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# TOWARDS OPTIMAL TRANSPORT FOR QUANTUM DENSITIES

EMANUELE CAGLIOTI, FRANÇOIS GOLSE, AND THIERRY PAUL

ABSTRACT. An analogue of the quadratic Wasserstein (or Monge-Kantorovich) distance between Borel probability measures on  $\mathbf{R}^d$  has been defined in [F. Golse, C. Mouhot, T. Paul: Commun. Math. Phys. 343 (2015), 165–205] for density operators on  $L^2(\mathbf{R}^d)$ , and used to estimate the convergence rate of various asymptotic theories in the context of quantum mechanics. The present work proves a Kantorovich type duality theorem for this quantum variant of the Monge-Kantorovich or Wasserstein distance, and discusses the structure of optimal quantum couplings. Specifically, we prove that optimal quantum couplings involve a gradient type structure similar to the Brenier transport map (which is the gradient of a convex function), or more generally, to the subdifferential of a l.s.c. convex function as in the Knott-Smith optimality criterion (see Theorem 2.12 in [C. Villani: “Topics in Optimal Transportation”, Amer. Math. Soc. 2003]).

## 1. INTRODUCTION

Let  $\mu, \nu \in \mathcal{P}(\mathbf{R}^d)$  (the set of Borel probability measures on  $\mathbf{R}^d$ ). Given a l.s.c. function  $C : \mathbf{R}^d \times \mathbf{R}^d \rightarrow [0, +\infty]$ , the Monge problem in optimal transport is to minimize the functional

$$I_C[T] = \int_{\mathbf{R}^d} C(x, T(x))\mu(dx) \in [0, +\infty]$$

over the set of Borel maps  $T : \mathbf{R}^d \rightarrow \mathbf{R}^d$  such that  $\nu = T\#\mu$  (the push-forward measure of  $\mu$  by  $T$ ). Here  $C(x, y)$  represents the cost of transporting the point  $x$  to the point  $y$ , so that  $I_C[T]$  represents the total cost of transporting the probability  $\mu$  on  $\nu$  by the map  $T$ . An optimal transportation map  $T$  may fail to exist in full generality, so that one can consider instead the following relaxed variant of the Monge problem, known as the Kantorovich problem:

$$\inf_{\pi \in \Pi(\mu, \nu)} \iint_{\mathbf{R}^d \times \mathbf{R}^d} C(x, y)\pi(dxdy)$$

where  $\Pi(\mu, \nu)$  is the set of couplings of  $\mu$  and  $\nu$ , i.e. the set of Borel probability measures on  $\mathbf{R}^d \times \mathbf{R}^d$  such that

$$\iint_{\mathbf{R}^d \times \mathbf{R}^d} (\phi(x) + \psi(y))\pi(dxdy) = \int_{\mathbf{R}^d} \phi(x)\mu(dx) + \int_{\mathbf{R}^d} \psi(x)\nu(dx)$$

for all  $\phi, \psi \in C_b(\mathbf{R}^d)$ . An optimal coupling  $\pi_{opt}$  always exists, so that the inf is always attained in the Kantorovich problem (see Theorem 1.3 in [7] or Theorem 4.1 in [8]). Of course, if an optimal map  $T$  exists for the Monge problem, the push-forward of the measure  $\mu$  by the map  $x \mapsto (x, T(x))$ , which can be (informally)

recast as

$$(1) \quad \pi(dxdy) := \mu(dx)\delta_{T(x)}(dy)$$

is an optimal coupling for the Kantorovich problem.

In the special case where  $C(x, y) = |x - y|^2$  (the square Euclidean distance between  $x$  and  $y$ )

$$\inf_{\pi \in \Pi(\mu, \nu)} \sqrt{\iint_{\mathbf{R}^d \times \mathbf{R}^d} |x - y|^2 \pi(dxdy)} = \text{dist}_{\text{MK}, 2}(\mu, \nu)$$

is a distance on

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

referred to as the Monge-Kantorovich, or the Wasserstein distance of exponent 2 (see chapter 7 in [7], or chapter 6 in [8], or chapter 7 in [1]). In that case, there is “almost” an optimal transport map, in the following sense:  $\pi \in \Pi(\mu, \nu)$  is an optimal coupling for the Kantorovich problem if and only if there exists a proper<sup>1</sup> convex l.s.c. function  $\phi: \mathbf{R}^d \rightarrow \mathbf{R} \cup \{+\infty\}$  such that

$$\text{supp}(\pi) \subset \text{graph}(\partial\phi)$$

(where  $\partial\phi$  denotes the subdifferential of  $\phi$ ). This is the Knott-Smith optimality criterion (Theorem 2.12 (i) in [7]). If  $\mu$  satisfies the condition

$$(2) \quad B \text{ is Borel measurable and } \mathcal{H}^{d-1}(B) < \infty \implies \mu(B) = 0,$$

there exists a unique optimal coupling  $\pi$  of the form (1) for the Kantorovich problem, with  $T = \nabla\phi$ , where  $\phi$  is a proper convex l.s.c. function<sup>2</sup> on  $\mathbf{R}^d$ . This is the Brenier optimal transport theorem (stated as Theorem 2.12 (ii) in [7]), and the a.e. defined map  $\nabla\phi$  is referred to as the Brenier optimal transport map.

Recently, an analogue of the Monge-Kantorovich-Wasserstein distance  $\text{dist}_{\text{MK}, 2}$  has been defined in [3] on the set  $\mathcal{D}(\mathfrak{H})$  of density operators on the Hilbert space  $\mathfrak{H} := L^2(\mathbf{R}^d)$ . (Recall that a density operator on  $\mathfrak{H}$  is a linear operator  $R$  on  $\mathfrak{H}$  such that  $R = R^* \geq 0$  and  $\text{trace}(R) = 1$ .) This definition is based on the following well known analogies between classical and quantum mechanics:

- (a) Bounded continuous functions  $f \equiv f(q, p)$  on the phase space  $\mathbf{R}_q^d \times \mathbf{R}_p^d$  should be replaced with bounded operators on the Hilbert space  $\mathfrak{H} = L^2(\mathbf{R}_q^d)$  of square-integrable functions defined on the configuration space  $\mathbf{R}_q^d$ ;
- (b) The (Lebesgue) integral of (integrable) functions on  $\mathbf{R}_q^d \times \mathbf{R}_q^d$  should be replaced with the trace of (trace-class) operators on  $\mathfrak{H}$ ;
- (c) The coordinates  $q_j$  (for  $j = 1, \dots, d$ ) on the null section of the phase space  $\mathbf{R}_q^d \times \mathbf{R}_p^d$  should be replaced by the (unbounded) self-adjoint operators  $Q_j$  on  $\mathfrak{H}$  defined by

$$\text{Dom}(Q_j) := \left\{ \psi \in \mathfrak{H} \text{ s.t. } \int_{\mathbf{R}^d} q_j^2 |\psi(q)|^2 dq < \infty \right\}, \quad (Q_j \psi)(q) := q_j \psi(q)$$

for all  $j = 1, \dots, d$ ;

<sup>1</sup>I.e. not identically equal to  $+\infty$ .

<sup>2</sup>In particular  $\nabla\phi$  is defined a.e. on  $\mathbf{R}^d$ .

(d) The coordinates  $p_j$  (for  $j = 1, \dots, d$ ) on the fibers of the phase space  $\mathbf{R}_q^d \times \mathbf{R}_p^d$  should be replaced with the (unbounded) self-adjoint operators  $P_j$  on  $\mathfrak{H}$  defined by

$$\text{Dom}(P_j) := \left\{ \psi \in \mathfrak{H} \text{ s.t. } \int_{\mathbf{R}^d} |\partial_{q_j} \psi(q)|^2 dq < \infty \right\}, \quad (P_j \psi)(q) := -i\hbar \partial_{q_j} \psi(q)$$

for all  $j = 1, \dots, d$ ;

(e) The first order differential operators  $f \mapsto \{q_j, f\}$  and  $f \mapsto \{p_j, f\}$ , where  $\{\cdot, \cdot\}$  is the Poisson bracket on  $\mathbf{R}_q^d \times \mathbf{R}_p^d$  such that

$$\{p_j, p_k\} = \{q_j, q_k\} = 0, \quad \{p_j, q_k\} = \delta_{jk} \quad \text{for } j, k = 1, \dots, d$$

should be replaced with the derivations on  $\mathcal{L}(\mathfrak{H})$  defined by

$$A \mapsto \frac{i}{\hbar} [Q_j, A] \quad \text{and} \quad A \mapsto \frac{i}{\hbar} [P_j, A]$$

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

Following these principles, the quadratic transportation cost from  $(x, \xi)$  to  $(y, \eta)$  in  $\mathbf{R}^d \times \mathbf{R}^d$  should be replaced with the differential operator on  $\mathbf{R}_x^d \times \mathbf{R}_y^d$

$$(3) \quad C := \sum_{j=1}^d ((x_j - y_j)^2 - \hbar^2 (\partial_{x_j} - \partial_{y_j})^2).$$

Henceforth we denote by  $H$  the Hamiltonian

$$(4) \quad H := \sum_{j=1}^d (Q_j^2 + P_j^2) = |x|^2 - \hbar^2 \Delta_x$$

of the quantum harmonic oscillator. Given  $R, S \in \mathcal{D}_2(\mathfrak{H})$ , the set of density operators  $\rho$  on  $\mathfrak{H}$  such that  $\text{trace}(\rho^{1/2} H \rho^{1/2}) < \infty$ , the quantum analogue of the Monge-Kantorovich-Wasserstein distance  $\text{dist}_{\text{MK},2}$  is defined by the quantum Kantorovich problem (see Definition 2.2 in [3])

$$(5) \quad MK_{\hbar}(R, S) := \inf_{F \in \mathcal{C}(R, S)} \sqrt{\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2} C F^{1/2})},$$

where  $\mathcal{C}(R, S)$  is the set of quantum couplings of  $R$  and  $S$ , i.e.

$$\mathcal{C}(R, S) := \{F \in \mathcal{D}(\mathfrak{H} \otimes \mathfrak{H}) \text{ s.t. } \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((A \otimes I + I \otimes B)F) = \text{trace}_{\mathfrak{H}}(AR + BS)\}.$$

(See Definition 2.1 in [3].) The functional  $MK_{\hbar}$  is a particularly convenient tool to obtain a convergence rate for the mean-field limit in quantum mechanics that is uniform in the Planck constant  $\hbar$  (see Theorem 2.4 in [3], and Theorem 3.1 in [4] for precise statements of these results).

The striking analogy between the Wasserstein distance  $\text{dist}_{\text{MK},2}$  and the quantum functional  $MK_{\hbar}$  suggests the following question: what is the structure of optimal quantum couplings in the definition (5) of the  $MK_{\hbar}(R, S)$ ? For instance, is there an analogue of the notion of Brenier optimal transport map, or of the Knott-Smith optimality criterion involving the graph of the subdifferential of a proper convex l.s.c. function? Clearly, we are missing a quantum analogue of the original variational problem considered by Monge, or, equivalently, of the coupling (1), so that this last question seems far from obvious.

## 2. MAIN RESULTS

The key argument in deriving the structure (1) of optimal couplings for the Kantorovich problem involves a min-max type result known as ‘‘Kantorovich duality’’. For each  $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^d)$ , one has

$$(6) \quad \min_{\pi \in \Pi(\mu, \nu)} \iint_{\mathbf{R}^d \times \mathbf{R}^d} |x - y|^2 \pi(dx dy) = \int_{\mathbf{R}^d} |z|^2 \mu(dz) + \int_{\mathbf{R}^d} |z|^2 \nu(dz) - 2 \min_{\phi \in \mathcal{B}} \left( \int_{\mathbf{R}^d} \phi(z) \mu(dz) + \int_{\mathbf{R}^d} \phi^*(z) \nu(dz) \right)$$

where

$$\phi^*(y) := \sup_{x \in \mathbf{R}} (x \cdot y - \phi(x))$$

is the Legendre dual of  $\phi$ , while

$\mathcal{B} := \{\phi : \mathbf{R}^d \rightarrow \mathbf{R} \cup \{+\infty\} \text{ proper convex l.s.c. s.t. } \phi \in L^1(\mathbf{R}^d, \mu) \text{ and } \phi^* \in L^1(\mathbf{R}^d, \nu)\}$ . (See Theorem 1.3, Proposition 2.1 and Theorem 2.9 in [7].)

**Theorem 2.1** (Quantum duality). *Let  $R, S \in \mathcal{D}_2(\mathfrak{H})$ . Then*

$$\min_{F \in \mathcal{C}(R, S)} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2} C F^{1/2}) = \sup_{(A, B) \in \mathfrak{K}} \text{trace}_{\mathfrak{H}}(RA + SB),$$

where

$$\mathfrak{K} := \{(A, B) \in \mathcal{L}(\mathfrak{H}) \times \mathcal{L}(\mathfrak{H}) \text{ s.t. } A = A^*, B = B^* \text{ and } A \otimes I + I \otimes B \leq C\}.$$

In the definition of  $\mathfrak{K}$ , the inequality

$$A \otimes I + I \otimes B \leq C$$

means that

$$\langle \psi | A \otimes I + I \otimes B | \psi \rangle \leq \langle \psi | C | \psi \rangle$$

for all  $\psi \in \text{Form-Dom}(C)$ , which is given by

$$(7) \quad \text{Form-Dom}(C) := \{\psi \in \mathfrak{H} \otimes \mathfrak{H} \text{ s.t. } (x_j - y_j)\psi \text{ and } (\partial_{x_j} - \partial_{y_j})\psi \in \mathfrak{H} \otimes \mathfrak{H}, 1 \leq j \leq d\}.$$

The definition of the form domain of a self-adjoint operator can be found for instance in section VIII.6, Example 2 of [5].

Notice that the inf on the right hand side of the quantum duality formula is attained, while the sup on the right hand side is in general not attained. Finding optimal operators  $A$  and  $B$  requires modifying the definition of  $\mathfrak{K}$ .

**Gelfand triple associated to a nonnegative trace-class operator.** We shall use repeatedly the following construction. Given a separable Hilbert space  $\mathcal{H}$  and  $T \in \mathcal{L}^1(\mathcal{H})$  such that  $T = T^* \geq 0$ , let  $(\xi_n)_{n \geq 1}$  be a complete orthonormal basis of  $\mathcal{H}$  of eigenvectors of  $T$ . Set

$$(8) \quad \mathcal{J}_0[T] := \text{span}\{\xi_n \text{ s.t. } \langle \xi_n | T | \xi_n \rangle > 0\},$$

and

$$(9) \quad (\phi | \psi)_T := \langle \phi | T^{-1} | \psi \rangle, \quad \phi, \psi \in \mathcal{J}_0[T].$$

Let  $\mathcal{J}[T]$  designate the completion of  $\mathcal{J}_0[T]$  for the inner product  $(\cdot | \cdot)_T$ . Obviously

$$(10) \quad \mathcal{J}[T] \subset \overline{\mathcal{J}_0[T]} = \text{Ker}(T)^\perp \subset \mathcal{J}[T]'$$

(where  $\overline{\mathcal{J}_0[T]}$  is the closure of  $\mathcal{J}_0[T]$  in  $\mathfrak{H}$ ), and  $T^{-1/2}$ , defined on  $\mathcal{J}_0[T]$ , has a unique continuous extension which is the unitary transformation

$$(11) \quad T^{-1/2} : \mathcal{J}[T] \rightarrow \text{Ker}(T)^\perp \quad \text{with adjoint} \quad T^{-1/2} : \text{Ker}(T)^\perp \rightarrow \mathcal{J}[T]'.$$

In other words, one has a Gelfand triple

$$\mathcal{J}[T] \subset_c \text{Ker}(T)^\perp \subset \mathcal{J}[T]'.$$

(Notice that the embedding  $\mathcal{J}[T] \subset \text{Ker}(T)^\perp$  is compact since  $T^{1/2}$  is a Hilbert-Schmidt, and therefore compact, operator on  $\mathfrak{H}$ .) With the unitary transformation (11), one defines the isometric isomorphism

$$(12) \quad \mathcal{L}(\mathcal{J}[T], \mathcal{J}[T]') \ni \mathfrak{Z} \mapsto T^{1/2} \mathfrak{Z} T^{1/2} = Z \in \mathcal{L}(\text{Ker}(T)^\perp).$$

Under this isomorphism,  $\mathfrak{Z}^*$  is obviously mapped to  $Z^*$ .

**Definition 2.2.** For each  $R, S \in \mathcal{D}_2(\mathfrak{H})$ , let  $\tilde{\mathfrak{R}}(R, S)$  be the set of  $(\mathfrak{v}, \mathfrak{w})$  with  $\mathfrak{v} \in \mathcal{L}(\mathcal{J}[R], \mathcal{J}[R]')$  and  $\mathfrak{w} \in \mathcal{L}(\mathcal{J}[S], \mathcal{J}[S]')$  such that

(a) the operators  $V = R^{1/2} \mathfrak{v} R^{1/2}$  and  $W = S^{1/2} \mathfrak{w} S^{1/2}$  satisfy

$$2R^{1/2} H R^{1/2} \geq V = V^* \in \mathcal{L}^1(\text{Ker}(R)^\perp)$$

$$2R^{1/2} H R^{1/2} \geq W = W^* \in \mathcal{L}^1(\text{Ker}(S)^\perp);$$

(b) for each  $\Phi \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S]$ , one has

$$\langle \Phi | \mathfrak{v} \otimes I + I \otimes \mathfrak{w} | \Phi \rangle \leq \langle \Phi | C | \Phi \rangle.$$

Passing from  $\mathfrak{R}(R, S)$  to  $\tilde{\mathfrak{R}}(R, S)$  is equivalent to seeking the optimal Kantorovich potential  $\phi$  in (6) in  $L^1(\mathbf{R}^d, \mu)$  as in Theorems 1.3 or Theorem 2.9 of [7], instead of  $C_b(\mathbf{R}^d)$  — see the last sentence in Theorem 1.3 of [7], together with Remark 1.6 in that same reference.

**Theorem 2.3** (Existence of optimal  $\mathfrak{a}, \mathfrak{b}$ ). For all  $R, S \in \mathcal{D}_2(\mathfrak{H})$ ,

$$\min_{F \in \mathcal{C}(R, S)} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2} C F^{1/2}) = \max_{(\mathfrak{a}, \mathfrak{b}) \in \tilde{\mathfrak{R}}(R, S)} \text{trace}_{\mathfrak{H}}(R^{1/2} \mathfrak{a} R^{1/2} + S^{1/2} \mathfrak{b} S^{1/2}).$$

In the classical setting, let  $\phi : \mathbf{R}^d \mapsto \mathbf{R} \cup \{+\infty\}$  be a proper convex l.s.c. function, and let  $\mu \in \mathcal{P}(\mathbf{R}^d)$  satisfying the condition (2) and

$$(13) \quad \int_{\mathbf{R}^d} (|x|^2 + |\nabla \phi(x)|^2 + |\phi(x)| + |\phi^*(\nabla \phi(x))|) \mu(dx) < \infty.$$

Then

$$(14) \quad \pi(dx dy) := \mu(dx) \delta(y - \nabla \phi(x))$$

is an optimal coupling of the measures  $\mu$  and  $\nu := \nabla \phi \# \mu$  for the Kantorovich problem with the cost  $C(x, y) = |x - y|^2$ .

There is an almost analogous property in the quantum setting.

**Theorem 2.4** (Optimality criterion). Let  $R, S \in \mathcal{D}_2(\mathfrak{H})$ , and let  $(\mathfrak{a}, \mathfrak{b}) \in \tilde{\mathfrak{R}}(R, S)$ . Let  $(\Phi_j)_{j \geq 1}$  be a sequence of vectors in  $\mathfrak{H} \otimes \mathfrak{H}$  satisfying

$$\Phi_j \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S] \quad \text{and} \quad \langle \Phi_j | \Phi_k \rangle = \delta_{jk}, \quad j, k \geq 1,$$

Let

$$F = \sum_{j \geq 1} \lambda_j |\Phi_j\rangle \langle \Phi_j|, \quad \text{with } \lambda_j \geq 0 \quad \text{for all } j \geq 1,$$

such that

$$\sum_{j \geq 1} \lambda_j = 1 \quad \text{and} \quad \sum_{j \geq 1} \lambda_j \langle \Phi_j | (H + R^{-1}) \otimes I + I \otimes (S^{-1} + H) | \Phi_j \rangle < \infty.$$

(1) If

$$\lambda_j \langle \Phi_j | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_j \rangle = 0 \quad \text{for all } j \geq 1,$$

then  $F$  is an optimal coupling, i.e.

$$\begin{aligned} MK_{\hbar}(\text{trace}_2(F), \text{trace}_1(F))^2 &= \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2} C F^{1/2}) \\ &= \text{trace}_{\mathfrak{H}}(\text{trace}_2(F)^{1/2} \mathbf{a} \text{trace}_2(F)^{1/2} + \text{trace}_1(F)^{1/2} \mathbf{b} \text{trace}_1(F)^{1/2}). \end{aligned}$$

(2) Conversely, if  $F$  is an optimal element of  $\mathcal{C}(R, S)$ , and if  $(\mathbf{a}, \mathbf{b})$  is an optimal pair in  $\tilde{\mathfrak{K}}(R, S)$ , i.e.

$$MK_{\hbar}(R, S)^2 = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2} C F^{1/2}) = \text{trace}_{\mathfrak{H}}(R^{1/2} \mathbf{a} R^{1/2} + R^{1/2} \mathbf{b} R^{1/2}),$$

then

$$\lambda_j \langle \Phi_j | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_j \rangle = 0 \quad \text{for all } j \geq 1.$$

In the classical setting, the structure (14) of optimal couplings is a straightforward consequence of (13). Indeed, the set of points where the Young inequality

$$\phi(x) + \phi^*(y) \geq x \cdot y$$

becomes an equality is included in  $\text{graph}(\partial\phi)$ . This suggests the idea of looking for a quantum analogue of the Brenier optimal transport map in the optimality criterion in Theorem 2.4. The canonical commutation relations

$$(15) \quad [Q_j, Q_k] = [P_j, P_k] = 0, \quad [P_j, Q_k] = -i\hbar\delta_{jk}, \quad j, k = 1, \dots, d$$

for the position  $Q_j$  and momentum  $P_j$  operators (whose definition is recalled in statements (c)-(d) of section 1), or equivalently statement (e) in section 1, are of key importance in the definition of a quantum analogue of the Brenier optimal transport map. Set

$$\mathcal{D}_{Q_j} A := \frac{i}{\hbar} [P_j, A] \quad \text{and} \quad \mathcal{D}_{P_j} A := -\frac{i}{\hbar} [P_j, A], \quad j = 1, \dots, d,$$

for each unbounded operator  $A$  on  $\mathfrak{H}$ . Obviously  $\mathcal{D}_{Q_j} A$  and  $\mathcal{D}_{P_j} A$  are themselves unbounded operators on  $\mathfrak{H}$ , and are defined as weak derivatives in analysis (i.e. by duality, as in the case of the derivatives of distributions)..

**Theorem 2.5** (Quantum Transport). *Let  $R, S \in \mathcal{D}_2(\mathfrak{H})$  with*

$$\text{Ker}(R) = \text{Ker}(S) = \{0\},$$

and assume that

$$(16) \quad \begin{aligned} \phi \in \mathcal{J}_0[R] &\implies Q_j \phi \text{ and } P_j \phi \in \mathcal{J}[R], \\ \psi \in \mathcal{J}_0[S] &\implies Q_j \psi \text{ and } P_j \psi \in \mathcal{J}[S]. \end{aligned}$$

Let  $(\Phi_j)_{j \geq 1}$  be a sequence of vectors in  $\mathfrak{H} \otimes \mathfrak{H}$  such that

$$\Phi_j \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S] \quad \text{and} \quad \langle \Phi_j | \Phi_k \rangle = \delta_{jk}, \quad j, k \geq 1,$$

and let

$$F = \sum_{j \geq 1} \lambda_j |\Phi_j\rangle \langle \Phi_j|, \quad \text{with} \quad \sum_{j \geq 1} \lambda_j = 1, \quad \text{and} \quad \lambda_j > 0 \quad \text{for all } j \geq 1,$$

satisfying

$$F \in \mathcal{C}(R, S), \quad \text{and} \quad \sum_{j \geq 1} \lambda_j \langle \Phi_j | (H + R^{-1}) \otimes I + I \otimes (S^{-1} + H) | \Phi_j \rangle < \infty.$$

If  $F$  is an optimal coupling of  $R, S$  and  $(\mathbf{a}, \mathbf{b}) \in \tilde{\mathfrak{K}}(R, S)$  an optimal pair, i.e.

$$MK_h(R, S)^2 = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2} C F^{1/2}) = \text{trace}_{\mathfrak{H}}(R^{1/2} \mathbf{a} R^{1/2} + R^{1/2} \mathbf{b} R^{1/2}),$$

then

$$(17) \quad \begin{aligned} \langle \Phi_m | \mathcal{D}_{Q_k}(H - \mathbf{a}) \otimes I - I \otimes Q_k | \Phi_n \rangle &= \langle \Phi_m | \mathcal{D}_{P_k}(H - \mathbf{a}) \otimes I - I \otimes P_k | \Phi_n \rangle = 0, \\ \langle \Phi_m | Q_k \otimes I - I \otimes \mathcal{D}_{Q_k}(H - \mathbf{b}) | \Phi_n \rangle &= \langle \Phi_m | P_k \otimes I - I \otimes \mathcal{D}_{P_k}(H - \mathbf{b}) | \Phi_n \rangle = 0, \end{aligned}$$

for all  $k = 1, \dots, d$  and all  $m, n \geq 1$ .

As mentioned above, these identities hold in the weak sense: see the proof of Theorem 2.5 for more details. Equivalently, these identities can be recast as

$$\begin{aligned} & F^{1/2} (\mathcal{D}_{Q_k}(H - \mathbf{a}) \otimes I - I \otimes Q_k) F^{1/2} \\ &= \sum_{m, n \geq 1} \sqrt{\lambda_m \lambda_n} \langle \Phi_m | \mathcal{D}_{Q_k}(H - \mathbf{a}) \otimes I - I \otimes Q_k | \Phi_n \rangle | \Phi_m \rangle \langle \Phi_n | = 0, \\ & F^{1/2} (\mathcal{D}_{P_k}(H - \mathbf{a}) \otimes I - I \otimes P_k) F^{1/2} \\ &= \sum_{m, n \geq 1} \sqrt{\lambda_m \lambda_n} \langle \Phi_m | \mathcal{D}_{P_k}(H - \mathbf{a}) \otimes I - I \otimes P_k | \Phi_n \rangle | \Phi_m \rangle \langle \Phi_n | = 0. \end{aligned}$$

These identities are obviously analogous to the condition

$$(\nabla \phi(x) - y) \pi(dx dy) = 0$$

obtained in the setting of classical optimal transport in the case where the convex function  $\phi$  is smooth, so that  $\partial \phi(x) = \{\nabla \phi(x)\}$  (see the Brenier or the Knott-Smith theorems, stated as Theorem 2.12 (i)-(ii) in [7]). In the case where  $x = (q, p)$  and  $y = (q', p')$ , the equality above becomes

$$(\nabla_q \phi(q, p) - q') \pi(dq dp dq' dp') = (\nabla_p \phi(q, p) - p') \pi(dq dp dq' dp') = 0.$$

In the identities obtained in the quantum case  $I \otimes Q_k$  and  $I \otimes P_k$  are analogous of  $q'_k$  and  $p'_k$  respectively, while  $\mathcal{D}_{Q_k}(H - \mathbf{a}) \otimes I$  and  $\mathcal{D}_{P_k}(H - \mathbf{a}) \otimes I$  are analogous to  $\nabla_q \phi(q, p)$  and to  $\nabla_p \phi(q, p)$  respectively.

### 3. PROOF OF THEOREM 2.1

Set  $E := \mathcal{L}(\mathfrak{H} \otimes \mathfrak{H})$ . Define  $f, g: E \rightarrow \mathbf{R} \cup \{+\infty\}$  by the formulas

$$f(T) := \begin{cases} 0 & \text{if } T = T^* \geq -C, \\ +\infty & \text{otherwise.} \end{cases}$$

and

$$g(T) := \begin{cases} \text{trace}_{\mathfrak{H}}(RA + SB) & \text{if } T = T^* = A \otimes I + I \otimes B, \\ +\infty & \text{otherwise.} \end{cases}$$

When  $T = T^*$ , the constraint  $T \geq -C$  is to be understood as follows:

$$\langle \phi | T | \phi \rangle \geq -\langle \phi | C | \phi \rangle \quad \text{for each } \phi \in \text{Form-Dom}(C).$$

Clearly  $f$  and  $g$  are convex; besides

$$f(0) = g(0) = 0$$



and  $f$  is continuous at 0. Indeed, the Heisenberg uncertainty inequality implies that  $C \geq 2d\hbar I$ , so that

$$T = T^* \text{ and } \|T\| < d\hbar \implies T \geq -2d\hbar I \geq -C.$$

Hence

$$T = T^* \text{ and } \|T\| < d\hbar \implies f(T) = 0$$

so that  $f$  is continuous at 0.

By the Fenchel-Rockafellar duality theorem (Theorem 1.12 in [2])

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

Let us compute  $f^*$  and  $g^*$ . First

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

If  $\Lambda$  is not  $\geq 0$ , there exists  $T_0 = T_0^* \geq 0$  such that  $\langle \Lambda, T_0 \rangle = -\alpha < 0$ , so that

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

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

$$\langle \Lambda, C \rangle := \sup_{\substack{T \in E \\ 0 \leq T = T^* \leq C}} \langle \Lambda, T \rangle \in [0, +\infty].$$

With this definition

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

Next

$$g^*(\Lambda) = \sup_{T \in E} (\langle \Lambda, T \rangle - g(T)) = \sup_{\substack{T = T^* \in E \\ T = A \otimes I + I \otimes B}} (\langle \Lambda, T \rangle - \text{trace}(RA + SB)).$$

If there exists  $A = A^* \in \mathcal{L}(\mathfrak{H})$  and  $B = B^* \in \mathcal{L}(\mathfrak{H})$  such that

$$\langle \Lambda, A \otimes I + I \otimes B \rangle > \text{trace}(RA + SB)$$

then

$$g^*(\Lambda) \geq \sup_{n \geq 1} (n\langle \Lambda, A \otimes I + I \otimes B \rangle - n \text{trace}_{\mathfrak{H}}(RA + SB)) = +\infty$$

Likewise, if

$$\langle \Lambda, A \otimes I + I \otimes B \rangle < \text{trace}_{\mathfrak{H}}(RA + SB)$$

then

$$g^*(\Lambda) \geq \sup_{n \geq 1} (\langle \Lambda, -n(A \otimes I + I \otimes B) \rangle - \text{trace}_{\mathfrak{H}}(-n(RA + SB))) = +\infty.$$

Hence

$$g^*(\Lambda) = \begin{cases} 0 & \text{if } \langle \Lambda, A \otimes I + I \otimes B \rangle = \text{trace}_{\mathfrak{H}}(RA + SB), \\ +\infty & \text{otherwise.} \end{cases}$$

(Notice that, if

$$T = A \otimes I + I \otimes B = A' \otimes I + I \otimes B',$$

then

$$A - A' = B' - B = \kappa I \quad \text{for some } \kappa \in \mathbf{R},$$

so that

$$\text{trace}_{\mathfrak{H}}(RA + SB) = \text{trace}_{\mathfrak{H}}(RA' + SB') \quad \text{since } \text{trace}_{\mathfrak{H}}(R) = \text{trace}_{\mathfrak{H}}(S) = 1.$$

Hence the linear functional  $\Lambda$  is well defined on the set of elements of  $E$  of the form  $A \otimes I + I \otimes B$ .)

By the Fenchel-Rockefeller duality theorem recalled above,

$$\begin{aligned} \inf_{T \in E} (f(T) + g(T)) &= \inf_{\substack{A=A^*, B=B^* \in \mathcal{L}(\mathfrak{H}) \\ A \otimes I + I \otimes B \geq -C}} \text{trace}_{\mathfrak{H}}(RA + SB) \\ &= \max_{\Lambda \in E'} (-f^*(-\Lambda) - g^*(\Lambda)) = \max_{\substack{0 \leq \Lambda \in E' \\ \langle \Lambda, A \otimes I + I \otimes B \rangle = \text{trace}_{\mathfrak{H}}(RA + SB)}} -\langle \Lambda, C \rangle \end{aligned}$$

or equivalently, after exchanging the signs,

$$\sup_{\substack{A=A^*, B=B^* \in \mathcal{L}(\mathfrak{H}) \\ A \otimes I + I \otimes B \leq C}} \text{trace}_{\mathfrak{H}}(RA + SB) = \min_{\substack{0 \leq \Lambda \in E' \\ \langle \Lambda, A \otimes I + I \otimes B \rangle = \text{trace}_{\mathfrak{H}}(RA + SB)}} \langle \Lambda, C \rangle.$$

The constraint  $A \otimes I + I \otimes B \leq C$  is to be understood as explained above.

One can further restrict the min on the right hand side with the following observations.

**Lemma 3.1.** *Let  $0 \leq \Lambda \in E'$ . Then there exists  $Q \in \mathcal{L}^1(\mathfrak{H})$  such that*

$$Q = Q^* \geq 0, \quad \text{and} \quad \|Q\|_{\mathcal{L}^1} \leq \|\Lambda\|,$$

and  $L \in E'$  such that

$$L \geq 0, \quad L|_{\mathcal{K}(\mathfrak{H} \otimes \mathfrak{H})} = 0, \quad \text{and} \quad \|L\| \leq \|\Lambda\|$$

satisfying

$$\Lambda = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q \bullet) + L$$

*Proof.* Since  $\mathcal{L}^1(\mathfrak{H} \otimes \mathfrak{H}) = \mathcal{K}(\mathfrak{H} \otimes \mathfrak{H})'$ , one has

$$\Lambda|_{\mathcal{K}(\mathfrak{H} \otimes \mathfrak{H})} = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q \bullet)$$

and

$$\Lambda \geq 0 \implies Q = Q^* \geq 0.$$

Then<sup>3</sup>

$$\|Q\|_{\mathcal{L}^1} = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q) = \sup_{n \geq 1} \sum_{k=1}^n \langle e_n | Q | e_n \rangle = \sup_{n \geq 1} \left\langle \Lambda, \sum_{k=1}^n |e_n\rangle \langle e_n| \right\rangle \leq \langle \Lambda, I \rangle = \|\Lambda\|.$$

Define

$$L := \Lambda - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q \bullet).$$

so that

$$L|_{\mathcal{K}(\mathfrak{H} \otimes \mathfrak{H})} = 0$$

by construction. Since  $Q = Q^* \geq 0$  belongs to  $\mathcal{L}^1$ , let  $(e_n)_{n \geq 0}$  be a complete orthonormal system of eigenvectors of  $Q$ , and let  $P_n$  be the orthogonal projection on  $\text{span}(e_0, \dots, e_n)$ . For each  $T = T^* \geq 0$  in  $E$ ,

$$\begin{aligned} 0 &\leq \langle \Lambda, (I - P_n)T(I - P_n) \rangle = \langle \Lambda, T \rangle - \langle \Lambda, TP_n \rangle - \langle \Lambda, P_n T \rangle + \langle \Lambda, P_n T P_n \rangle \\ &= \langle \Lambda, T \rangle - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q(TP_n + P_n T - P_n T P_n)) = \langle \Lambda, T \rangle - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(P_n Q P_n T) \\ &\quad \rightarrow \langle \Lambda, T \rangle - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(QT) = \langle L, T \rangle \end{aligned}$$

<sup>3</sup>If  $0 \leq \ell \in E'$ , then  $\|\ell\| = \langle \ell, I \rangle$ . Indeed, for all  $T = T^* \in E$ , one has  $-\|T\|I \leq T \leq \|T\|I$ , so that one has  $-\|T\|\langle \ell, I \rangle \leq \langle \ell, T \rangle \leq \|T\|\langle \ell, I \rangle$ . In particular, for all  $T = T^* \in E$ , one has  $\langle \ell, T \rangle \in \mathbf{R}$ . For all  $T \in E$  (not necessarily self-adjoint), write  $\Re(T) = \frac{1}{2}(T + T^*)$  and  $\Im(T) := \frac{1}{2}i(T^* - T)$ . If  $\langle \ell, T \rangle \neq 0$ , there exists  $\alpha \in \mathbf{C}$  s.t.  $|\alpha| = 1$  and  $\langle \ell, \alpha T \rangle = |\langle \ell, T \rangle|$ . Hence  $\langle \ell, \Im(\alpha T) \rangle = 0$  so that  $|\langle \ell, T \rangle| = \langle \ell, \Re(\alpha T) \rangle \leq \langle \ell, I \rangle \|\Re(\alpha T)\| \leq \frac{1}{2} \langle \ell, I \rangle (\|\alpha T\| + \|(\alpha T)^*\|) = \langle \ell, I \rangle \|T\|$ . Hence  $\|\ell\| \leq \langle \ell, I \rangle$ , while it is obvious that  $\langle \ell, I \rangle \leq \|\ell\|$ .

as  $n \rightarrow \infty$ , since  $Q \in \mathcal{L}^1(\mathfrak{H})$ , so that

$$P_n Q P_n \rightarrow Q \quad \text{in } \mathcal{L}^1(\mathfrak{H} \otimes \mathfrak{H}) \text{ as } n \rightarrow \infty.$$

Hence  $L \geq 0$ . In particular (see footnote above), one has

$$\|L\| = \langle L, I \rangle = \langle \Lambda, I \rangle - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q) \leq \langle \Lambda, I \rangle = \|\Lambda\|.$$

□

**Lemma 3.2.** *Let  $0 \leq \Lambda \in E'$  satisfy*

$$\langle \Lambda, A \otimes I + I \otimes B \rangle = \text{trace}_{\mathfrak{H}}(RA + SB), \quad \text{for all } A = A^* \text{ and } B = B^* \in \mathcal{L}(\mathfrak{H}).$$

*Then  $\Lambda$  is of the form*

$$\Lambda = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q \bullet), \quad \text{with } Q = Q^* \geq 0 \text{ and } \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q) = 1.$$

*In particular,  $Q$  is a coupling of  $R$  and  $S$ .*

*Proof.* Let  $(e_1, e_2, \dots)$  be a complete orthonormal system in  $\mathfrak{H}$  (at variance with the notation used in the proof of the previous lemma), and let  $P_n$  be the orthogonal projection on  $\text{span}(e_1, \dots, e_n)$ . Consider

$$T_n := (I - P_n) \otimes P_n + P_n \otimes (I - P_n), \quad n \geq 1.$$

Since  $P_n \otimes P_n \geq 0$ , one has

$$0 \leq T_n \leq I \otimes P_n + P_n \otimes I \leq I \otimes I.$$

Hence

$$\begin{aligned} \langle \Lambda, T_n \rangle &\leq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q((I - P_n) \otimes I + I \otimes (I - P_n))) + \langle L, T_n \rangle \\ &\leq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((Q_1 + Q_2)(I - P_n)) + \langle L, I \rangle \rightarrow \langle L, I \rangle = \langle \Lambda, I \rangle - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q), \end{aligned}$$

so that

$$\overline{\lim}_{n \rightarrow \infty} \langle \Lambda, T_n \rangle \leq \langle \Lambda, I \rangle - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q) = 1 - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q).$$

(Taking  $A = I$  and  $B = 0$  shows that  $\langle \Lambda, I \otimes I \rangle = \text{trace}_{\mathfrak{H}}(R) = 1$ .)

On the other hand,  $(I - P_n) \otimes (I - P_n) \geq 0$ , so that

$$T_n \leq I \otimes P_n + P_n \otimes I - 2P_n \otimes P_n;$$

hence

$$\begin{aligned} \langle \Lambda, T_n \rangle &= \text{trace}_{\mathfrak{H}}((R + S)P_n) - 2\langle \Lambda, P_n \otimes P_n \rangle \\ &= \text{trace}_{\mathfrak{H}}((R + S)P_n) - 2\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q(P_n \otimes P_n)) \end{aligned}$$

since  $P_n \otimes P_n$  is a finite-rank operator (and therefore a compact operator). Hence

$$\lim_{n \rightarrow \infty} \langle \Lambda, T_n \rangle = \text{trace}_{\mathfrak{H}}(R + S) - 2\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q) = 2(1 - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q)).$$

Hence

$$\lim_{n \rightarrow \infty} \langle \Lambda, T_n \rangle = 2(1 - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q)) \leq 1 - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q) = \overline{\lim}_{n \rightarrow \infty} \langle \Lambda, T_n \rangle$$

so that

$$1 = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q) \quad \text{and} \quad \|L\| = \langle \Lambda, I \rangle - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q) = 1 - \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q) = 0.$$

□

Hence, the minimizing linear functional  $\Lambda$  in the duality formula above is represented by  $Q \in \mathcal{L}^1(\mathfrak{H} \otimes \mathfrak{H})$ . The constraints on  $\Lambda$  imply that

$$Q = Q^* \geq 0, \quad \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(Q(A \otimes I + I \otimes B)) = \text{trace}_{\mathfrak{H}}(RA + SB),$$

which is equivalent to the condition  $Q \in \mathcal{Q}(R, S)$ . Hence

$$\sup_{\substack{A=A^*, B=B^* \in \mathcal{L}(\mathfrak{H}) \\ A \otimes I + I \otimes B \leq C}} \text{trace}_{\mathfrak{H}}(RA + SB) = \min_{Q \in \mathcal{Q}(R, S)} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(QC),$$

with the notation

$$\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(QC) := \sup_{\substack{T=T^* \in E \\ T \leq C}} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(QT),$$

where the constraint  $T \leq C$  has the meaning recalled above.

#### 4. PROOF OF THEOREM 2.3

Let  $(A_k, B_k) \in \mathcal{L}(\mathfrak{H}) \times \mathcal{L}(\mathfrak{H})$  be a maximizing sequence, i.e.

$$\text{trace}(RA_k + SB_k) \rightarrow \sup_{\substack{A=A^*, B=B^* \in \mathcal{L}(\mathfrak{H}) \\ A \otimes I + I \otimes B \leq \frac{1}{2}C}} \text{trace}(RA + SB) =: \tau \in [0, +\infty),$$

$$A_k = A_k^*, B_k = B_k^* \in \mathcal{L}(\mathfrak{H}), \quad A_k \otimes I + I \otimes B_k \leq C \quad \text{as } k \rightarrow \infty.$$

##### Step 1: normalizing the maximizing sequence.

Set

$$a_k := 2H - A_k, \quad b_k := 2H - B_k,$$

where  $H$  has been defined in (4). Thus

$$\begin{aligned} a_k \otimes I + I \otimes b_k &\geq 2(H \otimes I + I \otimes H) - C \\ &= \sum_{j=1}^d ((P_j \otimes I + I \otimes P_j)^2 + (Q_j \otimes I + I \otimes Q_j)^2) =: \Sigma \geq 0. \end{aligned}$$

The operator  $\Sigma$  satisfies the same uncertainty inequality as  $C$ :

$$\begin{aligned} \Sigma &= \sum_{j=1}^d ((Q_j \otimes I + I \otimes Q_j) + i(P_j \otimes I + I \otimes P_j))((Q_j \otimes I + I \otimes Q_j) - i(P_j \otimes I + I \otimes P_j)) \\ &\quad + \sum_{j=1}^d i([P_j, Q_j] \otimes I + I \otimes [P_j, Q_j]) \geq 2d\hbar I \otimes I. \end{aligned}$$

Since  $R, S \in \mathcal{D}_2(\mathfrak{H})$ , there exist two complete orthonormal systems  $(e_j)_{j \geq 0}$  and  $(f_j)_{j \geq 0}$  of eigenvectors of  $R$  and  $S$  respectively, such that

$$R = \sum_{j \geq 0} \lambda_j |e_j\rangle\langle e_j|, \quad S = \sum_{j \geq 0} \mu_j |f_j\rangle\langle f_j|$$

with

$$\lambda_j, \mu_j \geq 0, \quad \sum_{j \geq 0} \lambda_j = \sum_{j \geq 0} \mu_j = 1,$$

and

$$\sum_{j \geq 0} (\lambda_j \langle e_j | H | e_j \rangle + \mu_j \langle f_j | H | f_j \rangle) < \infty.$$

Let

$$\alpha_k := \sup\{\alpha \in \mathbf{R} \text{ s.t. } a_k \geq \alpha I\} \in [-\|A_k\|, 2\langle e_0 | H | e_0 \rangle] \subset (-\infty, +\infty).$$

(Since  $a_k = 2H - A_k$  and  $H = H^* \geq 0$ , one has  $a_k \geq -A_k \geq -\|A_k\|I$ . On the other hand

$$\langle e_0 | a_k | e_0 \rangle = 2\langle e_0 | H | e_0 \rangle - \langle e_0 | A_k | e_0 \rangle \leq 2\langle e_0 | H | e_0 \rangle$$

since  $A_k = A_k^* \geq 0$ , so that  $a_k \geq \alpha I$  implies that  $\alpha \leq 2\langle e_0 | H | e_0 \rangle$ . Therefore, one has  $\alpha_k \leq 2\langle e_0 | H | e_0 \rangle$ .)

By definition of  $\alpha_k$ , there exists  $\phi_n \in \text{Dom}(H)$  such that

$$\|\phi_n\|_{\mathfrak{H}} = 1 \quad \text{and} \quad \langle \phi_n | a_k | \phi_n \rangle \rightarrow \alpha_k \quad \text{as } n \rightarrow \infty \quad \text{for each } k \geq 1.$$

Hence

$$\langle \phi_n | a_k | \phi_n \rangle I + b_k \geq 2d\hbar I \quad \text{for each } n \geq 1,$$

so that

$$\alpha_k I + b_k \geq 2d\hbar I.$$

On the other hand, again by definition of  $\alpha_k$ , one has

$$a_k - \alpha_k I \geq 0.$$

Setting

$$\hat{a}_k := a_k - \alpha_k I + d\hbar I, \quad \hat{b}_k := b_k + \alpha_k I - d\hbar I,$$

one has

$$\hat{a}_k \otimes I + I \otimes \hat{b}_k = a_k \otimes I + I \otimes b_k \geq \Sigma,$$

$$\hat{a}_k = \hat{a}_k^* \geq d\hbar I, \quad \hat{b}_k = \hat{b}_k^* \geq d\hbar I,$$

and

$$\begin{aligned} 0 &\leq \text{trace}_{\mathfrak{H}}(R\hat{a}_k + S\hat{b}_k) = \text{trace}_{\mathfrak{H}}(Ra_k + Sb_k) \\ &= 2\text{trace}_{\mathfrak{H}}((R+S)H) - \text{trace}_{\mathfrak{H}}(RA_k + SB_k) \\ &\rightarrow 2\text{trace}_{\mathfrak{H}}((R+S)H) - \tau \end{aligned}$$

as  $k \rightarrow \infty$ .

**Step 2: defining the unbounded operators  $\mathfrak{a}$  and  $\mathfrak{b}$** 

Hence

$$\begin{aligned} 0 \leq \text{trace}(R^{1/2}\hat{a}_k R^{1/2}) &\leq \sup_k \text{trace}(R\hat{a}_k) < \infty, \\ 0 \leq \text{trace}(S^{1/2}\hat{b}_k S^{1/2}) &\leq \sup_k \text{trace}(S\hat{b}_k) < \infty, \end{aligned}$$

so that

$$R^{1/2}\hat{a}_k R^{1/2} \xrightarrow{*} V \quad \text{and} \quad S^{1/2}\hat{b}_k S^{1/2} \xrightarrow{*} W \quad \text{in } \mathcal{L}^1(\mathfrak{H})$$

as  $k \rightarrow \infty$ .

Since

$$\hat{a}_k = \hat{a}_k^* \geq d\hbar I \quad \text{and} \quad \hat{b}_k = \hat{b}_k^* \geq d\hbar I,$$

one has

$$V = V^* \geq d\hbar R \quad \text{and} \quad W = W^* \geq d\hbar S.$$

In particular

$$\text{Ker}(V) \subset \text{Ker}(R) \quad \text{and} \quad \text{Ker}(W) \subset \text{Ker}(S).$$

On the other hand

$$\text{Im}(V) \subset \text{Im}(R^{1/2}) = \text{Im}(R) \quad \text{and} \quad \text{Im}(W) \subset \text{Im}(S^{1/2}) = \text{Im}(S).$$

Since

$$\begin{aligned} \text{Ker}(V)^\perp &= \overline{\text{Im}(V)} \subset \overline{\text{Im}(R)} = \text{Ker}(R)^\perp, \\ \text{Ker}(W)^\perp &= \overline{\text{Im}(W)} \subset \overline{\text{Im}(S)} = \text{Ker}(S)^\perp, \end{aligned}$$

(see Corollary 2.18 (iv) in [2]) one has

$$\begin{aligned} \text{Ker}(V) &= \text{Ker}(R) \quad \text{and} \quad \overline{\text{Im}(V)} = \text{Ker}(R)^\perp, \\ \text{Ker}(W) &= \text{Ker}(S) \quad \text{and} \quad \overline{\text{Im}(W)} = \text{Ker}(S)^\perp. \end{aligned}$$

In particular

$$V \in \mathcal{L}^1(\text{Ker}(R)^\perp) \quad \text{and} \quad W \in \mathcal{L}^1(\text{Ker}(S)^\perp).$$

Let  $\mathfrak{v} \in \mathcal{L}(\mathcal{J}[R], \mathcal{J}[R]')$  and  $\mathfrak{w} \in \mathcal{L}(\mathcal{J}[S], \mathcal{J}[S]')$  be the operators associated to  $V$  and  $W$  by (12); since  $V = V^*$  and  $W = W^*$ , one has

$$\mathfrak{v}^* = \mathfrak{v} \quad \text{and} \quad \mathfrak{w}^* = \mathfrak{w}.$$

Denote by  $(e'_j)_{j \geq 0}$  and  $(f'_j)_{j \geq 0}$  orthonormal subsequences of  $(e_j)_{j \geq 0}$  and  $(f_j)_{j \geq 0}$  which are complete in  $\text{Ker}(R)^\perp$  and  $\text{Ker}(S)^\perp$  respectively. For each  $n \geq 0$ , let

$$\mathcal{V}_n := \text{span}(e'_0, \dots, e'_n), \quad \mathcal{W}_n := \text{span}(f'_0, \dots, f'_n)$$

and let  $\Pi_n$  be the  $\mathfrak{H} \otimes \mathfrak{H}$ -orthogonal projection on  $\mathcal{V}_n \otimes \mathcal{W}_n$ . Since

$$\text{trace}((R+S)H) < \infty,$$

one has

$$\langle e'_k \otimes f'_l | \Sigma | e'_k \otimes f'_l \rangle < \infty \quad \text{for each } k, l, \geq 0,$$

while

$$\langle e'_m | a_k | e'_m \rangle < \infty \quad \text{and} \quad \langle f'_m | b_k | f'_m \rangle < \infty$$

for all  $k, m \geq 0$ . For each  $k$ ,

$$\hat{a}_k \otimes I + I \otimes \hat{b}_k \geq \Sigma,$$

and therefore

$$\langle \Phi | \hat{a}_k \otimes I + I \otimes \hat{b}_k - \Sigma | \Phi \rangle \geq 0 \quad \text{for all } \Phi \in \bigcup_{n \geq 0} \mathcal{V}_n \otimes \mathcal{W}_n = \mathcal{J}_0[R] \otimes \mathcal{J}_0[S].$$

Passing to the limit as  $k \rightarrow \infty$  in this inequality, we conclude that

$$\langle \Phi | \mathfrak{v} \otimes I + I \otimes \mathfrak{w} - \Sigma | \Phi \rangle \geq 0 \quad \text{for all } \Phi \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S].$$

Let  $\mathfrak{a} = \mathfrak{a}^* \in \mathcal{L}(\mathcal{J}[R], \mathcal{J}[R]')$  and  $\mathfrak{b} = \mathfrak{b}^* \in \mathcal{L}(\mathcal{J}[S], \mathcal{J}[S]')$  be the operators associated to  $2R^{1/2}HR^{1/2} - V \in \mathcal{L}^1((\text{Ker}(R)^\perp))$  and to  $2S^{1/2}HS^{1/2} - W \in \mathcal{L}^1((\text{Ker}(S)^\perp))$  respectively. The last inequality on  $\mathfrak{v}$  and  $\mathfrak{w}$  implies that  $(\mathfrak{a}, \mathfrak{b}) \in \tilde{\mathfrak{K}}(R, S)$ .

**Step 3: relaxing the constraint**

In this step we prove the following: for each  $(\bar{a}, \bar{b}) \in \tilde{\mathfrak{K}}(R, S)$  and each  $F \in \mathcal{C}(R, S)$ , one has

$$\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2}CF^{1/2}) \geq \text{trace}_{\mathfrak{H}}(R^{1/2}\bar{a}R^{1/2} + S^{1/2}\bar{b}S^{1/2})$$

We shall argue instead in terms of the operators

$$\bar{v} = \bar{v}^* \in \mathcal{L}(\mathcal{J}[R], \mathcal{J}[R]') \quad \text{and} \quad \bar{w} = \bar{w}^* \in \mathcal{L}(\mathcal{J}[S], \mathcal{J}[S]')$$

associated by (12) to the operators  $2R^{1/2}HR^{1/2} - R^{1/2}\bar{a}R^{1/2} \in \mathcal{L}^1(\text{Ker}(R)^\perp)$  and  $2S^{1/2}HS^{1/2} - S^{1/2}\bar{b}S^{1/2} \in \mathcal{L}^1(\text{Ker}(S)^\perp)$  respectively. These operators satisfy the inequality<sup>4</sup>

$$\Pi_n(\bar{v} \otimes I + I \otimes \bar{w})\Pi_n \geq \Pi_n \Sigma \Pi_n \geq \Pi_n \Sigma' \Pi_n$$

for each  $n \geq 0$  and each  $\Sigma' \in \mathcal{L}(\mathfrak{H} \otimes \mathfrak{H})$  such that  $\Sigma' \leq \Sigma$ . Since  $F \in \mathcal{L}^1(\mathfrak{H} \otimes \mathfrak{H})$ , one has

$$\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F \Pi_n \Sigma' \Pi_n) \rightarrow \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F \Sigma') \quad \text{as } n \rightarrow \infty.$$

according to Example 3 in chapter 2 of [6], since

$$\Pi_n \Sigma' \Pi_n \rightarrow \Sigma' \quad \text{strongly in } \mathcal{L}(\mathfrak{H} \otimes \mathfrak{H}) \text{ as } n \rightarrow \infty.$$

Indeed, for each  $\Psi \in \mathfrak{H} \otimes \mathfrak{H}$ , one has

$$\Pi_n \Psi \rightarrow \Psi \quad \text{in } \mathfrak{H} \otimes \mathfrak{H} \text{ as } n \rightarrow \infty.$$

Hence

$$\begin{aligned} \|\Sigma' \Psi - \Pi_n \Sigma' \Pi_n \Psi\|_{\mathfrak{H} \otimes \mathfrak{H}} &\leq \|(I - \Pi_n) \Sigma' \Psi\|_{\mathfrak{H} \otimes \mathfrak{H}} + \|\Pi_n \Sigma' (I - \Pi_n) \Psi\|_{\mathfrak{H} \otimes \mathfrak{H}} \\ &\leq \|(I - \Pi_n) \Sigma' \Psi\|_{\mathfrak{H} \otimes \mathfrak{H}} + \|\Sigma' (I - \Pi_n) \Psi\|_{\mathfrak{H} \otimes \mathfrak{H}} \rightarrow 0 \end{aligned}$$

as  $n \rightarrow \infty$ . Therefore

$$\varliminf_{n \rightarrow \infty} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F \Pi_n(\bar{v} \otimes I + I \otimes \bar{w})\Pi_n) \geq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F \Sigma'),$$

and since this holds for each  $0 \leq \Sigma' = \Sigma'^* \leq \Sigma$ , one has

$$\varliminf_{n \rightarrow \infty} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F \Pi_n(\bar{v} \otimes I + I \otimes \bar{w})\Pi_n) \geq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2} \Sigma F^{1/2}).$$

(Take  $\Sigma'$  of the form

$$\Sigma'_N := \sum_{n=1}^N \sigma_n |\Psi_n\rangle \langle \Psi_n|$$

<sup>4</sup>With the defining equalities

$$\begin{aligned} \Pi_n(\bar{v} \otimes I)\Pi_n &:= (R^{-1/2} \otimes I)\Pi_n(\bar{V} \otimes I)(R^{-1/2} \otimes I)\Pi_n, \\ \Pi_n(I \otimes \bar{w})\Pi_n &:= (I \otimes S^{-1/2})\Pi_n(I \otimes \bar{W})(I \otimes S^{-1/2})\Pi_n. \end{aligned}$$

where  $(\Psi_n)_{n \geq 0}$  is a complete orthonormal system of eigenvectors of  $\Sigma$  in  $\mathfrak{H} \otimes \mathfrak{H}$ , and  $\Sigma \Psi_n = \sigma_n \Psi_n$  for each  $n \geq 0$ , and observe that

$$\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F \Sigma'_N) = \sum_{n=1}^N \sigma_n \langle \Psi_n | F | \Psi_n \rangle \rightarrow \sum_{n \geq 1} \sigma_n \langle \Psi_n | F | \Psi_n \rangle = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2} \Sigma F^{1/2})$$

as  $N \rightarrow \infty$ .)

Call  $\mathfrak{p}_n$  and  $\mathfrak{q}_n$  respectively the orthogonal projections on  $\mathcal{V}_n$  and  $\mathcal{W}_n$  in  $\mathfrak{H}$ . Then<sup>5</sup>

$$\Pi_n(\bar{v} \otimes I + I \otimes \bar{w}) \Pi_n \leq \mathfrak{p}_n \bar{v} \mathfrak{p}_n \otimes I + I \otimes \mathfrak{q}_n \bar{w} \mathfrak{q}_n.$$

Indeed, one has separately

$$\Pi_n(\bar{v} \otimes I) \Pi_n \leq \mathfrak{p}_n \bar{v} \mathfrak{p}_n \otimes I, \quad \text{and} \quad \Pi_n(I \otimes \bar{w}) \Pi_n \leq I \otimes \mathfrak{q}_n \bar{w} \mathfrak{q}_n.$$

This is seen easily, for instance by the following argument. Let  $\Phi$  be any element of  $\text{Ker}(R)^\perp \otimes \text{Ker}(S)^\perp$ , which we decompose on the complete orthonormal system  $(e'_k \otimes f'_l)_{k, l \geq 0}$ :

$$\Phi = \sum_{k, l \geq 0} \Phi_{kl} e'_k \otimes f'_l, \quad \sum_{k, l \geq 0} |\Phi_{kl}|^2 = \|\Phi\|_{\mathfrak{H} \otimes \mathfrak{H}}^2 < \infty.$$

Then

$$\begin{aligned} \langle \Phi | \Pi_n(\bar{v} \otimes I) \bar{\Pi}_n | \Phi \rangle &= \sum_{0 \leq j, k, l \leq n} \overline{\Phi_{jl}} \Phi_{kl} \langle \bar{v} e'_j | e'_k \rangle_{\mathcal{V}', \mathcal{V}} \\ &\leq \sum_{\substack{0 \leq j, k \leq n \\ l \geq 0}} \overline{\Phi_{jl}} \Phi_{kl} \langle \bar{v} e'_j | e'_k \rangle_{\mathcal{V}', \mathcal{V}} = \langle \Phi | \mathfrak{p}_n \bar{v} \mathfrak{p}_n \otimes I | \Phi \rangle, \end{aligned}$$

since the matrix  $(\langle \bar{v} e'_j | e'_k \rangle_{\mathcal{V}', \mathcal{V}})_{0 \leq j, k \leq n}$  is Hermitian nonnegative. The analogous inequality for  $\bar{w}$  is proved similarly.

Hence

$$\begin{aligned} &\varliminf_{n \rightarrow \infty} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F \Pi_n(\bar{v} \otimes I + I \otimes \bar{w}) \Pi_n) \\ &\leq \varliminf_{n \rightarrow \infty} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F(\mathfrak{p}_n \bar{v} \mathfrak{p}_n \otimes I + I \otimes \mathfrak{q}_n \bar{w} \mathfrak{q}_n)) \\ &= \lim_{n \rightarrow \infty} \text{trace}_{\mathfrak{H}}(R \mathfrak{p}_n \bar{v} \mathfrak{p}_n + S \mathfrak{q}_n \bar{w} \mathfrak{q}_n) \\ &= \text{trace}_{\mathfrak{H}}(R^{1/2} \bar{v} R^{1/2} + S^{1/2} \bar{w} S^{1/2}). \end{aligned}$$

(Indeed

$$\text{trace}_{\mathfrak{H}}(R \mathfrak{p}_n \bar{v} \mathfrak{p}_n) = \sum_{j=0}^n \langle e'_j | R | e'_j \rangle \langle \bar{v} e'_j, e'_j \rangle \rightarrow \sum_{j \geq 0} \langle e'_j | R | e'_j \rangle \langle \bar{v} e'_j, e'_j \rangle = \text{trace}_{\mathfrak{H}}(R^{1/2} \bar{v} R^{1/2}),$$

as  $n \rightarrow \infty$ . The term  $\text{trace}_{\mathfrak{H}}(S \mathfrak{q}_n \bar{w} \mathfrak{q}_n)$  is treated similarly.)

Putting these inequalities together shows that

$$\begin{aligned} \text{trace}_{\mathfrak{H}}(R^{1/2}(2H - \bar{a})R^{1/2} + S^{1/2}(2H - \bar{b})S^{1/2}) &= \text{trace}_{\mathfrak{H}}(R^{1/2} \bar{v} R^{1/2} + S^{1/2} \bar{w} S^{1/2}) \\ &\geq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2} \Sigma F^{1/2}) = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2}(2(H \otimes I + I \otimes H) - C)F^{1/2}), \end{aligned}$$

and subtracting  $2 \text{trace}_{\mathfrak{H}}((R + S)H)$  from both sides of this inequality leads to the announced result.

<sup>5</sup>With  $\mathfrak{p}_n \bar{v} \mathfrak{p}_n := R^{-1/2} \mathfrak{p}_n \bar{V} R^{-1/2} \mathfrak{p}_n$  and  $\mathfrak{q}_n \bar{w} \mathfrak{q}_n := S^{-1/2} \mathfrak{q}_n \bar{W} S^{-1/2} \mathfrak{q}_n$ .



**Step 4: the squeezing argument**

Pick an optimal coupling  $F_{opt} \in \mathcal{C}(R, S)$ . (We recall that the existence of such a coupling is one of the conclusions of Theorem 2.1, and follows from the Fenchel-Rockafellar duality theorem.) One has the following chain of inequalities:

$$(18) \quad \sup_{(A,B) \in \mathfrak{K}(R,S)} \text{trace}_{\mathfrak{H}}(RA + SB) \leq \sup_{(\bar{a}, \bar{b}) \in \tilde{\mathfrak{K}}(R,S)} \text{trace}_{\mathfrak{H}}(R^{1/2}\bar{a} + S^{1/2}\bar{b})S^{1/2} \\ \leq \text{trace}_{\mathfrak{H}^{\otimes 2}}(F_{opt}^{1/2}CF_{opt}^{1/2}).$$

The second inequality has been proved in Step 3.

As for the first inequality, observe first that

$$(19) \quad \sup_{(A,B) \in \mathfrak{K}(R,S)} \text{trace}_{\mathfrak{H}}(RA + SB) = \sup_{(A,B) \in \hat{\mathfrak{K}}(R,S)} \text{trace}_{\mathfrak{H}}(RA + SB),$$

with the notation

$$\hat{\mathfrak{K}}(R, S) := \{(A, B) \in \mathfrak{K}(R, S) \text{ s.t. } A \leq 2H - d\hbar I, B \leq 2H - d\hbar I\}.$$

This is proved by the normalization argument in Step 1: pick

$$\rho := \sup\{\alpha \in \mathbf{R} \text{ s.t. } 2H - A \geq \alpha I\}.$$

Then  $\rho \in [-\|A\|, 2\langle e_0|H|e_0\rangle]$  and one has

$$A + (\rho - d\hbar)I \leq 2H - d\hbar I \quad \text{and} \quad B - (\rho - d\hbar)I \leq 2H - d\hbar I$$

by the same argument as in Step 1. (Indeed, by definition of  $\rho$ , there exists a sequence  $\phi_n \in \text{Dom}(H)$  such that  $\|\phi_n\|_{\mathfrak{H}} = 1$  and  $\langle \phi_n|2H - A|\phi_n\rangle \rightarrow \rho$  as  $n \rightarrow \infty$ . With the inequality  $A \otimes I + I \otimes B \leq C$ , this implies that

$$\rho I + \langle \phi_n|2H - B|\phi_n\rangle \geq \langle \phi_n|2(H \otimes I + I \otimes H) - C|\phi_n\rangle \geq 2d\hbar I,$$

since  $2(H \otimes I + I \otimes H) - C \geq 2d\hbar I \otimes I$ .) Observing that

$$(A, B) \in \mathfrak{K}(R, S) \implies (A + (\rho - d\hbar)I, B - (\rho - d\hbar)I) \in \hat{\mathfrak{K}}(R, S),$$

and that

$$\text{trace}_{\mathfrak{H}}(RA + SB) = \text{trace}_{\mathfrak{H}}(R(A + (\rho - d\hbar)I) + S(B - (\rho - d\hbar)I))$$

leads to (19).

Let  $\mathfrak{P}$  and  $\mathfrak{Q}$  be the  $\mathfrak{H}$ -orthogonal projections on  $\text{Ker}(R)$  and  $\text{Ker}(S)$  respectively. We claim that

$$(A, B) \in \hat{\mathfrak{K}}(R, S) \implies ((I - \mathfrak{P})A(I - \mathfrak{P}), (I - \mathfrak{Q})B(I - \mathfrak{Q})) \in \tilde{\mathfrak{K}}(R, S).$$

Indeed

$$(I - \mathfrak{P})A(I - \mathfrak{P}) = ((I - \mathfrak{P})A(I - \mathfrak{P}))^* \in \mathcal{L}(\text{Ker}(T)^\perp) \subset \mathcal{L}(\mathcal{J}[R], \mathcal{J}[R]') \\ (I - \mathfrak{Q})B(I - \mathfrak{Q}) = ((I - \mathfrak{Q})B(I - \mathfrak{Q}))^* \in \mathcal{L}(\text{Ker}(S)^\perp) \subset \mathcal{L}(\mathcal{J}[S], \mathcal{J}[S]').$$

because of the double continuous embedding (10). Then

$$2H \geq A \implies 2R^{1/2}HR^{1/2} \geq R^{1/2}AR^{1/2} = R^{1/2}(I - \mathfrak{P})A(I - \mathfrak{P})R^{1/2} \\ 2H \geq B \implies 2S^{1/2}HS^{1/2} \geq S^{1/2}BS^{1/2} = S^{1/2}(I - \mathfrak{Q})B(I - \mathfrak{Q})S^{1/2}$$

and

$$\begin{aligned} \text{trace}_{\mathfrak{H}}(2R^{1/2}HR^{1/2} - R^{1/2}(I - \mathfrak{P})A(I - \mathfrak{P})R^{1/2}) \\ \leq 2 \text{trace}_{\mathfrak{H}}(R^{1/2}HR^{1/2}) + \|A\| < \infty \\ \text{trace}_{\mathfrak{H}}(2S^{1/2}HS^{1/2} - S^{1/2}(I - \mathfrak{Q})B(I - \mathfrak{Q})S^{1/2}) \\ \leq 2 \text{trace}_{\mathfrak{H}}(S^{1/2}HS^{1/2}) + \|B\| < \infty \end{aligned}$$

so that

$$\begin{aligned} 2R^{1/2}HR^{1/2} - R^{1/2}(I - \mathfrak{P})A(I - \mathfrak{P})R^{1/2} \in \mathcal{L}^1(\text{Ker}(R)^\perp), \\ 2S^{1/2}HS^{1/2} - S^{1/2}(I - \mathfrak{Q})B(I - \mathfrak{Q})S^{1/2} \in \mathcal{L}^1(\text{Ker}(S)^\perp). \end{aligned}$$

Finally, the inequality

$$\langle \Phi | A \otimes I + I \otimes B | \Phi \rangle \leq \langle \Phi | C | \Phi \rangle$$

holds for all  $\Phi \in \text{Form-Dom}(C)$ . In particular, it holds for all  $\Phi \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S]$ , which is included in  $\text{Form-Dom}(C)$  because  $R, S \in \mathcal{D}_2(\mathfrak{H})$ . Observing that

$$\Phi \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S] \implies (\mathfrak{P} \otimes I)\Phi = (I \otimes \mathfrak{Q})\Phi = 0$$

leads to the desired implication.

In view of the obvious identity

$$\text{trace}_{\mathfrak{H}}(RA + SB) = \text{trace}_{\mathfrak{H}}(R^{1/2}(I - \mathfrak{P})A(I - \mathfrak{P})R^{1/2} + S^{1/2}(I - \mathfrak{Q})B(I - \mathfrak{Q})S^{1/2}),$$

we conclude that

$$(20) \quad \sup_{(A,B) \in \hat{\mathfrak{K}}(R,S)} \text{trace}(RA + SB) \leq \sup_{(\bar{a}, \bar{b}) \in \hat{\mathfrak{K}}(R,S)} \text{trace}(R^{1/2}\bar{a}R^{1/2} + S^{1/2}\bar{b}S^{1/2}).$$

Both inequalities (19) and (20) implies the chain of inequalities (18). By the quantum duality theorem (Theorem 2.1), all the inequalities in (18) are equalities:

$$(21) \quad \begin{aligned} \sup_{(A,B) \in \hat{\mathfrak{K}}(R,S)} \text{trace}_{\mathfrak{H}}(RA + SB) &= \sup_{(\bar{a}, \bar{b}) \in \hat{\mathfrak{K}}(R,S)} \text{trace}_{\mathfrak{H}}(R^{1/2}\bar{a} + S^{1/2}\bar{b}S^{1/2}) \\ &= \text{trace}_{\mathfrak{H} \otimes 2}(F_{opt}^{1/2}CF_{opt}^{1/2}). \end{aligned}$$

### Step 5: the pair $(\mathfrak{a}, \mathfrak{b}) \in \hat{\mathfrak{K}}(R, S)$ is optimal

For each finite rank  $P = P^* = P^2 \in \mathcal{L}(\mathfrak{H})$ , one has

$$\begin{aligned} \text{trace}_{\mathfrak{H}}(PR^{1/2}\mathfrak{v}R^{1/2}P) &= \text{trace}_{\mathfrak{H}}(PR^{1/2}\mathfrak{v}R^{1/2}) \\ &= \lim_{k \rightarrow \infty} \text{trace}_{\mathfrak{H}}(PR^{1/2}\hat{a}_kR^{1/2}) = \lim_{k \rightarrow \infty} \text{trace}_{\mathfrak{H}}(PR^{1/2}\hat{a}_kR^{1/2}P), \\ \text{trace}_{\mathfrak{H}}(PS^{1/2}\mathfrak{w}S^{1/2}P) &= \text{trace}_{\mathfrak{H}}(PS^{1/2}\mathfrak{w}S^{1/2}) \\ &= \lim_{k \rightarrow \infty} \text{trace}_{\mathfrak{H}}(PS^{1/2}\hat{b}_kS^{1/2}) = \lim_{k \rightarrow \infty} \text{trace}_{\mathfrak{H}}(PS^{1/2}\hat{b}_kS^{1/2}P), \end{aligned}$$

since

$$R^{1/2}\hat{a}_kR^{1/2} \xrightarrow{*} V = R^{1/2}\mathfrak{v}R^{1/2} \text{ and } S^{1/2}\hat{b}_kS^{1/2} \xrightarrow{*} W = S^{1/2}\mathfrak{w}S^{1/2}$$

in  $\mathcal{L}^1(\mathfrak{H})$  by construction.

Since  $\hat{a}_k = \hat{a}_k^* \geq 0$  and  $\hat{b}_k = \hat{b}_k^* \geq 0$  for each  $k \geq 0$ , one has

$$\begin{aligned} \text{trace}_{\mathfrak{H}}(PR^{1/2}\hat{a}_kR^{1/2}P) &= \|PR^{1/2}\hat{a}_kR^{1/2}P\|_1 \\ &\leq \|R^{1/2}\hat{a}_kR^{1/2}\|_1 = \text{trace}_{\mathfrak{H}}(R^{1/2}\hat{a}_kR^{1/2}), \\ \text{trace}_{\mathfrak{H}}(PS^{1/2}\hat{b}_kS^{1/2}P) &= \|PS^{1/2}\hat{b}_kS^{1/2}P\|_1 \\ &\leq \|S^{1/2}\hat{b}_kS^{1/2}\|_1 = \text{trace}_{\mathfrak{H}}(S^{1/2}\hat{b}_kS^{1/2}). \end{aligned}$$

Thus, for each finite rank  $P = P^* = P^2 \in \mathcal{L}(\mathfrak{H})$ , one has

$$\begin{aligned} \text{trace}_{\mathfrak{H}}(P(R^{1/2}\mathfrak{v}R^{1/2} + S^{1/2}\mathfrak{w}S^{1/2})P) &\leq \lim_{k \rightarrow \infty} \text{trace}_{\mathfrak{H}}(R^{1/2}\hat{a}_kR^{1/2} + S^{1/2}\hat{b}_kS^{1/2}) \\ &= 2 \text{trace}_{\mathfrak{H}}(R^{1/2}HR^{1/2} + S^{1/2}HS^{1/2}) - \tau. \end{aligned}$$

Indeed

$$\hat{a}_k = 2H - A_k - \alpha_k I + d\mathfrak{h}I \quad \text{and} \quad \hat{b}_k = 2H - B_k + \alpha_k I - d\mathfrak{h}I$$

so that

$$\begin{aligned} &\text{trace}_{\mathfrak{H}}(R^{1/2}\hat{a}_kR^{1/2} + S^{1/2}\hat{b}_kS^{1/2}) \\ &= 2 \text{trace}_{\mathfrak{H}}(R^{1/2}HR^{1/2} + S^{1/2}HS^{1/2}) - \text{trace}_{\mathfrak{H}}(R^{1/2}A_kR^{1/2} + S^{1/2}B_kS^{1/2}) \\ &\rightarrow 2 \text{trace}_{\mathfrak{H}}(R^{1/2}HR^{1/2} + S^{1/2}HS^{1/2}) - \tau \end{aligned}$$

by definition of the sequence  $(A_k, B_k)$ .

Since  $R^{1/2}\mathfrak{v}R^{1/2} \in \mathcal{L}^1(\mathfrak{H})$  and  $S^{1/2}\mathfrak{w}S^{1/2} \in \mathcal{L}^1(\mathfrak{H})$ , one has

$$\begin{aligned} \text{trace}_{\mathfrak{H}}(R^{1/2}\mathfrak{v}R^{1/2} + S^{1/2}\mathfrak{w}S^{1/2}) &= \sup_{\substack{P^2 = P = P^* \\ \text{rank}(P) < \infty}} \text{trace}_{\mathfrak{H}}(P(R^{1/2}\mathfrak{v}R^{1/2} + S^{1/2}\mathfrak{w}S^{1/2})P) \\ &\leq 2 \text{trace}_{\mathfrak{H}}(R^{1/2}HR^{1/2} + S^{1/2}HS^{1/2}) - \tau. \end{aligned}$$

Equivalently, in terms of  $\mathfrak{a}$  and  $\mathfrak{b}$ , one has

$$\text{trace}_{\mathfrak{H}}(R^{1/2}\mathfrak{a}R^{1/2} + S^{1/2}\mathfrak{b}S^{1/2}) \geq \tau$$

and we deduce from the first equality in (21) that

$$\text{trace}_{\mathfrak{H}}(R^{1/2}\mathfrak{a}R^{1/2} + S^{1/2}\mathfrak{b}S^{1/2}) \geq \sup_{(\bar{\mathfrak{a}}, \bar{\mathfrak{b}}) \in \tilde{\mathfrak{R}}(R, S)} \text{trace}_{\mathfrak{H}}(R^{1/2}\bar{\mathfrak{a}}R^{1/2} + S^{1/2}\bar{\mathfrak{b}}S^{1/2}).$$

Since  $(\mathfrak{a}, \mathfrak{b}) \in \tilde{\mathfrak{R}}(R, S)$ , the inequality above is an equality and the pair  $(\mathfrak{a}, \mathfrak{b})$  is optimal.

## 5. PROOF OF THEOREM 2.4

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

$$\mathcal{J}_0[R] \cup \mathcal{J}_0[S] \subset \text{Form-Dom}(H) := \{\psi \in H^1(\mathbf{R}^d) \text{ s.t. } |x|\psi \in \mathfrak{H}\},$$

so that

$$\mathcal{J}_0[R] \otimes \mathcal{J}_0[S] \subset \text{Form-Dom}(H \otimes I + I \otimes H) \subset \text{Form-Dom}(C).$$

Hence the expressions

$$\langle \Phi_j | H \otimes I | \Phi_j \rangle, \quad \langle \Phi_j | I \otimes H | \Phi_j \rangle, \quad \text{and} \quad \langle \Phi_j | C | \Phi_j \rangle$$

are well defined, and the condition

$$\sum_{j \geq 1} \lambda_j \langle \Phi_j | H \otimes I + I \otimes H | \Phi_j \rangle < \infty$$

implies that

$$0 \leq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2}CF^{1/2}) \leq 2 \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2}(H \otimes I + I \otimes H)F^{1/2}) < \infty.$$

**Step 1: defining the operators  $F^{1/2}CF^{1/2}$ ,  $F^{1/2}\mathfrak{a} \otimes IF^{1/2}$  and  $F^{1/2}I \otimes \mathfrak{b}F^{1/2}$ .**

The condition

$$\sum_{j \geq 1} \lambda_j \langle \Phi_j | R^{-1} \otimes I | \Phi_j \rangle = \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((R^{-1/2} \otimes I)F(R^{-1/2} \otimes I)) < \infty$$

implies that

$$F^{1/2}(R^{-1/2} \otimes I) = \mathfrak{F}_1 := \sum_{j \geq 1} \sqrt{\lambda_j} |\Phi_j\rangle \langle (R^{-1/2} \otimes I)\Phi_j| \in \mathcal{L}^2(\text{Ker}(R)^\perp \otimes \mathfrak{H}),$$

while

$$(R^{-1/2} \otimes I)F^{1/2} = \mathfrak{F}_1^* := \sum_{j \geq 1} \sqrt{\lambda_j} \langle (R^{-1/2} \otimes I)\Phi_j| \langle \Phi_j| \in \mathcal{L}^2(\text{Ker}(R)^\perp \otimes \mathfrak{H}).$$

In particular

$$\begin{aligned} F^{1/2} &= \mathfrak{F}_1(R^{1/2} \otimes I) \in \mathcal{L}^2(\mathcal{J}[R]' \otimes \mathfrak{H}; \text{Ker}(R)^\perp \otimes \mathfrak{H}), \\ F^{1/2} &= (R^{1/2} \otimes I)\mathfrak{F}_1^* \in \mathcal{L}^2((\text{Ker}(R)^\perp \otimes \mathfrak{H}; \mathcal{J}[R] \otimes \mathfrak{H}). \end{aligned}$$

Therefore

$$F^{1/2}(\mathfrak{a} \otimes I)F^{1/2} = \mathfrak{F}_1(R^{1/2}\mathfrak{a}R^{1/2} \otimes I)\mathfrak{F}_1^* \in \mathcal{L}^1(\text{Ker}(R)^\perp \otimes \mathfrak{H}).$$

By the same token

$$F^{1/2}(I \otimes \mathfrak{b})F^{1/2} = \mathfrak{F}_2(I \otimes S^{1/2}\mathfrak{b}S^{1/2})\mathfrak{F}_2^* \in \mathcal{L}^1(fH \otimes \text{Ker}(S)^\perp),$$

with

$$F^{1/2}(I \otimes S^{-1/2}) = \mathfrak{F}_2 := \sum_{j \geq 1} \sqrt{\lambda_j} |\Phi_j\rangle \langle (I \otimes S^{-1/2})\Phi_j| \in \mathcal{L}^2(\mathfrak{H} \otimes \text{Ker}(S)^\perp).$$

**Step 2: defining  $\text{trace}(F^{1/2}\mathfrak{a} \otimes IF^{1/2})$  and  $\text{trace}(F^{1/2}I \otimes \mathfrak{b}F^{1/2})$ .**

One has

$$\begin{aligned} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}(F^{1/2}\mathfrak{a} \otimes IF^{1/2}) &= \text{trace}_{\text{Ker}(R)^\perp \otimes \mathfrak{H}}(F^{1/2}\mathfrak{a} \otimes IF^{1/2}) \\ &= \text{trace}_{\text{Ker}(R)^\perp \otimes \mathfrak{H}}(\mathfrak{F}_1^*\mathfrak{F}_1(R^{1/2}\mathfrak{a}R^{1/2} \otimes I)) \\ &= \text{trace}_{\text{Ker}(R)^\perp}(\text{trace}_2(\mathfrak{F}_1^*\mathfrak{F}_1)R^{1/2}\mathfrak{a}R^{1/2}). \end{aligned}$$

Observe that

$$\mathfrak{F}_1^*\mathfrak{F}_1 = \sum_{j \geq 1} \lambda_j |(R^{-1/2} \otimes I)\Phi_j\rangle \langle (R^{-1/2} \otimes I)\Phi_j|,$$

and that

$$\begin{aligned} \text{trace}_2(|(R^{-1/2} \otimes I)\Phi_j\rangle \langle (R^{-1/2} \otimes I)\Phi_j|) &= \text{trace}_2((R^{-1/2} \otimes I)|\Phi_j\rangle \langle \Phi_j|(R^{-1/2} \otimes I)) \\ &= R^{-1/2} \text{trace}_2(|\Phi_j\rangle \langle \Phi_j|)R^{-1/2} \end{aligned}$$

for all  $j \geq 1$ . Hence

$$\begin{aligned} \text{trace}_2(\mathfrak{F}_1^*\mathfrak{F}_1) &= \sum_{j \geq 1} \lambda_j \text{trace}_2(|(R^{-1/2} \otimes I)\Phi_j\rangle \langle (R^{-1/2} \otimes I)\Phi_j|) \\ &= R^{-1/2} \left( \sum_{j \geq 1} \lambda_j \text{trace}_2(|\Phi_j\rangle \langle \Phi_j|) \right) R^{-1/2} = R^{-1/2} \text{trace}_2(F)R^{-1/2} \in \mathcal{L}^1(\text{Ker}(R)^\perp), \end{aligned}$$

so that

$$\text{trace}_{\text{Ker}(R)^\perp \otimes \mathfrak{H}}(F^{1/2} \mathbf{a} \otimes IF^{1/2}) = \text{trace}_{\text{Ker}(R)^\perp}((R^{-1/2} \text{trace}_2(F) R^{-1/2})(R^{1/2} \mathbf{a} R^{1/2})).$$

Likewise

$$\text{trace}_{\mathfrak{H} \otimes \text{Ker}(S)^\perp}(F^{1/2} I \otimes \mathbf{b} F^{1/2}) = \text{trace}_{\text{Ker}(S)^\perp}((S^{-1/2} \text{trace}_1(F) S^{-1/2})(S^{1/2} \mathbf{b} S^{1/2})).$$

**Step 3: computing**  $\text{trace}_{\mathfrak{H}}(\sqrt{\text{trace}_2(F)} \mathbf{a} \sqrt{\text{trace}_2(F)} + \sqrt{\text{trace}_1(F)} \mathbf{b} \sqrt{\text{trace}_1(F)})$ .

Since  $R^{1/2} \mathbf{a} R^{1/2} = (R^{1/2} \mathbf{a} R^{1/2})^* \in \mathcal{L}^1(\text{Ker}(R)^\perp)$ , one has

$$R^{1/2} \mathbf{a} R^{1/2} = \sum_{j \geq 1} \alpha_j |\phi_j\rangle \langle \phi_j|$$

where  $(\phi_j)_{j \geq 1}$  is an orthonormal system in  $\text{Ker}(R)^\perp$  while  $(\alpha_j)_{j \geq 1} \in \ell^1(\mathbf{N}^*)$ . On the other hand, since  $R^{-1/2} \text{trace}_2(F) R^{-1/2} \in \mathcal{L}^1(\text{Ker}(R)^\perp)$ , one has

$$\mathfrak{f}_1 := \text{trace}_2(F)^{1/2} R^{-1/2} \text{ and } \mathfrak{f}_1^* = R^{-1/2} \text{trace}_2(F)^{1/2} \in \mathcal{L}^2(\text{Ker}(R)^\perp)$$

by the same argument used to prove that  $\mathfrak{F}_1 \in \mathcal{L}^2(\text{Ker}(R)^\perp \otimes \mathfrak{H})$ . In particular

$$\begin{aligned} \text{trace}_2(F)^{1/2} &= \mathfrak{f}_1 R^{1/2} \in \mathcal{L}^2(\mathcal{J}[R]', \text{Ker}(R)^\perp), \\ \text{trace}_2(F)^{1/2} &= R^{1/2} \mathfrak{f}_1^* \in \mathcal{L}^2(\text{Ker}(R)^\perp, \mathcal{J}[R]'). \end{aligned}$$

Hence

$$\begin{aligned} &\text{trace}_{\text{Ker}(R)^\perp}((R^{-1/2} \text{trace}_2(F) R^{-1/2})(R^{1/2} \mathbf{a} R^{1/2})) \\ &= \sum_{j \geq 1} \alpha_j \langle \phi_j | R^{-1/2} \text{trace}_2(F) R^{-1/2} | \phi_j \rangle \\ &= \sum_{j \geq 1} \alpha_j \langle (\text{trace}_2(F))^{1/2} R^{-1/2} \phi_j | (\text{trace}_2(F))^{1/2} R^{-1/2} \phi_j \rangle \\ &= \text{trace}_{\mathfrak{H}}(\text{trace}_2(F)^{1/2} \mathbf{a} \text{trace}_2(F)^{1/2}). \end{aligned}$$

By the same token

$$\begin{aligned} &\text{trace}_{\text{Ker}(S)^\perp}((S^{-1/2} \text{trace}_1(F) S^{-1/2})(S^{1/2} \mathbf{b} S^{1/2})) \\ &= \text{trace}_{\mathfrak{H}}(\text{trace}_1(F)^{1/2} \mathbf{b} \text{trace}_1(F)^{1/2}) \end{aligned}$$

**Step 4: proving that**  $(\mathbf{a}|_{\mathcal{J}[\text{trace}_2(F)]}, \mathbf{b}|_{\mathcal{J}[\text{trace}_1(F)]}) \in \tilde{\mathfrak{K}}(\text{trace}_2(F), \text{trace}_1(F))$ .

Since

$$F = \sum_{j \geq 1} \lambda_j |\Phi_j\rangle \langle \Phi_j| \quad \text{with } \Phi_j \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S] \text{ for all } j \geq 1,$$

one has the following chain of implications:

$$\psi \in \text{Ker}(R) \implies \psi \otimes e \in \text{Ker}(F) \text{ for each } e \in \mathfrak{H} \implies \text{Ker}(R) \subset \text{Ker}(\text{trace}_2(F)).$$

Moreover

$$R^{-1/2} \text{trace}_2(F) R^{-1/2} \in \mathcal{L}(\text{Ker}(R)^\perp) \implies \mathcal{J}[\text{trace}_2(F)] \subset \mathcal{J}[R].$$

Since  $\mathbf{a} \in \mathcal{L}(\mathcal{J}[R], \mathcal{J}[R]')$ , one has  $\mathbf{a}|_{\mathcal{J}[\text{trace}_2(F)]} \in \mathcal{L}(\mathcal{J}[\text{trace}_2(F)], \mathcal{J}[\text{trace}_2(F)]')$  and, by the same token,  $\mathbf{b}|_{\mathcal{J}[\text{trace}_1(F)]} \in \mathcal{L}(\mathcal{J}[\text{trace}_1(F)], \mathcal{J}[\text{trace}_1(F)]')$ . The pair  $(\mathbf{a}, \mathbf{b})$  obviously satisfies condition (b) is the definition of  $\tilde{\mathfrak{K}}(\text{trace}_2(F), \text{trace}_1(F))$  since  $\mathcal{J}_0[\text{trace}_2(F)] \subset \mathcal{J}_0[R]$  and  $\mathcal{J}_0[\text{trace}_1(F)] \subset \mathcal{J}_0[S]$ . It also satisfies condition (a): indeed

$$\text{trace}_2(F)^{1/2} (2H - \mathbf{a}) \text{trace}_2(F)^{1/2} = \mathfrak{f}_1 (R^{1/2} (2H - \mathbf{a}) R^{1/2}) \mathfrak{f}_1^* \geq 0$$

since  $R^{1/2}(2H - \mathbf{a})R^{1/2} \geq 0$ , and

$$\text{trace}(\mathbf{f}_1(R^{1/2}(2H - \mathbf{a})R^{1/2})\mathbf{f}_1^*) \leq \|\mathbf{f}_1\|^2 \text{trace}(R^{1/2}(2H - \mathbf{a})R^{1/2}) < \infty$$

so that  $\text{trace}_2(F)^{1/2}\mathbf{a}\text{trace}_2(F)^{1/2} \in \mathcal{L}^1(\text{Ker}(\text{trace}_2(F))^\perp)$ . Arguing likewise, we conclude that  $(\mathbf{a}|_{\mathcal{J}[\text{trace}_2(F)]}, \mathbf{b}|_{\mathcal{J}[\text{trace}_1(F)]}) \in \tilde{\mathfrak{K}}(\text{trace}_2(F), \text{trace}_1(F))$ .

**Step 5: conclusion.**

We deduce from Steps 1-4 the identity

$$\begin{aligned} \text{trace}_{\text{Ker}(R)^\perp \otimes \text{Ker}(S)^\perp}(F^{1/2}(C - \mathbf{a} \otimes I - I \otimes \mathbf{b})F^{1/2}) &= \text{trace}_{\text{Ker}(R)^\perp \otimes \text{Ker}(S)^\perp}(F^{1/2}CF^{1/2}) \\ &\quad - \text{trace}_{\mathfrak{S}}(\sqrt{\text{trace}_2(F)}\mathbf{a}\sqrt{\text{trace}_2(F)} + \sqrt{\text{trace}_1(F)}\mathbf{b}\sqrt{\text{trace}_1(F)}) \\ &= \sum_{j \geq 1} \lambda_j \langle \Phi_j | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_j \rangle. \end{aligned}$$

In Step 3 of the proof of Theorem 2.3, we have seen that, for each coupling  $Q \in \mathcal{C}[\text{trace}_2(F), \text{trace}_1(F)]$  and each  $(\bar{a}, \bar{b}) \in \tilde{\mathfrak{K}}(\text{trace}_2(F), \text{trace}_1(F))$ , one has  $\text{trace}(Q^{1/2}CQ^{1/2}) \geq \text{trace}(\text{trace}_2(F)^{1/2}\bar{a}\text{trace}_2(F)^{1/2} + \text{trace}_1(F)^{1/2}\bar{b}\text{trace}_1(F)^{1/2})$ . The identity above shows that, if  $\langle \Phi_j | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_j \rangle = 0$  for each  $j \geq 1$ , then

$$\begin{aligned} &\text{trace}_{\text{Ker}(R)^\perp \otimes \text{Ker}(S)^\perp}(F^{1/2}CF^{1/2}) \\ &= \text{trace}_{\mathfrak{S}}(\sqrt{\text{trace}_2(F)}\mathbf{a}\sqrt{\text{trace}_2(F)} + \sqrt{\text{trace}_1(F)}\mathbf{b}\sqrt{\text{trace}_1(F)}). \end{aligned}$$

Hence

$$\text{trace}(F^{1/2}CF^{1/2}) = \inf_{Q \in \mathcal{C}(\text{trace}_2(F), \text{trace}_1(F))} \text{trace}(Q^{1/2}CQ^{1/2})$$

and

$$\begin{aligned} &\text{trace}(\text{trace}_2(F)^{1/2}\mathbf{a}\text{trace}_2(F)^{1/2} + \text{trace}_1(F)^{1/2}\mathbf{b}\text{trace}_1(F)^{1/2}) \\ &= \sup_{(\bar{a}, \bar{b}) \in \tilde{\mathfrak{K}}(\text{trace}_2(F), \text{trace}_1(F))} \text{trace}(\text{trace}_2(F)^{1/2}\bar{a}\text{trace}_2(F)^{1/2} + \text{trace}_1(F)^{1/2}\bar{b}\text{trace}_1(F)^{1/2}). \end{aligned}$$

Conversely, assume that

$$F = \sum_{j \geq 1} \lambda_j |\Phi_j\rangle\langle \Phi_j| \in \mathcal{C}(R, S),$$

with  $\Phi_j \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S]$  for all  $j \geq 1$  satisfying

$$\sum_{j \geq 1} \lambda_j \langle \Phi_j | R^{-1} \otimes I + I \otimes S^{-1} | \Phi_j \rangle < \infty,$$

is an optimal coupling, i.e. satisfies

$$\text{trace}(F^{1/2}CF^{1/2}) = \inf_{Q \in \mathcal{C}(R, S)} \text{trace}(Q^{1/2}CQ^{1/2}) = MK_h(R, S)^2.$$

Let  $(\mathbf{a}, \mathbf{b}) \in \tilde{\mathfrak{K}}(R, S)$  be an optimal couple such that

$$\text{trace}(F^{1/2}CF^{1/2}) = \text{trace}(R^{1/2}\mathbf{a}R^{1/2} + S^{1/2}\mathbf{b}S^{1/2}),$$

whose existence is guaranteed by Theorem 2.3. Then

$$\sum_{j \geq 1} \lambda_j \langle \Phi_j | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_j \rangle = 0$$

and since

$$\langle \Phi_j | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_j \rangle \geq 0$$

for all  $j \geq 1$  since  $\Phi_j \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S]$  and  $(\mathbf{a}, \mathbf{b}) \in \tilde{\mathfrak{K}}(R, S)$ , we conclude that

$$\lambda_j > 0 \implies \langle \Phi_j | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_j \rangle = 0,$$

which completes the proof.

## 6. PROOF OF THEOREM 2.5

Since  $(\mathbf{a}, \mathbf{b}) \in \tilde{\mathfrak{K}}(R, S)$ , one has

$$\langle \Psi | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Psi \rangle \geq 0 \quad \text{for all } \Psi \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S],$$

while

$$\langle \Phi_n | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_n \rangle \geq 0 \quad \text{for all } n \geq 1.$$

Thus, for each  $\Psi \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S]$  and each  $t \in \mathbf{R}$ , one has

$$\langle t\Phi_n + \Psi | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | t\Phi_n + \Psi \rangle \geq 0 \quad \text{for all } n \geq 1,$$

i.e

$$2t\Re \langle \Psi | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_n \rangle \geq -\langle \Psi | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Psi \rangle$$

for all  $t \in \mathbf{R}$ . Therefore,

$$\Re \langle \Psi | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_n \rangle = 0 \quad \text{for all } \Psi \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S].$$

Changing  $\Psi$  into  $i\Psi$  shows that

$$\langle \Psi | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_n \rangle = 0 \quad \text{for all } \Psi \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S].$$

In other words, we have proved that

$$(C - \mathbf{a} \otimes I - I \otimes \mathbf{b})\Phi_n = 0 \quad \text{in } \mathcal{J}[R]' \otimes \mathcal{J}[S]' \quad \text{for all } n \geq 0.$$

In particular

$$\begin{aligned} \langle (P_j \otimes I)\Phi_m | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_n \rangle &= 0, & \text{for all } m, n \geq 1 \text{ and } j = 1, \dots, d, \\ \langle (Q_j \otimes I)\Phi_m | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_n \rangle &= 0, & \text{for all } m, n \geq 1 \text{ and } j = 1, \dots, d. \end{aligned}$$

since  $(P_j \otimes I)\Phi_m, (Q_j \otimes I)\Phi_m \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S]$  by assumption (16). By the same token

$$\begin{aligned} \langle \Phi_m | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | (P_j \otimes I)\Phi_n \rangle &= 0, & \text{for all } m, n \geq 1 \text{ and } j = 1, \dots, d, \\ \langle \Phi_m | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | (Q_j \otimes I)\Phi_n \rangle &= 0, & \text{for all } m, n \geq 1 \text{ and } j = 1, \dots, d. \end{aligned}$$

Hence

$$\begin{aligned} -\langle (P_j \otimes I)\Phi_m | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_n \rangle + \langle \Phi_m | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | (P_j \otimes I)\Phi_n \rangle &= 0, \\ -\langle (Q_j \otimes I)\Phi_m | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | \Phi_n \rangle + \langle \Phi_m | C - \mathbf{a} \otimes I - I \otimes \mathbf{b} | (Q_j \otimes I)\Phi_n \rangle &= 0, \end{aligned}$$

for all  $m, n \geq 1$  and  $j = 1, \dots, d$ .

These equalities are the weak formulations of the identities

$$\langle \Phi_m | \mathcal{D}_{Q_j} \otimes I (C - \mathbf{a} \otimes I - I \otimes \mathbf{b}) | \Phi_n \rangle = \langle \Phi_m | \mathcal{D}_{P_j} \otimes I (C - \mathbf{a} \otimes I - I \otimes \mathbf{b}) | \Phi_n \rangle = 0$$

for all  $m, n \geq 1$  and  $j = 1, \dots, d$ .

Similarly  $(I \otimes P_j)\Phi_m$  and  $(I \otimes Q_j)\Phi_m \in \mathcal{J}_0[R] \otimes \mathcal{J}_0[S]$  by (16), and, proceeding as above, one concludes that

$$\langle \Phi_m | I \otimes \mathcal{D}_{Q_j} (C - \mathbf{a} \otimes I - I \otimes \mathbf{b}) | \Phi_n \rangle = \langle \Phi_m | I \otimes \mathcal{D}_{P_j} (C - \mathbf{a} \otimes I - I \otimes \mathbf{b}) | \Phi_n \rangle = 0$$

for all  $m, n \geq 1$  and  $j = 1, \dots, d$ .

It remains to compute

$$\begin{aligned}\mathcal{D}_{Q_j} \otimes I(C - \mathbf{a} \otimes I - I \otimes \mathbf{b}) &= (2Q_j - \mathcal{D}_{Q_j} \mathbf{a}) \otimes I - 2I \otimes Q_j \\ &= \mathcal{D}_{Q_j}(H - \mathbf{a}) \otimes I - I \otimes \mathcal{D}_{Q_j} H, \\ \mathcal{D}_{P_j} \otimes I(C - \mathbf{a} \otimes I - I \otimes \mathbf{b}) &= (2P_j - \mathcal{D}_{P_j} \mathbf{a}) \otimes I - 2I \otimes P_j \\ &= \mathcal{D}_{P_j}(H - \mathbf{a}) \otimes I - I \otimes \mathcal{D}_{P_j} H.\end{aligned}$$

Similarly

$$\begin{aligned}I \otimes \mathcal{D}_{Q_j}(C - \mathbf{a} \otimes I - I \otimes \mathbf{b}) &= I \otimes (2Q_j - \mathcal{D}_{Q_j} \mathbf{b}) - 2Q_j \otimes I \\ &= I \otimes \mathcal{D}_{Q_j}(H - \mathbf{b}) - \mathcal{D}_{Q_j} H \otimes I, \\ I \otimes \mathcal{D}_{P_j}(C - \mathbf{a} \otimes I - I \otimes \mathbf{b}) &= I \otimes (2P_j - \mathcal{D}_{P_j} \mathbf{b}) - 2P_j \otimes I \\ &= I \otimes \mathcal{D}_{P_j}(H - \mathbf{b}) - \mathcal{D}_{P_j} H \otimes I.\end{aligned}$$

Hence the identities above are recast as

$$\begin{aligned}&\langle \Phi_m | \mathcal{D}_{Q_j}(H - \mathbf{a}) \otimes I - I \otimes \mathcal{D}_{Q_j} H | \Phi_n \rangle \\ &= \langle \Phi_m | \mathcal{D}_{P_j}(H - \mathbf{a}) \otimes I - I \otimes \mathcal{D}_{P_j} H | \Phi_n \rangle = 0 \\ &\quad \text{for all } m, n \geq 1 \text{ and } j = 1, \dots, d,\end{aligned}$$

and

$$\begin{aligned}&\langle \Phi_m | \mathcal{D}_{Q_j} H \otimes I - I \otimes \mathcal{D}_{Q_j}(H - \mathbf{b}) | \Phi_n \rangle \\ &= \langle \Phi_m | \mathcal{D}_{P_j} H \otimes I - I \otimes \mathcal{D}_{P_j}(H - \mathbf{b}) | \Phi_n \rangle = 0 \\ &\quad \text{for all } m, n \geq 1 \text{ and } j = 1, \dots, d,\end{aligned}$$

which are precisely the identities (17).

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