in particular the existence of at least one optimal coupling $Q \in \mathcal{C}(p, S)$.

Proof. The proof is split in several steps.

Step 1: the functions f and g . Consider the Banach space $E := C_b(\mathbf{R}^{2d}, \mathcal{L}(\mathfrak{H}))$, with

$$\|T\|_E := \sup_{(x, \xi) \in \mathbf{R}^{2d}} \|T(x, \xi)\|,$$

and set

$$f(T) := \begin{cases} 0 & \text{if } T(x, \xi) = T(x, \xi)^* \geq -c_{\hbar}(x, \xi) \text{ for all } (x, \xi) \in \mathbf{R}^{2d}, \\ +\infty & \text{otherwise,} \end{cases}$$

while

$$g(T) := \begin{cases} \int_{\mathbf{R}^{2d}} ap(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}(BS) & \text{if } T(x, \xi) = T(x, \xi)^* = a(x, \xi)I_{\mathfrak{H}} + B, \\ +\infty & \text{for all } (x, \xi) \in \mathbf{R}^{2d}, \\ +\infty & \text{otherwise,} \end{cases}$$

The constraint $T(x, \xi) = T(x, \xi)^* \geq -c_{\hbar}(x, \xi)$ means that, for each $(x, \xi) \in \mathbf{R}^{2d}$, one has

$$\langle \phi(x, \xi) | T(x, \xi) + c_{\hbar}(x, \xi) | \phi(x, \xi) \rangle \geq 0$$

for all $\phi \in \text{Form-Dom}(c_{\hbar}(x, \xi))$. On the other hand, the nullspace of the linear map

$$C_b(\mathbf{R}^{2d}) \times \mathcal{L}(\mathfrak{H}) \ni (a, B) \mapsto \Gamma(a, B) \equiv a(x, \xi)I_{\mathfrak{H}} + B \in E$$

is

$$\text{Ker}(\Gamma) = \{(t, -tI_{\mathfrak{H}}), \quad t \in \mathbf{R}\}.$$

Since p is a probability density while $\text{trace}_{\mathfrak{H}}(S) = 1$, one has

$$g((a+t)I_{\mathfrak{H}} + (B-tI_{\mathfrak{H}})) = g(aI_{\mathfrak{H}} + B) + t \int_{\mathbf{R}^{2d}} p(x, \xi) dx d\xi - t \text{trace}_{\mathfrak{H}}(S) = g(aI_{\mathfrak{H}} + B),$$

and the prescription above defines g on $\text{Ran}(\Gamma) \simeq (C_b(\mathbf{R}^{2d}) \times \mathcal{L}(\mathfrak{H})) / \text{Ker}(\Gamma)$.

Observe that

$$\begin{aligned} g((aI_{\mathfrak{H}} + B)^*) &= g(\bar{a}I_{\mathfrak{H}} + B^*) = \int_{\mathbf{R}^{2d}} \overline{a(x, \xi)} p(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}(B^* S) \\ &= \overline{\int_{\mathbf{R}^{2d}} a(x, \xi) p(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}((SB)^*)} \\ &= \overline{\int_{\mathbf{R}^{2d}} a(x, \xi) p(x, \xi) dx d\xi + \overline{\text{trace}_{\mathfrak{H}}(SB)}} \\ &= \overline{g(aI_{\mathfrak{H}} + B)}, \end{aligned}$$

so that $(aI_{\mathfrak{H}} + B)^* = aI_{\mathfrak{H}} + B \implies g(aI_{\mathfrak{H}} + B) \in \mathbf{R}$. Thus the definition above implies that g takes its values in $\mathbf{R} \cup \{+\infty\}$.

The functions f and g are convex. Indeed, g is the extension by $+\infty$ of a \mathbf{R} -linear functional defined on the set of self-adjoint elements of $\text{Ran}(\Gamma)$, which is a linear subspace of E . As for f , it is the indicator function (in the sense of the definition in §4 of [20] on p. 28) of the convex set

$$\{T \in E \text{ s.t. } T(x, \xi) = T(x, \xi)^* \geq -c_{\hbar}(x, \xi) \text{ for all } (x, \xi) \in \mathbf{R}^{2d}\}$$

and is therefore convex. Besides $f(0) = g(0) = 0$, and f is continuous at 0. Indeed

$$c_{\hbar}(x, \xi) \geq d\hbar I_{\mathfrak{H}} \quad \text{for all } (x, \xi) \in \mathbf{R}^{2d},$$

so that, for each $T \in E$

$$\begin{aligned} T(x, \xi) &= T(x, \xi)^* \text{ and } \|T(x, \xi)\| < \frac{1}{2}d\hbar \text{ for all } (x, \xi) \in \mathbf{R}^{2d} \\ \implies T(x, \xi) &\geq -c_{\hbar}(x, \xi) \text{ for all } (x, \xi) \in \mathbf{R}^{2d} \implies f(T) = 0. \end{aligned}$$

In particular f is continuous at 0.

Step 2: applying convex duality. By the Fenchel-Rockafellar convex duality theorem (Theorem 1.12 in [4])

$$\inf_{T \in E} (f(T) + g(T)) = \max_{\Lambda \in E'} (-f^*(-\Lambda) - g^*(\Lambda)).$$

Here f^* and g^* are the Legendre duals of f and g , and are computed below.

First

$$f^*(-\Lambda) = \sup_{T \in E} (\langle -\Lambda, T \rangle - f(T)) = \sup_{\substack{T \in E \\ T(x, \xi) = T(x, \xi)^* \geq -c_{\hbar}(x, \xi)}} \langle -\Lambda, T \rangle.$$

If $\Lambda \in E'$ is not a nonnegative linear functional, there exists $T_0 \in E$ such that $T_0(x, \xi) = T_0(x, \xi)^* \geq 0$ such that $\langle \Lambda, T_0 \rangle = -\alpha < 0$. Since

$$nT_0(x, \xi) = nT_0(x, \xi)^* \geq 0 \geq -d\hbar I_{\mathfrak{H}} \geq -c_{\hbar}(x, \xi) \text{ for all } (x, \xi) \in \mathbf{R}^{2d},$$

one has

$$f^*(-\Lambda) \geq \sup_{n \geq 1} \langle -\Lambda, nT_0 \rangle = \sup_{n \geq 1} (n\alpha) = +\infty.$$

For $\Lambda \in E'$ such that $\Lambda \geq 0$, we define

$$\langle \Lambda, c_{\hbar} \rangle := \sup_{\substack{T \in E \\ T(x, \xi) = T(x, \xi)^* \leq c_{\hbar}(x, \xi)}} \langle \Lambda, T \rangle \in [0, +\infty].$$

(Observe indeed that $T = 0$ satisfies the constraints since $c_{\hbar}(x, \xi) = c_{\hbar}(x, \xi)^* \geq 0$ for each $(x, \xi) \in \mathbf{R}^{2d}$.) With this definition, one has clearly

$$f^*(-\Lambda) := \begin{cases} \langle \Lambda, c_{\hbar} \rangle & \text{if } \Lambda \geq 0, \\ 0 & \text{otherwise.} \end{cases}$$

Next

$$\begin{aligned} g^*(\Lambda) &= \sup_{T \in E} (\langle \Lambda, T \rangle - g(T)) \\ &= \sup_{\substack{T \in E \\ T(x, \xi) = T(x, \xi)^* = a(x, \xi)I_{\mathfrak{H}} + B}} \left(\langle \Lambda, T \rangle - \int_{\mathbf{R}^{2d}} a(x, \xi)p(x, \xi)dx d\xi - \text{trace}_{\mathfrak{H}}(BS) \right). \end{aligned}$$

If there exists $a \equiv a(x, \xi) \in C_b(\mathbf{R}^{2d}, \mathbf{R})$ and $B = B^* \in \mathcal{L}(\mathfrak{H})$ such that either

$$\langle \Lambda, aI_{\mathfrak{H}} + B \rangle > \int_{\mathbf{R}^{2d}} a(x, \xi)p(x, \xi)dx d\xi + \text{trace}_{\mathfrak{H}}(BS)$$

or

$$\langle \Lambda, aI_{\mathfrak{H}} + B \rangle < \int_{\mathbf{R}^{2d}} a(x, \xi)p(x, \xi)dx d\xi + \text{trace}_{\mathfrak{H}}(BS),$$

one has either

$$g(\Lambda) \geq \sup_{n \geq 1} \left(\langle \Lambda, n(aI_{\mathfrak{H}} + B) \rangle - n \int_{\mathbf{R}^{2d}} a(x, \xi)p(x, \xi)dx d\xi - n \text{trace}_{\mathfrak{H}}(BS) \right) = +\infty,$$

or

$$g(\Lambda) \geq \sup_{n \geq 1} \left(\langle \Lambda, n(-aI_{\mathfrak{H}} - B) \rangle + n \int_{\mathbf{R}^{2d}} a(x, \xi)p(x, \xi)dx d\xi + n \text{trace}_{\mathfrak{H}}(BS) \right) = +\infty.$$

Hence

$$g^*(\Lambda) := \begin{cases} 0 & \text{if } \langle \Lambda, aI_{\mathfrak{H}} + B \rangle = \int_{\mathbf{R}^{2d}} a(x, \xi) p(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}(BS) \\ & \text{for each } a \equiv a(x, \xi) \in C_b(\mathbf{R}^{2d}, \mathbf{R}) \text{ and } B = B^* \in \mathcal{L}(\mathfrak{H}), \\ +\infty & \text{otherwise.} \end{cases}$$

Notice that the prescription

$$\langle \Lambda, aI_{\mathfrak{H}} + B \rangle = \int_{\mathbf{R}^{2d}} a(x, \xi) p(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}(BS)$$

defines a unique linear functional on the set of $T \in \text{Ran } \Gamma$ such that $T(x, \xi)^* = T(x, \xi)$ for each $(x, \xi) \in \mathbf{R}^{2d}$ by the same argument as in Step 1.

Therefore, the Fenchel-Rockafellar duality theorem in this case results in the equality

$$\begin{aligned} \inf_{T \in E} (f(T) + g(T)) &= \inf_{\substack{a \in C_b(\mathbf{R}^{2d}, \mathbf{R}), B = B^* \\ a(x, \xi) I_{\mathfrak{H}} + B \geq -c_h(x, \xi)}} \left(\int_{\mathbf{R}^{2d}} a(x, \xi) p(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}(SB) \right) \\ &= \max_{\Lambda \in E'} (f^*(-\Lambda) + g^*(\Lambda)) = \max_{\substack{0 \leq \Lambda \in E', \langle \Lambda, aI_{\mathfrak{H}} + B \rangle \\ = \int a(x, \xi) p(x, \xi) dx d\xi + \text{trace}(SB)}} -\langle \Lambda, c_h \rangle \end{aligned}$$

or, equivalently

$$\begin{aligned} \sup_{\substack{a \in C_b(\mathbf{R}^{2d}, \mathbf{R}), B = B^* \\ a(x, \xi) I_{\mathfrak{H}} + B \leq c_h(x, \xi)}} \left(\int_{\mathbf{R}^{2d}} a(x, \xi) p(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}(SB) \right) \\ = \min_{\substack{0 \leq \Lambda \in E', \langle \Lambda, aI_{\mathfrak{H}} + B \rangle \\ = \int a(x, \xi) p(x, \xi) dx d\xi + \text{trace}(SB)}} \langle \Lambda, c_h \rangle. \end{aligned}$$

Step 3: representing the optimal Λ . Let $\Lambda \in E'$ satisfy the constraints in the min on the right hand side of the equality above.

Define a linear map $F_{\Lambda} : C_b(\mathbf{R}^{2d}) \rightarrow \mathcal{L}^1(\mathfrak{H})$ by the formula

$$\text{trace}_{\mathfrak{H}}(KF_{\Lambda}(a)) = \Lambda(aK), \quad \text{for each } K \in \mathcal{K}(\mathfrak{H}).$$

The map F_{Λ} is well defined since $K \mapsto \Lambda(aK)$ is a linear functional on $\mathcal{K}(\mathfrak{H})$ which is continuous for the norm topology, and since $\mathcal{K}(\mathfrak{H})' = \mathcal{L}^1(\mathfrak{H})$, this linear functional is represented by a trace-class operator $F_{\Lambda}(a)$. Since Λ is linear, the map F_{Λ} is linear.

Since $\Lambda \geq 0$, one has $F_{\Lambda}(a) = F_{\Lambda}(a)^* \geq 0$ for each $a \in C_b(\mathbf{R}^d)$ such that $a(x, \xi) \geq 0$ for each $(x, \xi) \in \mathbf{R}^{2d}$. Indeed, for $a \in C_b(\mathbf{R}^{2d}; \mathbf{R})$, set

$$T_1 := \frac{1}{2}(F_{\Lambda}(a) + F_{\Lambda}(a)^*), \quad T_2 := -\frac{1}{2}i(F_{\Lambda}(a) - F_{\Lambda}(a)^*).$$

Then, for each $K = K^* \in \mathcal{K}(\mathfrak{H})$, one has

$$\Lambda(aK) = \text{trace}_{\mathfrak{H}}(T_1 K) + i \text{trace}_{\mathfrak{H}}(T_2 K)$$

with

$$\overline{\text{trace}_{\mathfrak{H}}(T_j K)} = \text{trace}_{\mathfrak{H}}((T_j K)^*) = \text{trace}_{\mathfrak{H}}(K^* T_j^*) = \text{trace}_{\mathfrak{H}}(K T_j) = \text{trace}_{\mathfrak{H}}(T_j K)$$

for $j = 1, 2$. Since $a \in C_b(\mathbf{R}^{2d}; \mathbf{R})$ and $K = K^* \in \mathcal{L}(\mathfrak{H})$, one has

$$-\|a\|_{L^\infty} \|K\|_{I_{\mathfrak{H}}} \leq aK \leq \|a\|_{L^\infty} \|K\|_{I_{\mathfrak{H}}}$$

so that

$$-\|a\|_{L^\infty}\|K\| \leq \Lambda(aK) \leq \|a\|_{L^\infty}\|K\| \quad \text{since } \Lambda(I_{\mathfrak{H}}) = \int_{\mathbf{R}^{2d}} p(x, \xi) dx d\xi = 1.$$

In particular, $\Lambda(aK) \in \mathbf{R}$, so that $\text{trace}_{\mathfrak{H}}(T_2 K) = 0$ for each $K = K^* \in \mathcal{K}(\mathfrak{H})$. Since $T_2 = T_2^* \in \mathcal{L}^1(\mathfrak{H})$, specializing this identity to the case where K is the orthogonal projection on any eigenvector of T_2 shows that $T_2 = 0$. Thus

$$a \in C_b(\mathbf{R}^{2d}; \mathbf{R}) \implies F_\Lambda(a) = F_\Lambda(a)^*.$$

Moreover

$$a \in C_b(\mathbf{R}^{2d}; \mathbf{R}) \text{ and } a \geq 0 \implies \text{trace}_{\mathfrak{H}}(F_\Lambda(a)K) \geq 0 \text{ for each } K = K^* \geq 0 \text{ in } \mathcal{K}(\mathfrak{H})$$

and specializing this last inequality to the case where K is the orthogonal projection on any eigenvector of $F_\Lambda(a) = F_\Lambda(a)^* \in \mathcal{L}^1(\mathfrak{H})$ shows that all the eigenvalues of $F_\Lambda(a)$ are nonnegative, so that $F_\Lambda(a) \geq 0$.

Next we deduce from the defining identity for F_Λ , i.e.

$$\Lambda(aK) = \text{trace}_{\mathfrak{H}}(F_\Lambda(a)K) \text{ for each } a \in C_b(\mathbf{R}^{2d}; \mathbf{C}) \text{ and } K \in \mathcal{K}(\mathfrak{H}),$$

that

$$\|F_\Lambda(a)\|_1 \leq \|\Lambda\| \|a\|_{L^\infty(\mathbf{R}^{2d})}.$$

Then we specialize this defining identity to the case where $a \geq 0$ on \mathbf{R}^{2d} while $K = \Pi_n$ is the orthogonal projection on $\text{span}\{e_1, \dots, e_n\}$, with (e_1, e_2, \dots) a complete orthonormal system in \mathfrak{H} . One has

$$\Lambda(a\Pi_n) = \text{trace}_{\mathfrak{H}}(F_\Lambda(a)\Pi_n) \rightarrow \text{trace}_{\mathfrak{H}}(F_\Lambda(a)) = \|F_\Lambda(a)\|_1 \quad \text{as } n \rightarrow \infty,$$

while

$$a(I_{\mathfrak{H}} - \Pi_n) \geq 0 \text{ so that } \Lambda(a\Pi_n) \leq \Lambda(aI_{\mathfrak{H}}) = \int_{\mathbf{R}^{2d}} a(x, \xi)p(x, \xi) dx d\xi.$$

Hence

$$a \in C_b(\mathbf{R}^{2d}) \text{ and } a \geq 0 \implies \|F_\Lambda(a)\|_1 \leq \int_{\mathbf{R}^{2d}} a(x, \xi)p(x, \xi) dx d\xi.$$

More generally, for each $a \in C_b(\mathbf{R}^{2d}; \mathbf{R})$, one has $-|a| \leq a \leq |a|$ so that

$$|\text{trace}_{\mathfrak{H}}(F_\Lambda(a)|e_j\rangle\langle e_j|)| = |\Lambda(a|e_j\rangle\langle e_j|)| \leq \Lambda(|a||e_j\rangle\langle e_j|)$$

for each $j \geq 1$, where (e_1, e_2, \dots) is a complete orthonormal system of eigenvectors of $F_\Lambda(a) = F_\Lambda(a)^* \in \mathcal{L}^1(\mathfrak{H})$. Hence

$$\sum_{j=1}^n |\text{trace}_{\mathfrak{H}}(F_\Lambda(a)|e_j\rangle\langle e_j|)| \leq \Lambda\left(|a| \sum_{j=1}^n |e_j\rangle\langle e_j|\right) \leq \Lambda(|a|I_{\mathfrak{H}}),$$

and since

$$\sum_{j=1}^n |\text{trace}_{\mathfrak{H}}(F_\Lambda(a)|e_j\rangle\langle e_j|)| \rightarrow \|F_\Lambda(a)\|_1 \quad \text{as } n \rightarrow \infty,$$

we conclude that

$$\|F_\Lambda(a)\|_1 \leq \Lambda(|a|I_{\mathfrak{H}}) = \int_{\mathbf{R}^{2d}} |a(x, \xi)|p(x, \xi) dx d\xi.$$

Since $C_b(\mathbf{R}^{2d})$ is dense in $L^1(\mathbf{R}^{2d}, p dx d\xi)$, this inequality, applied to the real and the imaginary parts of a , shows that F_Λ is a continuous linear operator from

$L^1(\mathbf{R}^{2d}, p dx d\xi)$ to $\mathcal{L}^1(\mathfrak{H})$. Since $\mathcal{L}^1(\mathfrak{H})$ is separable and is the dual of the Banach space $\mathcal{K}(\mathfrak{H})$ (the norm closure in $\mathcal{L}(\mathfrak{H})$ of the set of finite rank operators), we conclude from the Dunford-Pettis theorem (Theorem 1 in §3 of chapter III in [11]) that $\mathcal{L}^1(\mathfrak{H})$ has the Radon-Nikodym property. By Theorem 5 in §1 of chapter III in [11], the operator F_Λ is Riesz-representable: in other words, there exists $q \in L^\infty(\mathbf{R}^{2d}, p dx d\xi; \mathcal{L}^1(\mathfrak{H}))$ such that

$$F_\Lambda(a) = \int_{\mathbf{R}^{2d}} a(x, \xi) q(x, \xi) p(x, \xi) dx d\xi, \quad \text{for all } a \in L^1(\mathbf{R}^{2d}, p dx d\xi).$$

Step 4: defining the optimal coupling. With Λ as in Step 3, we have seen that

$$a \in C_b(\mathbf{R}^{2d}) \text{ and } a \geq 0 \implies F_\Lambda(a) = \int_{\mathbf{R}^{2d}} a(x, \xi) q(x, \xi) p(x, \xi) dx d\xi \geq 0.$$

This implies that $q(x, \xi) = q(x, \xi)^* \geq 0$ for a.e. $(x, \xi) \in \mathbf{R}^{2d}$.

Next, one has

$$\Lambda(K) = \text{trace}_{\mathfrak{H}}(F_\Lambda(1)K) = \text{trace}_{\mathfrak{H}}(KS), \quad K \in \mathcal{K}(\mathfrak{H}),$$

so that

$$F_\Lambda(1) = \int_{\mathbf{R}^{2d}} q(x, \xi) p(x, \xi) dx d\xi = S \in \mathcal{L}^1(\mathfrak{H}) (= \mathcal{K}(\mathfrak{H})').$$

On the other hand, for each $a \in C_b(\mathbf{R}^{2d})$ such that $a \geq 0$, one has

$$\begin{aligned} \text{trace}_{\mathfrak{H}} \left(P_n \int_{\mathbf{R}^{2d}} a(x, \xi) q(x, \xi) p(x, \xi) dx d\xi \right) &= \text{trace}_{\mathfrak{H}}(F_\Lambda(a)P_n) = \Lambda(aP_n) \\ &\leq \Lambda(aI_{\mathfrak{H}}) = \int_{\mathbf{R}^{2d}} a(x, \xi) p(x, \xi) dx d\xi \end{aligned}$$

where P_n is the orthogonal projection on $\text{span}\{e_1, \dots, e_n\}$, with (e_1, e_2, \dots) being a complete orthonormal system of eigenvectors of

$$\int_{\mathbf{R}^{2d}} a(x, \xi) q(x, \xi) p(x, \xi) dx d\xi \in \mathcal{L}^1(\mathfrak{H}).$$

Letting $n \rightarrow \infty$, one has

$$\begin{aligned} &\text{trace}_{\mathfrak{H}} \left(P_n \int_{\mathbf{R}^{2d}} a(x, \xi) q(x, \xi) p(x, \xi) dx d\xi \right) \\ &\rightarrow \text{trace}_{\mathfrak{H}} \left(\int_{\mathbf{R}^{2d}} a(x, \xi) q(x, \xi) p(x, \xi) dx d\xi \right), \end{aligned}$$

so that

$$\int_{\mathbf{R}^{2d}} a(x, \xi) \text{trace}_{\mathfrak{H}}(q(x, \xi)) p(x, \xi) dx d\xi \leq \int_{\mathbf{R}^{2d}} a(x, \xi) p(x, \xi) dx d\xi.$$

Since this holds for each $a \in C_b(\mathbf{R}^{2d})$ such that $a \geq 0$, we conclude that

$$\text{trace}_{\mathfrak{H}}(q(x, \xi)) \leq 1 \quad \text{for } p(x, \xi) dx d\xi\text{-a.e. } (x, \xi) \in \mathbf{R}^{2d}.$$

Moreover

$$\int_{\mathbf{R}^{2d}} (1 - \text{trace}_{\mathfrak{H}}(q(x, \xi))) p(x, \xi) dx d\xi = 1 - \text{trace}_{\mathfrak{H}}(S) = 0,$$

so that

$$\text{trace}_{\mathfrak{H}}(q(x, \xi)) = 1 \quad \text{for } p(x, \xi) dx d\xi\text{-a.e. } (x, \xi) \in \mathbf{R}^{2d}.$$

In other words, we have proved that $(x, \xi) \mapsto Q(x, \xi) = p(x, \xi)q(x, \xi)$ defines an element of $\mathcal{C}(p, S)$.

Step 5: extending the representation formula for Λ . Let Λ be as in Step 3, and let Q be the coupling of p and S obtained at the end of Step 4. For each $B \in E$, we define

$$\langle L, B \rangle := \langle \Lambda, B \rangle - \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(B(x, \xi)Q(x, \xi)) dx d\xi.$$

Let us prove that

$$B \in E \text{ and } B(x, \xi) = B(x, \xi)^* \geq 0 \text{ for all } (x, \xi) \in \mathbf{R}^{2d} \implies \langle L, B \rangle \geq 0.$$

Pick $\epsilon > 0$, and let Q_ϵ be a simple $\mathcal{L}^1(\mathfrak{H})$ -valued function on \mathbf{R}^{2d} such that

$$\int_{\mathbf{R}^{2d}} \|Q(x, \xi) - Q_\epsilon(x, \xi)\|_1 dx d\xi < \epsilon.$$

Write

$$Q_\epsilon(x, \xi) = \sum_{j=1}^N \mathbf{1}_{\Omega_j}(x, \xi) Q_j, \quad 0 \leq Q_j = Q_j^* \in \mathcal{L}^1(\mathfrak{H}) \text{ for each } j = 0, \dots, N,$$

where Ω_j are bounded, pairwise disjoint measurable sets in \mathbf{R}^{2d} for $j = 1, \dots, N$. For each $j = 1, \dots, N$, let $(e_{j,1}, e_{j,2}, \dots)$ designate a complete orthonormal system of eigenvectors of Q_j , and let $P_{j,n}$ be the orthogonal projection on $\text{span}\{e_{j,1}, \dots, e_{j,n}\}$. Define

$$\Pi_n(x, \xi) = \sum_{j=1}^N \mathbf{1}_{\Omega_j}(x, \xi) P_{j,n}.$$

One easily checks that $\Pi_n(x, \xi) = \Pi_n(x, \xi)^* = \Pi_n(x, \xi)^2$ for each $(x, \xi) \in \mathbf{R}^{2d}$. Then, for each $B \in E$ such that $B(x, \xi) = B(x, \xi)^* \geq 0$ for all $(x, \xi) \in \mathbf{R}^{2d}$, one has

$$\begin{aligned} 0 &\leq \langle \Lambda, (I_{\mathfrak{H}} - \Pi_n)B(I_{\mathfrak{H}} - \Pi_n) \rangle = \langle \Lambda, B \rangle - \langle \Lambda, \Pi_n B + B \Pi_n - \Pi_n B \Pi_n \rangle \\ &= \langle \Lambda, B \rangle - \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((\Pi_n B + B \Pi_n - \Pi_n B \Pi_n)Q)(x, \xi) dx d\xi \\ &= \langle \Lambda, B \rangle - \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((\Pi_n B + B \Pi_n - \Pi_n B \Pi_n)Q_\epsilon)(x, \xi) dx d\xi \\ &\quad + \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((\Pi_n B + B \Pi_n - \Pi_n B \Pi_n)(Q_\epsilon - Q))(x, \xi) dx d\xi. \end{aligned}$$

By construction, keeping $\epsilon > 0$ fixed, $[\Pi_n(x, \xi), Q_\epsilon(x, \xi)] = 0$, so that, by cyclicity of the trace, one has

$$\begin{aligned} &\int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((\Pi_n B + B \Pi_n - \Pi_n B \Pi_n)Q_\epsilon)(x, \xi) dx d\xi \\ &= \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(B \Pi_n Q_\epsilon \Pi_n)(x, \xi) dx d\xi \rightarrow \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(B Q_\epsilon)(x, \xi) dx d\xi \end{aligned}$$

as $n \rightarrow \infty$, so that

$$\begin{aligned} 0 \leq \overline{\lim}_{n \rightarrow \infty} \langle \Lambda, (I_{\mathfrak{H}} - \Pi_n)B(I_{\mathfrak{H}} - \Pi_n) \rangle &= \langle \Lambda, B \rangle - \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(BQ)(x, \xi) dx d\xi \\ &+ \overline{\lim}_{n \rightarrow \infty} \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((\Pi_n B + B\Pi_n - \Pi_n B\Pi_n)(Q_\epsilon - Q))(x, \xi) dx d\xi \\ &+ \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(B(Q - Q_\epsilon))(x, \xi) dx d\xi. \end{aligned}$$

On the other hand

$$\begin{aligned} &\left| \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}((\Pi_n B + B\Pi_n - \Pi_n B\Pi_n)(Q_\epsilon - Q))(x, \xi) dx d\xi \right| \\ &\leq \int_{\mathbf{R}^{2d}} |\text{trace}_{\mathfrak{H}}((\Pi_n B + B\Pi_n - \Pi_n B\Pi_n)(Q_\epsilon - Q))(x, \xi)| dx d\xi \\ &\leq \int_{\mathbf{R}^{2d}} \|(\Pi_n B + B\Pi_n - \Pi_n B\Pi_n)(x, \xi)\| \| (Q_\epsilon - Q)(x, \xi) \|_1 dx d\xi \\ &\leq 3 \sup_{(x, \xi) \in \mathbf{R}^{2d}} \|B(x, \xi)\| \int_{\mathbf{R}^{2d}} \| (Q_\epsilon - Q)(x, \xi) \|_1 dx d\xi \\ &\leq 3\epsilon \sup_{(x, \xi) \in \mathbf{R}^{2d}} \|B(x, \xi)\| \end{aligned}$$

while, by the same token,

$$\left| \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(B(Q - Q_\epsilon))(x, \xi) dx d\xi \right| \leq \epsilon \sup_{(x, \xi) \in \mathbf{R}^{2d}} \|B(x, \xi)\|.$$

Finally

$$\langle \Lambda, B \rangle - \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(BQ)(x, \xi) dx d\xi \geq -4\epsilon \sup_{(x, \xi) \in \mathbf{R}^{2d}} \|B(x, \xi)\|$$

and since this holds for each $\epsilon > 0$, we conclude that the linear functional L defined at the beginning of Step 5 satisfies

$$B \in E \text{ and } B(x, \xi) = B(x, \xi)^* \geq 0 \text{ for all } (x, \xi) \in \mathbf{R}^{2d} \implies \langle L, B \rangle \geq 0.$$

By a classical argument, this implies that $\|L\| = \langle L, I_{\mathfrak{H}} \rangle$.

On the other hand

$$\begin{aligned} \langle L, I_{\mathfrak{H}} \rangle &= \langle L, I_{\mathfrak{H}} \rangle - \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(q(x, \xi))p(x, \xi) dx d\xi \\ &= \text{trace}_{\mathfrak{H}}(S) - \int_{\mathbf{R}^{2d}} p(x, \xi) dx d\xi = 0 \end{aligned}$$

so that $L = 0$. In other words, the representation formula

$$\langle \Lambda, B \rangle = \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(B(x, \xi)Q(x, \xi)) dx d\xi$$

holds for each $B \in E$, and not only for $B \in C_b(\mathbf{R}^{2d}; \mathcal{K}(\mathfrak{H}))$.

Step 6: computing $\langle \Lambda, c_{\hbar} \rangle$. As explained in Step 2

$$\langle \Lambda, c_{\hbar} \rangle = \sup_{\substack{T \in E \\ T(x, \xi) = T(x, \xi)^* \leq c_{\hbar}(x, \xi)}} \langle \Lambda, T \rangle.$$

For each $n \geq 1$, set

$$c_n(x, \xi) := (I_{\mathfrak{H}} + \frac{1}{n}c_{\hbar}(x, \xi))^{-1}c_{\hbar}(x, \xi) \in \mathcal{L}(\mathfrak{H}),$$

so that

$$0 \leq c_1(x, \xi) = c_1(x, \xi)^* \leq \dots \leq c_n(x, \xi) = c_n(x, \xi)^* \leq \dots \leq c_{\hbar}(x, \xi) = c_{\hbar}(x, \xi)^*.$$

Thus, by the conclusion of Step 5,

$$\langle \Lambda, c_n \rangle = \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)c_n(x, \xi)) dx d\xi \leq \langle \Lambda, c_{\hbar} \rangle$$

for each $n \geq 1$, so that, using Proposition A.3 in [15] as in the proof of Lemma 2.1,

$$\begin{aligned} & \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2}c_{\hbar}(x, \xi)Q(x, \xi)^{1/2}) dx d\xi \\ &= \lim_{n \rightarrow \infty} \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)c_n(x, \xi)) dx d\xi \\ &\leq \langle \Lambda, c_{\hbar} \rangle. \end{aligned}$$

On the other hand, let $(e_1(x, \xi), e_2(x, \xi), \dots)$ designate a complete orthonormal system in \mathfrak{H} of eigenfunctions of $c_{\hbar}(x, \xi)$, with $c_{\hbar}(x, \xi)e_j(x, \xi) = \lambda_j e_j(x, \xi)$ for $j \geq 1$. Since $c_{\hbar}(x, \xi)$ is twice the harmonic oscillator $H := -\frac{1}{2}\hbar^2 \Delta_x + \frac{1}{2}|x|^2$ unitarily translated in phase space by (x, ξ) , the eigenvalues λ_j are independent of (x, ξ) . Set

$$t_{kl}(x, \xi) := \langle e_k(x, \xi) | Q(x, \xi)^{1/2} | e_l(x, \xi) \rangle, \quad k, l \geq 1.$$

Since $(x, \xi) \mapsto Q(x, \xi)^{1/2} \in L^2(\mathbf{R}^{2d}; \mathcal{L}^2(\mathfrak{H}))$, one has

$$v_k(x, \xi) := \sum_{l \geq 1} t_{kl}(x, \xi) e_l(x, \xi) \in \text{Form-Dom}(c_{\hbar}(x, \xi)) \quad \text{for a.e. } (x, \xi) \in \mathbf{R}^{2d},$$

and

$$\begin{aligned} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2}c_{\hbar}(x, \xi)Q(x, \xi)^{1/2}) &= \sum_{k, l \geq 1} \lambda_l |t_{kl}(x, \xi)|^2 \\ &= \sum_{k \geq 1} \langle v_k(x, \xi) | c_{\hbar}(x, \xi) | v_k(x, \xi) \rangle < \infty \end{aligned}$$

for a.e. $(x, \xi) \in \mathbf{R}^{2d}$, since

$$\int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2}c_{\hbar}(x, \xi)Q(x, \xi)^{1/2}) dx d\xi < \infty.$$

Taking this last inequality for granted, we conclude as follows.

Let $a \equiv a(x, \xi) \in C_b(\mathbf{R}^{2d})$ and $B = B^* \in \mathcal{L}(\mathfrak{H})$ satisfy the constraint

$$a(x, \xi)I_{\mathfrak{H}} + B \leq c_{\hbar}(x, \xi), \quad (x, \xi) \in \mathbf{R}^{2d}$$

in the sense that

$$a(x, \xi)\|\phi\|_{\mathfrak{H}}^2 + \langle \phi | B | \phi \rangle \leq \langle \phi | c_{\hbar}(x, \xi) | \phi \rangle \quad \text{for each } \phi \in \text{Form-Dom}(c_{\hbar}(x, \xi)).$$

Since $v_k(x, \xi) \in \text{Form-Dom}(c_{\hbar}(x, \xi))$ for a.e. $(x, \xi) \in \mathbf{R}^{2d}$ and each $k \geq 1$

$$\begin{aligned} & a(x, \xi)p(x, \xi) + \text{trace}_{\mathfrak{H}}(Q(x, \xi)B) \\ &= a(x, \xi) \text{trace}_{\mathfrak{H}}(Q(x, \xi)) + \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2}BQ(x, \xi)^{1/2}) \\ &= a(x, \xi) \sum_{k \geq 1} \langle v_k(x, \xi) | v_k(x, \xi) \rangle + \sum_{k \geq 1} \langle v_k(x, \xi) | B | v_k(x, \xi) \rangle \\ &\leq \sum_{k \geq 1} \langle v_k(x, \xi) | c_{\hbar}(x, \xi) | v_k(x, \xi) \rangle = \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2}c_{\hbar}(x, \xi)Q(x, \xi)^{1/2}). \end{aligned}$$

Integrating in (x, ξ) shows that

$$\begin{aligned} & \int_{\mathbf{R}^{2d}} a(x, \xi)p(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}(SB) \\ &\leq \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2}c_{\hbar}(x, \xi)Q(x, \xi)^{1/2}) dx d\xi \end{aligned}$$

since, by construction,

$$\int_{\mathbf{R}^{2d}} Q(x, \xi) dx d\xi = S.$$

Thus

$$\begin{aligned} \langle \Lambda, c_{\hbar} \rangle &= \sup_{\substack{a \in C_b(\mathbf{R}^{2d}), B=B^* \in \mathcal{L}(\mathfrak{H}) \\ a(x, \xi)I_{\mathfrak{H}} + B \leq c_{\hbar}(x, \xi)}} \left(\int_{\mathbf{R}^{2d}} a(x, \xi)p(x, \xi) dx d\xi + \text{trace}_{\mathfrak{H}}(SB) \right) \\ &\leq \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2}c_{\hbar}(x, \xi)Q(x, \xi)^{1/2}) dx d\xi \leq \langle \Lambda, c_{\hbar} \rangle, \end{aligned}$$

where the first equality follows from convex duality as explained in Step 2, while the last inequality has been obtained above at the beginning of Step 6. This completes the proof.

It remains to prove that

$$\int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2}c_{\hbar}(x, \xi)Q(x, \xi)^{1/2}) dx d\xi < \infty.$$

Since

$$c_{\hbar}(x, \xi) \leq (|x|^2 + |\xi|^2)I_{\mathfrak{H}} + 4H$$

with $H = -\frac{1}{2}\hbar^2\Delta_y + \frac{1}{2}|y|^2$, one has

$$v_k(x, \xi) \in \text{Form-Dom}(H) \implies v_k(x, \xi) \in \text{Form-Dom}(c_{\hbar}(x, \xi)),$$

and

$$\langle v_k(x, \xi) | c_{\hbar}(x, \xi) | v_k(x, \xi) \rangle \leq 2(|x|^2 + |\xi|^2)\|v_k(x, \xi)\|_{\mathfrak{H}}^2 + 4\langle v_k(x, \xi) | H | v_k(x, \xi) \rangle.$$

Let (h_1, h_2, \dots) be a complete orthonormal system of eigenvectors of H in \mathfrak{H} (the Hermite functions), with eigenvalues μ_j . Since

$$\sum_{k \geq 1} \overline{t_{km}(x, \xi)} t_{kn}(x, \xi) = \langle e_m(x, \xi) | Q(x, \xi) | e_n(x, \xi) \rangle$$

by definition of $t_{kl}(x, \xi)$, one has

$$\begin{aligned} \sum_{k \geq 1} |\langle v_k(x, \xi) | h_j \rangle|^2 &= \sum_{k \geq 1} \sum_{m, n \geq 1} \overline{t_{km}(x, \xi)} t_{kn}(x, \xi) \langle e_m(x, \xi) | h_j \rangle \langle h_j | e_n(x, \xi) \rangle \\ &= \sum_{m, n \geq 1} \langle e_m(x, \xi) | Q(x, \xi) | e_n(x, \xi) \rangle \langle e_m(x, \xi) | h_j \rangle \langle h_j | e_n(x, \xi) \rangle = \langle h_j | Q(x, \xi) | h_j \rangle. \end{aligned}$$

Hence

$$\begin{aligned} \int_{\mathbf{R}^{2d}} \sum_{k \geq 1} \langle v_k(x, \xi) | H | v_k(x, \xi) \rangle dx d\xi &= \sum_{j \geq 1} \mu_j \int_{\mathbf{R}^{2d}} \langle h_j | Q(x, \xi) | h_j \rangle dx d\xi \\ &= \sum_{j \geq 1} \mu_j \langle h_j | S | h_j \rangle = \text{trace}_{\mathfrak{H}}(S^{1/2} | H | S^{1/2}) < \infty, \end{aligned}$$

and since

$$\sum_{k \geq 1} \|v_k(x, \xi)\|_{\mathfrak{H}}^2 = \text{trace}_{\mathfrak{H}}(Q(x, \xi)) = p(x, \xi),$$

one concludes that

$$\begin{aligned} &\int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(Q(x, \xi)^{1/2} c_{\hbar}(x, \xi) Q(x, \xi)^{1/2}) dx d\xi \\ &\leq 2 \int_{\mathbf{R}^{2d}} (|x|^2 + |\xi|^2) p(x, \xi) dx d\xi + 4 \text{trace}_{\mathfrak{H}}(S^{1/2} H S^{1/2}) < \infty. \end{aligned}$$

□

5. THE “APPROXIMATE” TRIANGLE INEQUALITY

The main result in this section is the following “approximate” triangle inequality for \mathfrak{d} on \mathfrak{D}_2 .

Theorem 5.1. *For all $\rho_1, \rho_2, \rho_3 \in \mathfrak{D}_2$, 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, for all $\rho_1, \rho_2, \rho_3 \in \mathfrak{D}_2$, one has

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

Indeed, Theorem 3.1 shows that the triangle inequality holds without the additional term $\sqrt{d\hbar}$ if $\rho_2 \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$; this extra term is needed only if $\rho_2 \in \mathcal{D}_2(\mathfrak{H})$, in which case

$$\sqrt{2d\hbar} \leq \mathfrak{d}(\rho_2, \rho_2).$$

We first recall the definition of the Husimi function of a bounded operator on \mathfrak{H} .

Definition 5.2. *For all $q, p \in \mathbf{R}^d$, the Schrödinger coherent state $|q, p\rangle$ is the wave function defined by the formula*

$$|q, p\rangle(x) := (\pi\hbar)^{-d/4} e^{-|x-q|^2/2\hbar} e^{-ip \cdot x/\hbar}, \quad x \in \mathbf{R}^d.$$

The Husimi function of $R \in \mathcal{L}(\mathfrak{H})$ is

$$\mathcal{H}[R](q, p) := \frac{1}{(2\pi\hbar)^d} \langle q, p | R | q, p \rangle.$$

We shall also need the notion of Töplitz operator, whose definition is recalled below.

Definition 5.3. For each Borel measure μ on \mathbf{R}^{2d} such that

$$(9) \quad 0 \leq \mu(dqdp) \leq K(1 + |q|^2 + |p|^2)dqdp$$

for some $K > 0$, one defines the unbounded self-adjoint operator

$$\mathcal{T}[\mu] = \int_{\mathbf{R}^{2d}} |q, p\rangle\langle q, p| \mu(dqdp)$$

with domain

$$\text{Dom}(\mathcal{T}) := \{\psi \in \mathfrak{H} \text{ s.t. } \mathcal{H}[|\psi\rangle\langle\psi|] \in L^2(\mathbf{R}^{2d}; \mu)\}$$

by the formula

$$\langle\phi|\mathcal{T}[\mu]|\psi\rangle := \int_{\mathbf{R}^{2d}} \overline{\langle q, p|\phi\rangle} \langle q, p|\psi\rangle \mu(dqdp), \quad \phi, \psi \in \text{Dom}(\mathcal{T}).$$

The map \mathcal{T} is extended by linearity to complex Borel measures on \mathbf{R}^{2d} (with finite total variation: see Theorem 6.4 in [21]).

Formulas (47), (48) and (54) in [13] imply that $\mathcal{H}[R] \in \mathcal{P}_2^{gc}(\mathbf{R}^{2d})$ for all $R \in \mathcal{D}_2(\mathfrak{H})$, while formula (55) in [13] implies that

$$\mathcal{T}[\mathcal{P}_2(\mathbf{R}^{2d})] \subset \mathcal{D}_2(\mathfrak{H}).$$

We also recall formula (54) in [13] in the form

$$\text{trace}_{\mathfrak{H}}(R^* \mathcal{T}[\mu]) = (2\pi\hbar)^d \int_{\mathbf{R}^{2d}} \overline{\mathcal{H}[R](q, p)} \mu(dqdp)$$

for each $R \in \mathcal{D}_2(\mathfrak{H})$ and each Radon measure μ satisfying (9).

The key to the approximate triangle inequality is the inequality below, of independent interest, whose proof is based on the duality theorem (Theorem 4.1) in the preceding section.

Theorem 5.4. For each $R, S \in \mathcal{D}_2(\mathfrak{H})$, one has

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

Notice that this inequality, and the inequality in Theorem 2.4 (2) of [14], which we recall in the form

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

for all $R \in \mathcal{D}_2(\mathfrak{H})$ and all $f \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$, specialized to $f = \mathcal{H}[S]$, imply that

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

which is the inequality in Theorem 2.3 (2) of [13].

Proof. Let $a \equiv a(q, p)$ in $C_b(\mathbf{R}^{2d}; \mathbf{R})$ and $B = B^* \in \mathcal{L}(\mathfrak{H})$ satisfy

$$a(q, p)I_{\mathfrak{H}} + B \leq c_{\hbar}(q, p) \quad \text{for a.e. } (q, p) \in \mathbf{R}^{2d}.$$

Then

$$a(q, p)|q, p\rangle\langle q, p| \otimes I_{\mathfrak{H}} + |q, p\rangle\langle q, p| \otimes B \leq |q, p\rangle\langle q, p| \otimes c_{\hbar}(q, p)$$

for all $(q, p) \in \mathbf{R}^{2d}$. Using formulas (46) and (48) in [13] shows that

$$\begin{aligned} \mathcal{T}[1] &= (2\pi\hbar)^d I_{\mathfrak{H}}, \quad \mathcal{T}[q] = (2\pi\hbar)^d x, \quad \mathcal{T}[p] = -i\hbar(2\pi\hbar)^d \nabla_x, \\ \mathcal{T}[|q|^2 + |p|^2] &= (2\pi\hbar)^d (|x|^2 - \hbar^2 \Delta_x + d\hbar I_{\mathfrak{H}}). \end{aligned}$$

Hence

$$\begin{aligned} \frac{1}{(2\pi\hbar)^d} \mathcal{T}[a] \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes B &\leq \frac{1}{(2\pi\hbar)^d} \int_{\mathbf{R}^{2d}} |q, p\rangle \langle q, p| \otimes c_{\hbar}(q, p) dq dp \\ &= C_{\hbar} + d\hbar I_{\mathfrak{H} \otimes \mathfrak{H}}. \end{aligned}$$

Thus, for each $T \in \mathcal{C}(R, S)$, one has

$$\begin{aligned} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(T^{\frac{1}{2}} C_{\hbar} T^{\frac{1}{2}} \right) + d\hbar &\geq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(T^{\frac{1}{2}} \left(\frac{1}{(2\pi\hbar)^d} \mathcal{T}[a] \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes B \right) T^{\frac{1}{2}} \right) \\ &= \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}} \left(\left(\frac{1}{(2\pi\hbar)^d} \mathcal{T}[a] \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes B \right) T \right) \\ &= \text{trace}_{\mathfrak{H}} \left(\frac{1}{(2\pi\hbar)^d} \mathcal{T}[a] R + BS \right) \\ &= \int_{\mathbf{R}^{2d}} a(q, p) \mathcal{H}[R](q, p) dq dp + \text{trace}_{\mathfrak{H}}(BS). \end{aligned}$$

Minimizing the left hand side in $T \in \mathcal{C}(R, S)$ leads to the inequality

$$\mathfrak{d}(R, S)^2 + d\hbar \geq \int_{\mathbf{R}^{2d}} a(q, p) \mathcal{H}[R](q, p) dq dp + \text{trace}_{\mathfrak{H}}(BS)$$

which holds for all $a \in C_b(\mathbf{R}^{2d}; \mathbf{R})$ and all $B = B^* \in \mathcal{L}(\mathfrak{H})$ such that

$$a(q, p) I_{\mathfrak{H}} + B \leq c_{\hbar}(q, p), \quad q, p \in \mathbf{R}^d.$$

Maximizing the right hand side of the penultimate inequality and applying the Kantorovich duality theorem implies that

$$\mathfrak{d}(R, S)^2 \geq \text{dist}_{\text{MK}, 2}(\mathcal{H}[R](q, p), S)^2 - d\hbar$$

which is the sought inequality. \square

With these results as preliminaries, we can now prove the approximate triangle inequality (Theorem 5.1).

Proof of Theorem 5.1. If $\rho_2 \in \mathcal{P}_2(\mathbf{R}^{2d})$, the triangle inequality holds for ρ_1, ρ_2, ρ_3 , and there is nothing left to prove. If $\rho_2 \in \mathcal{D}_2(\mathfrak{H})$, then $\mathcal{H}[\rho_2] \in \mathcal{P}_2^{ac}(\mathbf{R}^{2d})$. Therefore, the restricted triangle inequality in Theorem 3.1 implies that

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

By Theorem 5.4, one has

$$\begin{aligned} \mathfrak{d}(\rho_1, \mathcal{H}[\rho_2]) &\leq \sqrt{\mathfrak{d}(\rho_1, \rho_2)^2 + d\hbar} \\ \mathfrak{d}(\mathcal{H}[\rho_2], \rho_3) &\leq \sqrt{\mathfrak{d}(\rho_2, \rho_3)^2 + d\hbar} \end{aligned}$$

so that

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

Finally, we recall the elementary inequality

$$X \geq Y > 0 \implies \sqrt{X^2 + Y^2} \leq X + \frac{1}{2}Y.$$

Since $\rho_2 \in \mathcal{D}_2(\mathfrak{H})$, one has

$$\mathfrak{d}(\rho_1, \rho_2) \geq \sqrt{d\hbar}, \quad \mathfrak{d}(\rho_2, \rho_3) \geq \sqrt{d\hbar},$$

so that one can take $X = \mathfrak{d}(\rho_1, \rho_2)$ or $X = \mathfrak{d}(\rho_2, \rho_3)$ and $Y = d\hbar$ in the elementary inequality above, so that

$$\begin{aligned} \mathfrak{d}(\rho_1, \rho_3) &\leq \sqrt{\mathfrak{d}(\rho_1, \rho_2)^2 + d\hbar} + \sqrt{\mathfrak{d}(\rho_2, \rho_3)^2 + d\hbar} \\ &\leq \mathfrak{d}(\rho_1, \rho_2) + \mathfrak{d}(\rho_2, \rho_3) + d\hbar. \end{aligned}$$

□

We shall conclude this section with a consequence of the restricted triangle inequalities obtained above.

Theorem 5.5. *Let $R_{\hbar}, S_{\hbar} \in \mathcal{D}_2(\mathfrak{S})$ and $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^{2d})$ satisfy the condition*

$$\mathfrak{d}(\mu, R_{\hbar}) \rightarrow 0 \quad \text{and} \quad \mathfrak{d}(\nu, S_{\hbar}) \rightarrow 0 \quad \text{as } \hbar \rightarrow 0^+.$$

Then

$$\mathfrak{d}(R_{\hbar}, S_{\hbar}) \rightarrow \text{dist}_{\text{MK},2}(\mu, \nu) \quad \text{as } \hbar \rightarrow 0^+.$$

Remark. In Theorem 2.3 (2) of [13], we have seen that, if $\mathcal{H}[R_{\hbar}]$ and $\mathcal{H}[S_{\hbar}]$ converge weakly (in the sense of Radon measures with finite total variation) to $\mu \in \mathcal{P}(\mathbf{R}^{2d})$ and $\nu \in \mathcal{P}(\mathbf{R}^{2d})$ respectively, then

$$\text{dist}_{\text{MK},2}(\mu, \nu) \leq \varliminf_{\hbar \rightarrow 0^+} \mathfrak{d}(R_{\hbar}, S_{\hbar}).$$

(This is a straightforward consequence of the lower bound in Theorem 2.3 (2) of [13], of Proposition 7.1.3 in chapter 7 of [1], and of Theorem 6.8 in chapter II of [19] (the so-called Portmanteau theorem).) Theorem 5.5 strengthens this inequality into an equality, under an assumption on R_{\hbar} and S_{\hbar} expressed in terms of the ‘‘pseudometric’’ \mathfrak{d} itself.

Proof. By the (restricted) triangle inequality (Theorem 3.1)

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

Letting $\hbar \rightarrow 0^+$ in both sides of this inequality implies that

$$\varlimsup_{\hbar \rightarrow 0^+} \mathfrak{d}(R_{\hbar}, S_{\hbar}) \leq \mathfrak{d}(\mu, \nu).$$

On the other hand, Theorem 2.4 (2) of [14] implies that

$$\begin{aligned} \mathfrak{d}(R_{\hbar}, \mu)^2 &\geq \text{dist}_{\text{MK},2}(\mathcal{H}[R_{\hbar}], \mu)^2 - d\hbar, \\ \mathfrak{d}(\nu, S_{\hbar})^2 &\geq \text{dist}_{\text{MK},2}(\nu, \mathcal{H}[S_{\hbar}])^2 - d\hbar, \end{aligned}$$

so that our assumption on R_{\hbar} and S_{\hbar} implies that

$$\text{dist}_{\text{MK},2}(\mathcal{H}[R_{\hbar}], \mu) \rightarrow 0 \quad \text{and} \quad \text{dist}_{\text{MK},2}(\nu, \mathcal{H}[S_{\hbar}]) \rightarrow 0 \quad \text{as } \hbar \rightarrow 0^+.$$

With the inequality in Theorem 2.3 (2) of [13], i.e.

$$\mathfrak{d}(R_{\hbar}, S_{\hbar})^2 \geq \text{dist}_{\text{MK},2}(\mathcal{H}[R_{\hbar}], \mathcal{H}[S_{\hbar}])^2 - 2d\hbar,$$

we conclude that

$$\varliminf_{\hbar \rightarrow 0^+} \mathfrak{d}(R_{\hbar}, S_{\hbar})^2 \geq \lim_{\hbar \rightarrow 0^+} \text{dist}_{\text{MK},2}(\mathcal{H}[R_{\hbar}], \mathcal{H}[S_{\hbar}])^2 = \text{dist}_{\text{MK},2}(\mu, \nu)^2.$$

Therefore

$$\text{dist}_{\text{MK},2}(\mu, \nu) \leq \varliminf_{\hbar \rightarrow 0^+} \mathfrak{d}(R_{\hbar}, S_{\hbar}) \leq \varlimsup_{\hbar \rightarrow 0^+} \mathfrak{d}(R_{\hbar}, S_{\hbar}) \leq \text{dist}_{\text{MK},2}(\mu, \nu),$$

and this implies Theorem 5.5. □

In other words, the set $\mathcal{P}_2(\mathbf{R}^{2d})$ of Borel probability measures with finite second order moment on phase space is the set of limits points of $\mathcal{D}_2(\mathfrak{H})$ (the set of finite energy density operators on \mathfrak{H}) for the ‘‘pseudometric’’ \mathfrak{d} in the semiclassical limit, i.e. as $\hbar \rightarrow 0$, since Töplitz operators satisfy the assumptions of Theorem 5.5 by Theorem 2.4 (1) in [14]. Moreover, the pseudometric \mathfrak{d} ‘‘converges’’ to the Monge-Kantorovich-(Wasserstein) distance $\text{dist}_{\text{MK},2}$ in that limit.

In that sense, the construction of the pseudometric \mathfrak{d} essentially fulfills the objectives presented in the introduction.

6. CLASSICAL/QUANTUM OPTIMAL TRANSPORT AND SEMIQUANTUM LEGENDRE TRANSFORM

6.1. A classical/quantum optimal transport. Let $r \in \mathcal{P}_2(\mathbf{R}^{2d})$ be a probability density on \mathbf{R}^{2d} and $S \in \mathcal{D}_2(\mathbf{R}^d)$ a density operator on $L^2(\mathbf{R}^d)$.

We suppose that an optimal operator \tilde{B} and an optimal function \tilde{a} exists for the Kantorovich duality formulation of $\mathfrak{d}(r, S)$, as in Theorem 4.1, and that $\tilde{a} \in C_b(\mathbf{R}^{2d})$ and $\tilde{B} \in \mathcal{L}(\mathfrak{H})$. That is to say that

$$\tilde{a}(x, \xi) + \tilde{B} \leq (Z - z)^2 \text{ and } \mathfrak{d}(r, S)^2 = \int_{\mathbf{R}^{2d}} \tilde{a}(z)r(z)dz + \text{trace}_{L^2(\mathbf{R}^d)} \tilde{B}S.$$

Here we have used the notation $z = (x, \xi)$, $dz = dx d\xi$, and $Z = (y, -i\hbar\nabla_y)$ acting on $L^2(\mathbf{R}^d, dy)$.

Let us denote by $\Pi(z)$ an optimal coupling of r, S and let us define

$$\begin{aligned} a(z) &:= \frac{1}{2}(|z|^2 - \tilde{a}(z)) \\ B &:= \frac{1}{2}(|Z|^2 - \tilde{B}). \end{aligned}$$

One has

$$(a(z) + B - z \cdot Z) \geq 0 \text{ and } \text{trace}_{L^2(\mathbf{R}^d)} \int_{\mathbf{R}^{2d}} \Pi(z)^{\frac{1}{2}}(a(z) + B - z \cdot Z)\Pi(z)^{\frac{1}{2}}dz = 0.$$

Therefore, since $\Pi(z)^{\frac{1}{2}}(a(z) + B - z \cdot Z)\Pi(z)^{\frac{1}{2}} \geq 0$, the preceding equality implies that

$$\Pi(z)^{\frac{1}{2}}(a(z) + B - z \cdot Z)\Pi(z)^{\frac{1}{2}} = 0 \text{ for a.e. } z \in \mathbf{R}^{2d}.$$

In other words,

$$\Pi(z)^{\frac{1}{2}}(a(z) + B - z \cdot Z)^{\frac{1}{2}} \left(\Pi(z)^{\frac{1}{2}}(a(z) + B - z \cdot Z)^{\frac{1}{2}} \right)^* = 0$$

which implies that

$$(a(z) + B - z \cdot Z)^{\frac{1}{2}}\Pi(z)^{\frac{1}{2}} = 0$$

and

$$(10) \quad (a(z) + B - z \cdot Z)\Pi(z) = 0.$$

Hence, the range of Π consists in functions $\mathbb{R}^{2d} \ni z \mapsto \psi_z \in L^2(\mathbb{R}^d)$ such that

$$(11) \quad (a(z) + B - z \cdot Z)\psi_z = 0 :$$

the vectors ψ_z belong to the kernel of $B + a(z) - z \cdot Z$ for a.e. $z \in \mathbf{R}^{2d}$.

Moreover $\Pi(z) \geq 0$ for every $z \in \mathbf{R}^{2d}$ and $\text{trace}_{L^2(\mathbf{R}^d)} \Pi(z) = r(z)$. Hence

$$r(z) > 0 \Rightarrow \text{Im } \Pi(z) \neq \{0\}$$

so that there exists an eigenvector ψ_z of $B - z \cdot Z$ of eigenvalue $-a(z)$ for r - a.e. $z \in \mathbf{R}^{2d}$.

But $B + a(z) - z \cdot Z \geq 0$. Therefore, for r - a.e. $z \in \mathbf{R}^{2d}$,

$$-a(z) \text{ is the lowest eigenvalue of } B - z \cdot Z.$$

Theorem 6.1. *Let \tilde{a} and \tilde{B} be two bounded optimal Kantorovich potentials for $\mathfrak{d}(r, S)$.*

Then, for r -almost every $(x, \xi) \in \mathbf{R}^{2d}$,

$$\tilde{a}(x, \xi) \text{ is the highest eigenvalue of } c_{\hbar}(x, \xi) - \tilde{B}.$$

If the fundamental of $B - z \cdot Z$ is non degenerate in the sense that the eigenspace corresponding to the lowest eigenvalue of $B - z \cdot Z$ has dimension 1, then $\Pi(z)$ is proportional to $|\psi_z\rangle\langle\psi_z|$ and therefore, since $\Pi(z)$ is a coupling between r and S ,

$$\Pi(z) = r(z)|\psi_z\rangle\langle\psi_z|$$

and

$$S = \int_{\mathbf{R}^{2d}} r(z)|\psi_z\rangle\langle\psi_z|dz.$$

We just proved the following result.

Theorem 6.2. *Let \tilde{a} and \tilde{B} be two bounded optimal Kantorovich potentials for $\mathfrak{d}(r, S)$.*

Let us suppose moreover that, for each $z \in \mathbf{R}^{2d}$, the lowest eigenspace of $\tilde{B} - c_{\hbar}(z)$ is nondegenerate and let ψ_z be its ground state.

Then S admits the following representation

$$S = \int_{\mathbf{R}^{2d}} r(z)|\psi_z\rangle\langle\psi_z|dz.$$

Theorem 6.2 suggests to associate to any probability density μ the following operator

$$(12) \quad \mu \longrightarrow \text{OP}_{\hbar}^{r, S}[\mu] := \int_{\mathbf{R}^{2d}} |\psi_z\rangle\langle\psi_z| \mu(dz).$$

The arrow in (12) can be seen as the “optimal transport”, from classical probability densities to quantum density matrices, transporting r to S .

Note that, for any density μ ,

$$\text{trace OP}_{\hbar}^{r, S}[\mu] = \int_{\mathbf{R}^{2d}} \mu(dz).$$

Finally, using (10), we easily show, by analogy with the proof of [6, Theorem 2.6 (1) (a)], that, when $a \in C^1(\mathbf{R}^{2d})$, $(\nabla a)r \in C_b(\mathbf{R}^{2d})$ and $\psi_z \in \text{Dom}(\frac{1}{i\hbar}[Z, B])$ for all $z \in \text{supp}(r)$,

$$\begin{aligned} 0 &= \Pi(z) \frac{1}{i\hbar} [JZ, (a(z) + B - z \cdot Z) \Pi(z)] = \Pi_z \frac{1}{i\hbar} [JZ, a(z) + B - z \cdot Z] \Pi(z) \\ &= \Pi(z) (\frac{1}{i\hbar} [JZ, B] - z) \Pi(z) \end{aligned}$$

and

$$\begin{aligned} 0 &= \Pi(z) \{Jz, (a(z) + B - z \cdot Z) \Pi(z)\} = \Pi(z) \{Jz, a(z) + B - z \cdot Z\} \Pi(z) \\ &= \Pi(z) (\nabla a(z) - Z) \Pi(z). \end{aligned}$$

Here J the symplectic matrix defined by $\{f, g\} = \nabla f \cdot J \nabla g$ i.e. $J = \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}$.

Therefore the (classical and quantum) ‘‘gradient’’ aspect appears in the following expressions

$$(13) \quad \begin{cases} \langle \psi_z | Z | \psi_z \rangle &= \nabla a(z) \\ z &= \langle \psi_z | Z | \nabla^Q B \psi_z \rangle \end{cases}$$

where, as introduced and motivated in [6, Section 1 formula (11)], $\nabla^Q := \frac{1}{i\hbar} [JZ, \cdot]$.

Let us finish this section by an example. Suppose that S is the Töplitz operator of symbol r , as defined in Definition 5.3:

$$S = \mathcal{T}(r).$$

In this case, one knows, [14, Theorem 2.4 (1)] (note a difference of normalization: in [14], $E_\hbar^2 = \frac{1}{2} \mathfrak{d}^2$),

$$\mathfrak{d}(r, S)^2 = d\hbar = \int_{\mathbf{R}^{2d}} \tilde{a}(z) r(z) dz + \text{trace}(\tilde{B}S) \text{ with } \tilde{a} = 0, \tilde{B} = d\hbar I_{\mathfrak{S}}.$$

Since $(x - y)^2 + (\xi + i\hbar \nabla_y)^2 \geq d\hbar I_{\mathfrak{S}} = \tilde{a} I_{\mathfrak{S}} + \tilde{B}$, \tilde{a} and \tilde{B} are optimal and the ‘‘renormalized’’ potentials a and B are just:

$$a(z) = \frac{1}{2} |z|^2 \text{ and } B = \frac{1}{2} (|Z|^2 - d\hbar I_{\mathfrak{S}}).$$

Hence

$$a(z) + B - z \cdot Z = \frac{1}{2} (-\nabla_y + y - (x + i\xi)) (\nabla_y + y - (x - i\xi))$$

so that the solution of (11) is in this case

$$\psi_z(y) = (\pi\hbar)^{-d/4} e^{-\frac{(y-x)^2}{2\hbar}} e^{i\frac{\xi \cdot y}{\hbar}}$$

and Theorem 6.2 expresses back that $S = \mathcal{T}(r)$:

$$\text{OP}_\hbar^{\mu, \mathcal{T}(\mu)} = \mathcal{T}$$

for any probability density μ .

6.2. A semiquantum Legendre transform. As we have seen, for r -a.e. $z \in \mathbf{R}^{2d}$, $-a(z)$ is the fundamental of the operator $B - z \cdot Z$. Therefore, by the variational characterization of the lowest eigenvalue,

$$-a(z) = \inf_{\substack{\phi \in \text{Dom}(B - z \cdot Z) \\ \|\phi\|_{\mathfrak{S}} = 1}} (\langle \phi | B | \phi \rangle - z \cdot \langle \phi | Z | \phi \rangle),$$

since, for each $z \in \mathbf{R}^{2d}$, $B - z \cdot Z$ is a bounded perturbation of $|Z - z|^2$, the harmonic oscillator H shifted by z , so that its spectrum is pure point, and $-a(z)$ is its lowest eigenvalue.

In other words,

$$(14) \quad a(z) = \sup_{\substack{\phi \in \text{Dom}(B - z \cdot Z) \\ \|\phi\|_{\mathfrak{S}} = 1}} (z \cdot \langle \phi | Z | \phi \rangle - \langle \phi | B | \phi \rangle) \text{ for } r\text{- a.e. } z \in \mathbf{R}^{2d}$$

To be faced to the classical definition of the Legendre transform

$$a(z) = \sup_{z'} (z \cdot z' - b(z')).$$

Definition 6.3. For B such that $-\hbar^2\Delta_x + |x|^2 - B \in \mathcal{L}(L^2(\mathbf{R}^d))$, let us define the semi-quantum Legendre dual of B as the function on $L^2(\mathbf{R}^{2d})$ defined by

$$B^*(z) := \sup_{\substack{\phi \in \text{Dom}(B) \\ \|\phi\|_B = 1}} (z \cdot \langle \phi | Z | \phi \rangle - \langle \phi | B | \phi \rangle).$$

Note that, since B is a bounded perturbation of the harmonic oscillator $-\hbar^2\Delta_y + |y|^2$, $\text{Dom}(B) = \text{Dom}(B - z \cdot Z) = \text{Dom}(-\hbar^2\Delta_y + |y|^2)$.

Definition 6.3 together with (14) leads to our final result.

Theorem 6.4. Let $a(z) = \frac{1}{2}(|z|^2 - \tilde{a}(z))$ and $B = \frac{1}{2}(|Z|^2 - \tilde{B})$ where $\tilde{a}(z)$ and \tilde{B} are bounded optimal Kantorovich potentials for $\mathfrak{d}(r, S)$. Then,

$$a = B^* \quad r - \text{almost everywhere in } \mathbf{R}^{2d}.$$

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