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# Order $p$ quantum Wasserstein distances from couplings

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Optimal transport provides a powerful mathematical framework with applications spanning numerous fields. A cornerstone within this domain is the  $p$ -Wasserstein distance, which serves to quantify the cost of transporting one probability measure to another. While recent attempts have sought to extend this measure to the realm of quantum states, existing definitions often present certain limitations, such as not being faithful. In this work, we present a new definition of quantum Wasserstein distances. This definition, leveraging the coupling method and a metric applicable to pure states, draws inspiration from a property characterising the classical Wasserstein distance — its determination based on its value on point masses. Subject to certain continuity properties, our definition exhibits numerous attributes expected of an optimal quantum rendition of the Wasserstein distance. Notably, our approach seamlessly integrates metrics familiar to quantum information theory, such as the trace distance. Moreover, it provides an organic extension for metrics, like Nielsen’s complexity metric, allowing their application to mixed states with a natural operational interpretation. Furthermore, we analyze this metric’s attributes in the context of random quantum states and unveil phase transitions concerning the complexity of subsystems of random states.

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## I. INTRODUCTION

Optimal transport has established itself as a powerful tool in various areas of science and pure mathematics, such as machine learning [FZM<sup>+</sup>15], information theory [RS15], partial differential equations [Vil08] and economics [Gal18]. In light of this, it should come as no surprise that the last years have seen a surge of interest in the quantum generalisation of optimal transport [PMTL21, CM14, CYL<sup>+</sup>19, GMP15, PT21, FECZ22, DPMRF23, GJL21, DR20, BPTV24].

One of the central concepts of classical optimal transport is the  $p$ -Wasserstein distances  $\mathcal{W}_p$ , which are a family of distances on the set of probability measures on a metric space. Roughly speaking, if we imagine a probability measure as describing a distribution of mass, these distances measure the cost of transporting one measure onto another in terms of a cost function on the underlying metric space. They can recover many widely studied metrics in probability spaces in a unified way. For instance, the total variation distance corresponds to the Wasserstein distance obtained when we equip the space with the discrete metric. In the classical setting [Vil08], they admit many different equivalent characterisations, which we can broadly categorise into a *geometrical formulation*, a *dual formulation* and a *coupling formulation*.

There now exist many different proposals of quantum Wasserstein distances that take one of the approaches mentioned above [PMTL21, PT23, PT21, CM14, CM19, RD19, CEFZ23, FECZ22, GMP15]. Important examples of definitions that follow the geometric route are the definitions by Carlen and Maas [CM14, CM17], which have been extensively studied in a series of works [RD19, CM19, DR20]. Roughly speaking, the geometric framework gives a natural generalisation of  $\mathcal{W}_2$  in terms of a Riemannian metric on the set of full rank states such that the relative entropy with respect to a reference state arises as a gradient flow. However, it has the undesirable feature of depending on an underlying semigroup converging to a reference state.

A good example of a distance that is based on a dual approach is the definition of de Palma et al [PMTL21]. Whereas the geometric approach is well-suited to generalise the case  $p = 2$ , this approach works well for  $p = 1$ , and the authors were able to define a natural quantum generalisation of  $\mathcal{W}_1$  with respect to the Hamming distance on the hypercube. The dual approach works by first defining a good generalisation of a so-called Lipschitz constant of observables, which in some sense measures how much the expectation value of the observable can change between two points when normalised by the underlying metric. From this, defining the distance induced by such observables is straightforward through duality. This generalisation has also found numerous applications in quantum information and computation [PR22, DPMRF23, RF21, KPM<sup>+</sup>22, PT23, PKP23].

Finally, some works have followed the coupling approach [CEFZ23, FECZ22, PT21, CYL<sup>+</sup>19]. Recall that given two random variables, a coupling is a joint distribution whose marginals are the two random variables. In the classical setting, the Wasserstein distance can be defined as the infimum of the expected cost of transporting one random variable onto the other, where the infimum is taken over all couplings of the two random variables. The main advantage of the coupling approach is that it yields a definition of  $W_p$  for all values of  $p$ . Existing approaches that attempt to quantise the coupling approach have significant downsides and usually do not satisfy one or more of the key properties expected from the Wasserstein distance. For example, the definition of [CEFZ23] is not a semidistance, and the definition of [PT21] is not faithful.

In this work, we propose a new definition of the quantum Wasserstein distance based on the coupling approach. Our novel definition departs from the observation that, classically, the Wasserstein distance is completely determined by its value on point masses. As pure states are quantum analogues of point masses, we propose a coupling definition of the quantum  $p$ -Wasserstein distance induced by a metric on pure states and then consider an optimisation over all separable couplings of the underlying states.

We show that, as long as the metric on pure states satisfies some simple continuity properties, the induced quantum  $p$ -Wasserstein has many desirable properties expected from a good quantisation of the Wasserstein distance. In particular, we show that our definition recovers widely studied metrics on the set of quantum states, such as the trace distance, and is closely related to de Palma's quantum Wasserstein distance of order 1. Furthermore, we show that it offers a natural way of extending distances from pure to mixed states in a way that preserves all the symmetries of the

original metric and recovers its value on pure states. We also discuss some interesting ways in which our quantised distance behaves differently from its classical counterpart.

As an application of our new definition, we give a generalisation of Nielsen’s complexity geometry [Nie06] to mixed states that has a natural operational interpretation of measuring the complexity of mapping one mixed state to another. We then study the behaviour of this metric for various ensembles of random quantum states and identify phase transitions in the expected Wasserstein distance between them. More concretely, we show that if we look at reduced density matrices of regions whose size is at most one-ninth of the total size, then the complexity distance is exponentially small. In contrast, for large enough subsystems, the distance is maximal. This result can be interpreted as formalizing the intuitive notion that small enough subsystems of random states are essentially maximally mixed and trivial from a complexity point of view, whereas large enough subsystems are highly entangled and complex.

We also study De Palma et al’s  $W_1^H$  distance under random quantum states, showing that they are essentially maximally far apart. Previous works [RF21] hinted at the possibility that the  $W_1^H$  captures how well states can be distinguished by local observables. However, as random states cannot be distinguished by local observables, and as our results show that random states can be distinguished by the  $W_1^H$  distance, we see that this original intuition is false. This mirrors a result found concurrently in [PKP23]. This shows that the  $W_1^H$  distance, and in turn the set of Lipschitz observables defined from its dual, have a significantly richer structure than previously expected.

Finally, we discuss an operational interpretation of our newly introduced distance and quantify the noise of a channel in terms of its hypercontractivity under the  $W_p^d$  distance.

## II. BASIC CONCEPTS AND NOTATION

### A. Classical optimal transport

In the classical setting, the domain of optimal transport introduced in [Mon81] is well-developed and finds applications in a wide variety of areas. The focus is to understand the cost of transporting one measure onto another and find the minimal cost of such transportation. More formally, for measurable spaces  $\mathcal{X}, \mathcal{Y}$  with probability measures  $\mu, \nu$  respectively, we assign a cost  $c : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}_{\geq 0}$  which represents the cost  $c(x, y)$  of moving one unit of measure from  $x$  to  $y$ . From here we optimise the total cost of transporting  $\mu$  onto  $\nu$  for each coupling [Kan42]  $\gamma$  of  $\mu$  and  $\nu$ .

**Definition 1.** *Let  $\mu, \nu$  be probability measures on measurable spaces  $\mathcal{X}, \mathcal{Y}$  respectively. A **coupling** of  $\mu$  and  $\nu$  is a measure  $\gamma$  on  $\mathcal{X} \times \mathcal{Y}$  such that for all measurable sets  $\mathcal{A} \subseteq \mathcal{X}$ , we have  $\gamma(\mathcal{A} \otimes \mathcal{Y}) = \mu(\mathcal{A})$ , and all measurable sets  $\mathcal{B} \subseteq \mathcal{Y}$  we have  $\gamma(\mathcal{X} \otimes \mathcal{B}) = \nu(\mathcal{B})$ . Denote by  $\mathcal{C}(\mu, \nu)$  the set of couplings of  $\mu$  with  $\nu$ .*

In other words, a coupling is a measure  $\gamma$  on  $\mathcal{X} \otimes \mathcal{Y}$  with marginals  $\mu$  and  $\nu$ . For a cost function  $c$  on  $\mathcal{X} \times \mathcal{Y}$ , we can then define the **transport cost** of a coupling  $\gamma$  as

$$\mathcal{T}(\gamma) = \int_{\mathcal{X} \times \mathcal{Y}} c(x, y) d\gamma(x, y). \quad (1)$$

The optimal transport cost of transporting  $\mu$  and  $\nu$  is then given by minimising (1) over all couplings  $\gamma$ . Throughout we will only consider the case where  $\mathcal{X} = \mathcal{Y}$ ,  $\mathcal{X}$  is equipped with a metric  $d$ , and the cost function  $c$  is a power of the metric  $d$ . This leads to the definition of a classical Wasserstein distance [Vil03, p. 207].

**Definition 2.** *Let  $(\mathcal{X}, d)$  be a measurable metric space with probability measures  $\mu, \nu$ . Given  $p \geq 1$ , the  **$p^{\text{th}}$ -order Wasserstein distance** between  $\mu$  and  $\nu$  is given by*

$$\mathcal{W}_p(\mu, \nu) = \left( \inf_{\gamma \in \mathcal{C}(\mu, \nu)} \int_{\mathcal{X} \times \mathcal{X}} d(x, y)^p d\gamma(x, y) \right)^{1/p}. \quad (2)$$

This notion also extends to  $p = \infty$  in the following way:

**Definition 3.** *Let  $(\mathcal{X}, d)$  be a measurable metric space with probability measures  $\mu, \nu$ . The **infinite-order Wasserstein distance** between  $\mu$  and  $\nu$  is given by*

$$\mathcal{W}_\infty(\mu, \nu) = \inf_{\gamma \in \mathcal{C}(\mu, \nu)} \sup_{(x, y) \in \text{supp}(\gamma)} d(x, y). \quad (3)$$

It is desirable to generalise these distances to quantities on quantum states to mirror many of their classical applications. We're particularly interested in generalisations of the case where the underlying metric  $d$  is the discrete metric, for which  $\mathcal{W}_p$  is the total variation distance, and the case where the underlying metric is the Hamming distance on the hypercube, for which  $\mathcal{W}_1$  is Ornstein's  $\bar{d}$ -distance [Orn73]. These are arguably the most widely used distances in this context so far and a good generalisation should also recover them.

## B. Quantum information framework

We represent a quantum system by a Hilbert space  $\mathcal{H}$  of finite dimension. Pure states on this system are modelled as elements  $|\psi\rangle$  of the projective space  $\mathbb{P}\mathcal{H}$ . We notate the Hermitian conjugate of such a pure state by  $\langle\psi|$ , and then in a slight abuse of notation we write  $|\psi\rangle\langle\psi|$  for the projection onto  $|\psi\rangle$ , taking the convention  $\text{Tr}[|\psi\rangle\langle\psi|] = 1$ .

Mixed states on this system are then convex combinations of pure states, written as a finite sum

$$\rho = \sum_j q_j |\psi_j\rangle\langle\psi_j| \quad (4)$$

where  $\sum_j q_j = 1$  and  $q_j > 0$ . Equivalently, the set of mixed states on  $\mathcal{H}$  is defined as the set of Hermitian positive semidefinite linear operators of trace 1, otherwise known as density operators, and we will denote this set by  $\mathcal{D}(\mathcal{H})$ .

Note that in the case  $\rho = |\psi\rangle\langle\psi|$ , we will also refer to  $\rho$  as a pure state. It will be clear from context whether the term 'pure state' refers to an element of the projective Hilbert space or a density operator. Similarly, the term 'state' could refer to either a pure state  $|\psi\rangle$  or a mixed state  $\rho$ , and the meaning will be clear from the context.

The combination of two systems  $\mathcal{H}_1$  and  $\mathcal{H}_2$  is represented by their tensor product  $\mathcal{H}_1 \otimes \mathcal{H}_2$ . Their projective space is then  $\mathbb{P}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ . Similarly, the set of density operators on this bipartite system is  $\mathcal{D}(\mathcal{H}_1 \otimes \mathcal{H}_2)$ .

The quantum equivalent of taking the marginal is the partial trace operation. Using this, we can define a quantum coupling of states  $\rho, \sigma$ .

**Definition 4.** Let  $\rho, \sigma$  be quantum states on Hilbert spaces  $\mathcal{H}_1, \mathcal{H}_2$  respectively. A **quantum coupling** of  $\rho$  with  $\sigma$  is a quantum state  $\tau$  on  $\mathcal{H}_1 \otimes \mathcal{H}_2$  such that

$$\text{Tr}_2 \tau = \rho \quad \text{and} \quad \text{Tr}_1 \tau = \sigma. \quad (5)$$

Once again, in this manuscript, we only consider the case where  $\mathcal{H}_1 = \mathcal{H}_2$ . Throughout this work, we will also reference a few key objects from quantum information theory and quantum computation.

**Definition 5.** For states  $\rho$  and  $\sigma$  on Hilbert space  $\mathcal{H}$ , their **trace distance** is half the trace norm of their difference, defined by

$$d_1(\rho, \sigma) = \frac{1}{2} \|\rho - \sigma\|_1 = \frac{1}{2} \text{Tr} \left[ \sqrt{(\rho - \sigma)^\dagger (\rho - \sigma)} \right]. \quad (6)$$

We also have the equivalence

$$d_1(\rho, \sigma) = \sup_{P^\dagger = P, 0 \leq P \leq I} \text{Tr}[P(\rho - \sigma)]. \quad (7)$$

**Definition 6.** Let  $\mathcal{U}(n)$  be the group of  $n \times n$  unitary matrices. The **Haar measure** on  $\mathcal{U}(n)$ , denoted  $\mu_{\text{Haar}}$ , is the unique measure on the group  $\mathcal{U}(n)$  which is invariant under left-multiplication and for which  $\mu_{\text{Haar}}(\mathcal{U}(n)) = 1$ .

**Definition 7.** The  $2 \times 2$  **Pauli operators**  $\sigma_x, \sigma_y, \sigma_z$  are given by the matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (8)$$

seen as unitary transformations with respect to the computational basis. On the  $n$ -fold tensor product of  $\mathbb{C}^2$ , a **Pauli string** is a product  $\sigma_1 \otimes \dots \otimes \sigma_n$  where each  $\sigma_i \in \{\mathbb{I}, \sigma_x, \sigma_y, \sigma_z\}$ . The **weight** of such a string is the number of indices for which  $\sigma_i \neq \mathbb{I}$ , so the weight of  $\mathbb{I} \otimes \sigma_x \otimes \mathbb{I}$  is one and the weight of  $\sigma_x \otimes \sigma_y \otimes \sigma_z$  is three.

### III. MOTIVATIONS AND DEFINITIONS

To generalise the Wasserstein distances to the quantum setting in a way that is useful, it is desirable to replicate as many basic properties of the classical definition as possible. To allow this, we note a key property of the classical Wasserstein distances. For all orders  $p \geq 1$  and all  $x, y \in \mathcal{X}$ , the  $\mathcal{W}_p$  distance between point masses agrees with the metric distance. That is, for Dirac measures  $\delta_x$  and  $\delta_y$ , we have

$$\mathcal{W}_p(\delta_x, \delta_y) = d(x, y). \quad (9)$$

It follows, therefore, that the classical Wasserstein distances are determined by their values on point masses. We also see that we can recover the underlying metric  $d$  from the Wasserstein distance.

This property of determination by point masses is the key motivation of this work. For any quantum Wasserstein distance which is defined for general order  $p$ , the distances between the quantum versions of point masses (pure states) should be independent of  $p$ , and should agree with the underlying metric on the space if one exists.

To replicate this property, consider a Hilbert space  $\mathcal{H}$  with projective space  $\mathbb{P}\mathcal{H}$ , equipped with metric  $d$ . In this setting, for all orders  $p \geq 1$  and states  $|\psi\rangle$  and  $|\varphi\rangle$  we would expect a quantum Wasserstein distance  $W_p^d$  to satisfy

$$W_p^d(|\psi\rangle\langle\psi|, |\varphi\rangle\langle\varphi|) = d(|\psi\rangle, |\varphi\rangle) \quad (10)$$

taking the convention that  $|\psi\rangle\langle\psi|$  and  $|\varphi\rangle\langle\varphi|$  both have unit trace. Given this motivation for a property the distance should satisfy, it remains to generalise the definition of a transport cost in (1) to the quantum setting. One possible generalisation is given in the definition below.

**Definition 8.** Let  $\mathcal{H}$  be a finite-dimensional Hilbert space with projective space  $\mathbb{P}\mathcal{H}$ , and let  $\rho, \sigma \in \mathcal{D}(\mathcal{H})$ . We define a **quantum transport plan** between  $\rho$  and  $\sigma$  as any finite set of triples  $\{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}_j$  such that

$$\sum_j q_j |\psi_j\rangle\langle\psi_j| = \rho \quad \text{and} \quad \sum_j q_j |\varphi_j\rangle\langle\varphi_j| = \sigma. \quad (11)$$

where  $q_j > 0$ , and taking convention  $\text{Tr}|\psi_j\rangle\langle\psi_j| = \text{Tr}|\varphi_j\rangle\langle\varphi_j| = 1$ . This is equivalent to an expression of a separable quantum coupling  $\tau$  of  $\rho$  and  $\sigma$  as a convex combination of pure bipartite states

$$\tau = \sum_j q_j |\psi_j\rangle\langle\psi_j| \otimes |\varphi_j\rangle\langle\varphi_j|. \quad (12)$$

We denote the set of all quantum transport plans between  $\rho$  and  $\sigma$  by  $\mathcal{Q}(\rho, \sigma)$ . By convention, we say that two elements  $(q, |\psi\rangle, |\varphi\rangle)$ ,  $(q', |\psi\rangle, |\varphi\rangle)$  never appear in the same transport plan: any plan written as such is implied to contain the element  $(q + q', |\psi\rangle, |\varphi\rangle)$  in their place.

This equivalence between transport plans and ways of writing couplings reflects the classical case, although we note that one quantum coupling could give rise to multiple quantum transport plans. For example, the separable quantum coupling  $\tau = |0\rangle\langle 0| \otimes \frac{1}{2}$  between  $|0\rangle\langle 0|$  and  $\frac{1}{2}$  on a two-qubit space gives rise to transport plans  $\{(1/2, |0\rangle, |0\rangle), (1/2, |0\rangle, |1\rangle)\}$  and  $\{(1/2, |0\rangle, |+\rangle), (1/2, |0\rangle, |-\rangle)\}$ .

In building quantum transport plans, we can also refer to **partial quantum transport plans**. This is a quantum transport plan where  $\rho$  and  $\sigma$  are instead positive semidefinite operators of equal trace at most 1, and the partial plan transports the ‘partial state’  $\rho$  onto the ‘partial state’  $\sigma$ .

We can then use this notion of a quantum transport plan to replicate the classical definitions of transport cost and Wasserstein distance in the quantum setting.

**Definition 9.** Let  $\mathcal{H}$  be a finite-dimensional Hilbert space and let  $d$  be a distance on  $\mathbb{P}\mathcal{H}$ . Let  $p \geq 1$ . For any transport plan  $Q = \{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}_j$  we define its  $p^{\text{th}}$ -order quantum transport cost as

$$T_p^d(Q) = \sum_j q_j d(|\psi_j\rangle, |\varphi_j\rangle)^p. \quad (13)$$

The  $p^{\text{th}}$ -order quantum Wasserstein distance on  $\mathcal{D}(\mathcal{H})$  is then defined as

$$W_p^d(\rho, \sigma) = \left( \inf_{Q \in \mathcal{Q}(\rho, \sigma)} T_p^d(Q) \right)^{1/p}. \quad (14)$$

We will see in Proposition 16 that the infimum in this definition is equivalent to the minimum, in the case that  $d$  is continuous. Note that we have restricted to separable couplings above. This is because it is not obvious how to extend the transportation cost for entangled pure states. In Appendix B 2 we discuss one possible way and then argue that at, at least for  $p = 1$ , entangled couplings are not advantageous and we can restrict to separable couplings without loss of generality.

As with many other ordered distances, we can also define the infinite-order quantum Wasserstein distance.

**Definition 10.** Let  $\mathcal{H}$  be a finite-dimensional Hilbert space and let  $d$  be a distance on  $\mathbb{P}\mathcal{H}$ . For any states  $\rho, \sigma \in \mathcal{D}(\mathcal{H})$ , we define their **infinite-order quantum Wasserstein distance** as

$$W_\infty^d(\rho, \sigma) = \inf_{Q \in \mathcal{Q}(\rho, \sigma)} \sup_j d(|\psi_j\rangle, |\varphi_j\rangle) \quad (15)$$

for quantum transport plans  $Q = \{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}_j$ .

As a natural consequence of the convex nature of these definitions, we see that this family of Wasserstein distances is monotone in  $p$ . Indeed, for any transport plan  $Q$  between  $\rho$  and  $\sigma$  we have for  $p_1 < p_2$  that

$$T_{p_1}(Q)^{1/p_1} = \left( \sum_j q_j d(|\psi_j\rangle, |\varphi_j\rangle)^{p_1} \right)^{1/p_1} \quad (16)$$

$$\leq \left( \left( \sum_j q_j (d(|\psi_j\rangle, |\varphi_j\rangle)^{p_1})^{p_2/p_1} \right)^{1/p_1} \right)^{p_1/p_2} \quad (17)$$

$$= \left( \sum_j q_j d(|\psi_j\rangle, |\varphi_j\rangle)^{p_2} \right)^{1/p_2} \quad (18)$$

$$= T_{p_2}(Q)^{1/p_2} \quad (19)$$

by an application of Jensen's inequality. Taking the infimum over  $Q \in \mathcal{Q}(\rho, \sigma)$ , we get

$$W_{p_1}^d(\rho, \sigma) \leq W_{p_2}^d(\rho, \sigma). \quad (20)$$

The same applies when  $p_2 = \infty$ , as  $T_{p_1}(Q)^{1/p_1} \leq \max_j d(|\psi_j\rangle, |\varphi_j\rangle)$ .

This definition is given for all  $1 \leq p \leq \infty$ . However, at least in the classical case, the most important cases to consider for interesting applications are  $p = 1, 2$ , and  $\infty$  [PZ19, Vil08, Tra18].

Although many desirable properties of these  $W_p^d$  are proven in Sec. IV, establishing a triangle inequality remains a difficult open problem. This is true of many attempts to establish a quantum generalisation of the classical Wasserstein distances, and further discussion of attempts to establish this are discussed in Appendix C. However, by looking at the dual picture in Sec. IV A, we establish a closely related norm on the space of traceless Hermitian operators for which  $W_1^d$  is an upper bound, and which agrees with the original distance  $d$  on differences between pure states. For order  $p = 1$  this norm allows a trade-off between ease of proving the triangle inequality, and operational interpretation in terms of moving mass. This dual formulation closely mirrors the Kantorovich-Rubinstein theorem in the classical case [Vil03, p. 34]. Furthermore, we show in Sec. V that it allows us to essentially recover the trace distance and the definition of [PMTL21], thus our results on the dual definition give strong evidence that this  $W_p^d$  a good quantum generalisation.

## A. Other approaches

Many proposals have been suggested for generalisations of the classical Wasserstein distance to quantum states, in various contexts, to varying degrees of success. Arguably the most desirable classical metrics to generalise are the discrete metric on a finite space and the Hamming distance on the hypercube.

The most prominent example is perhaps the first-order distance defined in [PMTL21] which generalises the  $W_1$  distance on the hypercube whose underlying geometry is the Hamming distance. They define states  $\rho, \sigma$  on  $(\mathbb{C}^d)^{\otimes n}$  to be *neighbouring* if there exists some qudit  $i$  for which  $\text{Tr}_i[\rho - \sigma] = 0$ . In other words,  $\rho$  and  $\sigma$  are the same when

qudit  $i$  is traced out. The norm  $\|\cdot\|_{W_1^H}$  traceless Hermitian operators is then defined such that its unit ball is the convex hull of all differences between neighbouring states. This means  $\|\rho - \sigma\|_{W_1^H}$  can be written as

$$\|\rho - \sigma\|_{W_1^H} = \min \left\{ \sum_{i=1}^n c_i : c_i > 0, \sum_{i=1}^n (\rho^{(i)} - \sigma^{(i)}) = \rho - \sigma, \text{Tr}_i[\rho^{(i)} - \sigma^{(i)}] = 0 \right\}. \quad (21)$$

This is a true metric and it has led to many applications such as in quantum spin systems [PT23] and variational quantum algorithms [DPMRF23]. However, the approach taken is very specific to the Hamming distance and does not lend itself to general transport costs.

For order  $p = 2$ , a number of definitions have been proposed in various contexts, such as [GMP15] which defines a second-order optimal transport cost in the context of mean field limits that was shown in [CGP21] to have links with the Brenier formulation of classical optimal transport [Vil03, p. 238].

More precisely, for a set of Hermitian operators  $\{R_1, \dots, R_K\}$  on  $\mathcal{H}$ , the second-order transport cost of a coupling  $\Pi$  on  $\mathcal{H} \otimes \mathcal{H}$  by

$$\mathcal{C}(\Pi) = \sum_{i=1}^K \text{Tr}[(R_i \otimes \mathbb{I} - \mathbb{I} \otimes R_i)\Pi(R_i \otimes \mathbb{I} - \mathbb{I} \otimes R_i)] \quad (22)$$

from which a second-order Wasserstein distance is derived by taking the square root of the infimum of the cost of all couplings between  $\rho$  and  $\sigma$  in the usual way. Defining quantity  $d(|\psi\rangle, |\varphi\rangle) = \sum_{i=1}^K \|R_i|\psi\rangle\|^2 + \|R_i|\varphi\rangle\|^2 - 2\langle\psi|R_i|\psi\rangle\langle\varphi|R_i|\varphi\rangle$ , we see that this is a variation of our definition above, although with a specific  $d$  which is not a true metric, and with the infimum taken over all couplings as opposed to just those which are separable.

Following the Brenier formulation more closely, the distance in [CM14] is also a second-order distance and has been used [DR20] to prove a quantum version of the HWI inequality. Specifically, the 2-Wasserstein distance is defined here as the geodesic distance on the set of full-rank states equipped with a Riemannian metric defined by the continuity equation. This definition is a world away from our framework, as it leans heavily into the intricacies of the classical dynamical formulation.

We should also mention the definition in [CYL<sup>+</sup>19] and refined in [MH22] which defines a second-order cost based on couplings with a specific cost function given by an asymmetric projection. While it is conjectured that this gives a true distance, we show in Appendix A that this definition cannot be extended to other underlying geometries, such as analogues of the Hamming distance on multipartite spaces. Further approaches include the more flexible [PT21], an alternative to [GMP15], which defines a second-order distance based on couplings that is not faithful. It has been conjectured [PT22] that a natural modification of this quantity is a true distance, though this remains an open problem. A similarly flexible approach appears in [FECZ22], following a naïve translation of the classical formulation into the quantum setting. This definition takes a cost matrix  $C$  on  $\mathcal{H} \otimes \mathcal{H}$ , and defines a Wasserstein distance by

$$W_p(\rho, \sigma) = \left( \inf_{\tau \in \mathcal{C}(\rho, \sigma)} \text{Tr}[C^p \tau] \right)^{1/p} \quad (23)$$

where  $\mathcal{C}(\rho, \sigma)$  is the set of quantum couplings of  $\rho$  with  $\sigma$ . The particular case of  $C$  being the projection onto the asymmetric subspace is studied in detail and coincides with the definition in [CYL<sup>+</sup>19]. In the general case, however, this is not shown to be a semidistance.

Each of the approaches seems to be generalising one particular aspect or application of Wasserstein distances to the noncommutative setting, be it obtaining a distance for a given value of  $p$  or a given underlying geometry of the Hilbert space. However, it is not clear how they relate to each other or how to extend them beyond their original setting. The definition in this work adapts to any order  $p$  and any underlying metric  $d$  on the set of pure states of the Hilbert space provided that  $d$  satisfies a few basic continuity properties. This broad flexibility allows us to talk about the moments of the cost of moving between classical-quantum sources in great generality (Sec. VIB) and also allows us to talk about the noise of an operator by comparing transport distances of different orders in an analogue of hypercontractivity (Sec. VIC).

To avoid confusion, we give in Table I a summary of all relevant Wasserstein distances used throughout this work.

#### IV. GENERAL PROPERTIES

The goals of this section are to prove some fundamental attributes of  $W_p^d$  which will give an idea of how it behaves in the case of general  $d$ . Throughout we will require some basic regularity conditions on  $d$ . As we will see in more detail in



Notation	Definition
$W_p^d(\mu, \nu)$	The <b>classical</b> Wasserstein distance of order $p$ between measures $\mu, \nu$ on metric space $(X, d)$ ; see Equations (2) and (3).
$W_p^d(\rho, \sigma)$	The <b>classical</b> Wasserstein distance of order $p$ between measures $\mu, \nu$ on Hilbert space $\mathcal{H}$ and metric $d$ on $\mathbb{P}\mathcal{H}$ ; see Equations (14) and (15).
$\ \rho - \sigma\ _{W_1^H}$	The quantum Wasserstein norm of order one from [PMTL21]; see Equation (22).
$W_p^H(\rho, \sigma)$	The quantum Wasserstein distance of order $p$ on $\mathcal{H} = (\mathbb{C}^d)^{\otimes n}$ defined by metric $d_H( \psi\rangle,  \varphi\rangle) = \  \psi\rangle\langle\psi  -  \varphi\rangle\langle\varphi \ _{W_1^H}$ ; see Sec. V A. Write $W_{p=1}^H$ when $p = 1$ to avoid confusion with norm $\ \cdot\ _{W_1^H}$ .
$W_p^1(\rho, \sigma)$	The quantum Wasserstein distance of order $p$ on $\mathcal{H} = \mathbb{C}^D$ defined by the trace distance $d_1( \psi\rangle,  \varphi\rangle) = \  \psi\rangle\langle\psi  -  \varphi\rangle\langle\varphi \ _1$ ; see Sec. V B.
$W_p^C(\rho, \sigma)$	The quantum Wasserstein distance of order $p$ on $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$ defined by the complexity geometry metric $d_C$ [Nie06]; see Sec. V C.

TABLE I. An overview of the Wasserstein distances used in this work, and the relevant notation.

the discussion following Cor. 13, not every metric  $d$  on the set of pure states induces a faithful Wasserstein distance. Thus, we will restrict to metrics with respect to which the 2-norm on the set of traceless self-adjoint operators is Hölder continuous. In other words, we require that there exists  $\alpha \in (0, 1]$  and  $C > 0$  for which for all  $|\psi\rangle, |\varphi\rangle \in \mathbb{P}\mathcal{H}$  we have

$$Cd(|\psi\rangle, |\varphi\rangle)^\alpha \geq \||\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|\|_2. \quad (24)$$

Note that as we work in finite dimension, the 2-norm is chosen here without loss of generality. In the case  $\alpha = 1$ , this is equivalent to the 2-norm being Lipschitz with respect to  $d$ . The constant  $C$  is a function of the metric space  $(\mathbb{P}\mathcal{H}, d)$  and so can depend on the dimension of  $\mathcal{H}$ . For some other properties such as continuity, we will require that  $d$  be continuous, noting that on  $\mathcal{H}$  of finite dimension this is equivalent to  $d$  being uniformly continuous.

Given the main philosophical motivation of this definition, that the transport distance between point masses in the classical setting is given by the underlying metric, it's important to show the quantum equivalent here. That is, for all orders  $p$  the quantum Wasserstein distance between pure states agrees with the underlying metric.

**Proposition 11.** *Let  $\mathcal{H}$  be a finite-dimensional Hilbert space with distance  $d$  on  $\mathbb{P}\mathcal{H}$ . Then for pure states  $|\psi\rangle\langle\psi|, |\varphi\rangle\langle\varphi|$ , we have*

$$W_p^d(|\psi\rangle\langle\psi|, |\varphi\rangle\langle\varphi|) = d(|\psi\rangle, |\varphi\rangle). \quad (25)$$

*Proof.* As  $|\psi\rangle\langle\psi|$  and  $|\varphi\rangle\langle\varphi|$  are pure, the only permitted transport plan is  $Q = \{(1, |\psi\rangle, |\varphi\rangle)\}$ , which has cost

$$T_p^d(Q) = d(|\psi\rangle, |\varphi\rangle)^p \quad (26)$$

and therefore we have  $W_p^d(|\psi\rangle\langle\psi|, |\varphi\rangle\langle\varphi|) = d(|\psi\rangle, |\varphi\rangle)$ .  $\square$

**Proposition 12.** *Let  $\mathcal{H}$  be a finite-dimensional Hilbert space with distance  $d$  on  $\mathbb{P}\mathcal{H}$  with respect to which the 2-norm is Hölder continuous with constant  $C > 0$  and exponent  $\alpha \in (0, 1]$ . Then for all  $\rho, \sigma \in \mathcal{D}(\mathcal{H})$ , we have*

$$W_p^d(\rho, \sigma) \geq \frac{1}{C} \|\rho - \sigma\|_2^{1/\alpha}. \quad (27)$$

*Proof.* We have  $Cd(|\psi\rangle, |\varphi\rangle)^\alpha \geq \||\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|\|_2$  on  $\mathbb{P}\mathcal{H}$ , for  $C > 0$  and  $\alpha \in (0, 1]$ . Let  $\{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}$  be a quantum transport plan between  $\rho$  and  $\sigma$ . The functions  $x \mapsto x^p$  and  $X \mapsto \|X\|_2^{1/\alpha}$  for traceless  $X$  are both convex.

Hence

$$\sum_j q_j d(|\psi_j\rangle, |\varphi_j\rangle)^p \geq \left( \sum_j q_j d(|\psi_j\rangle, |\varphi_j\rangle) \right)^p \quad (28)$$

$$\geq \left( \sum_j q_j \frac{1}{C} \left\| |\psi_j\rangle\langle\psi_j| - |\varphi_j\rangle\langle\varphi_j| \right\|_2^{1/\alpha} \right)^p \quad (29)$$

$$\geq \left( \frac{1}{C} \left\| \sum_j q_j (|\psi_j\rangle\langle\psi_j| - |\varphi_j\rangle\langle\varphi_j|) \right\|_2^{1/\alpha} \right)^p \quad (30)$$

$$= \frac{1}{C^p} \|\rho - \sigma\|_2^{p/\alpha}. \quad (31)$$

Hence taking the infimum and the  $p^{\text{th}}$  root, we have  $W_p^d(\rho, \sigma) \geq \frac{1}{C} \|\rho - \sigma\|_2^{1/\alpha}$ .  $\square$

This allows us to prove some of the metric properties of the  $W_p^d$  distance, namely nondegeneracy and zero self-distance. Symmetry in this definition is clear. Note that these fundamental properties have not always been present in previous definitions such as in [PT21] where the definition has non-zero self-distance.

**Corollary 13.** *Let  $d$  be a distance on  $\mathbb{P}\mathcal{H}$  with respect to which the 2-norm is Hölder continuous. For all  $\rho, \sigma \in \mathcal{D}(\mathcal{H})$ , we have  $W_p^d(\rho, \sigma) \geq 0$  with equality iff  $\rho = \sigma$ .*

*Proof.*  $W_p^d(\rho, \sigma) \geq 0$  is clear, and equality when  $\rho = \sigma$  can be obtained from the taking transport plan  $\{(c_j, |\psi_j\rangle, |\psi_j\rangle)\}$  where  $\rho = \sum_j c_j |\psi_j\rangle\langle\psi_j|$  is a spectral decomposition. Faithfulness is a direct consequence of Proposition 12.  $\square$

For a general distance  $d$ , not necessarily satisfying property (24), we get from the same proof above that  $W_p^d(\rho, \sigma) \geq 0$  and  $W_p^d(\rho, \rho) = 0$ . It is not guaranteed, however, that a general distance on  $\mathbb{P}\mathcal{H}$  leads to a nondegenerate  $W_p^d$ . For example, let  $\mathcal{H} = \mathbb{C}^2$  with the standard basis  $\{|0\rangle, |1\rangle\}$ . For any non-negative real-valued function  $f$  on  $\mathbb{P}\mathcal{H}$  with  $f(|0\rangle) = 0$  and  $f$  positive elsewhere, we can define a metric  $d$  as follows:

$$d(|\psi\rangle, |\varphi\rangle) = \begin{cases} 0 & \text{if } |\psi\rangle = |\varphi\rangle \\ f(|\psi\rangle) + f(|\varphi\rangle) & \text{otherwise.} \end{cases} \quad (32)$$

This forms a version of the SNCF metric, also known as the centralised railway metric [DD13, p. 327], with  $|0\rangle$  at the centre. This is a metric in which travel is only permitted along rays emanating from a central point. We will consider  $f$  such that

$$f\left(\sqrt{\frac{n-1}{n}}|0\rangle + \sqrt{\frac{1}{n}}|1\rangle\right) = f\left(\sqrt{\frac{n-1}{n}}|1\rangle - \sqrt{\frac{1}{n}}|0\rangle\right) = \frac{1}{n} \quad (33)$$

for  $n \in \mathbb{N}$  and  $f(|\psi\rangle) = 2$  otherwise. This gives  $W_1^d(|0\rangle, \frac{\mathbb{1}}{2}) = 0$  by the sequence of transport plans

$$\left\{ \left( \frac{1}{2}, |0\rangle, \sqrt{\frac{n-1}{n}}|0\rangle + \sqrt{\frac{1}{n}}|1\rangle \right), \left( \frac{1}{2}, |0\rangle, \sqrt{\frac{n-1}{n}}|1\rangle - \sqrt{\frac{1}{n}}|0\rangle \right) \right\} \quad (34)$$

for  $n \in \mathbb{N}$ , each with cost  $\frac{1}{n}$ . We have shown that the Hölder continuity condition is sufficient for  $W_p^d$  to be nondegenerate, but it is not immediately obvious whether or not it is necessary.

Furthermore, all symmetries of  $(\mathbb{P}\mathcal{H}, d)$  are inherited by the quantum Wasserstein distances.

**Proposition 14.** *Let  $1 \leq p \leq \infty$  and  $d$  be a metric on  $\mathbb{P}\mathcal{H}$ . The group of unitary symmetries of the underlying metric  $d$  is exactly the group of conjugational symmetries of  $W_p^d$ .*

*Proof.* Let  $U$  be a symmetry of  $d$ .  $U$  is invertible, therefore there's a direct correspondence

$$\{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\} \longleftrightarrow \{(q_j, U|\psi_j\rangle, U|\varphi_j\rangle)\} \quad (35)$$

between quantum transport plans from  $\rho$  to  $\sigma$  and from  $U\rho U^\dagger$  to  $U\sigma U^\dagger$ . The distance  $d$  is invariant under  $U$  so cost is preserved under this correspondence, therefore the optimal cost is also preserved.

Conversely, let unitary  $V$  be a conjugational symmetry of  $W_p^d$ . Then for all  $|\psi\rangle, |\varphi\rangle \in \mathbb{P}\mathcal{H}$ , we have

$$d(|\psi\rangle, |\varphi\rangle) = W_p^d(|\psi\rangle\langle\psi|, |\varphi\rangle\langle\varphi|) = W_p^d(V|\psi\rangle\langle\psi|V^\dagger, V|\varphi\rangle\langle\varphi|V^\dagger) = d(V|\psi\rangle, V|\varphi\rangle) \quad (36)$$

and so  $V$  is a symmetry of  $d$ .  $\square$

This allows us to prove a result on data processing for mixed unitary channels. The data processing inequality is a central concept in both classical and quantum information theory, and represents the idea that you can't create new information by processing old data: all the information you have about an object is encoded in the rawest data you have. This concept also exists in classical optimal transport: for measures  $\mu$  on a metric space  $(X, d)$ , measurable sets  $A, B$  and a measurable map  $f : X \rightarrow X$ , we define the *pushforward*  $f_*\mu$  by  $f_*\mu(B) = \mu(f^{-1}(B))$ . If  $f$  is 1-Lipschitz, then  $W_p^d(\mu, \nu) \geq W_p^d(f_*\mu, f_*\nu)$ . We can also recover this idea for mixed unitary channels of symmetries of the space as follows:

**Proposition 15.** *Suppose  $\Phi$  is a mixed unitary channel written as*

$$\Phi(\rho) = \sum_{k \in K} a_k U_k \rho U_k^\dagger \quad a_k \geq 0, \sum_{k \in K} a_k = 1 \quad (37)$$

for which each  $U_k$  is a symmetry of  $d$ . Then for all orders  $1 \leq p \leq \infty$  and all states  $\rho, \sigma$ , we have  $W_p^d(\rho, \sigma) \geq W_p^d(\Phi(\rho), \Phi(\sigma))$ .

*Proof.* Let  $Q = \{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}_{j \in J}$  be any  $p^{\text{th}}$ -order transport plan between  $\rho$  and  $\sigma$ . We can then define a transport plan  $Q' = \{(q_j a_k, U_k |\psi_j\rangle, U_k |\varphi_j\rangle)\}_{j \in J, k \in K}$  between  $\Phi(\rho)$  and  $\Phi(\sigma)$  which has the same  $p^{\text{th}}$ -order transport cost as  $Q$ . Taking the infimum over  $Q$  gives the result.  $\square$

It is also possible to guarantee the existence of an optimal transport plan when the underlying distance  $d$  is continuous and to bound the number of elements of an optimal transport plan. This applies in particular when  $d$  is induced by a norm: that is to say, that there exists a norm  $\|\cdot\|_d$  on the self-adjoint traceless operators on  $\mathcal{H}$  such that  $d(|\psi\rangle, |\varphi\rangle) = \|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|\|_d$  everywhere.

**Proposition 16.** *Let  $d$  be a continuous distance on  $\mathbb{P}\mathcal{H}$  and let  $\mathcal{H}$  have dimension  $D$ . The infimum in (14) is attained with a transport plan containing at most  $2D^2$  elements.*

*Proof.* Suppose  $\{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}_{j \in J}$  is a transport plan between  $\rho$  and  $\sigma$  with more than  $2D^2$  elements. Let  $\mathcal{M}_D^{\text{sa}}$  be the space of self-adjoint operators on  $D$  dimensions. The space  $\mathcal{M}_D^{\text{sa}} \times \mathcal{M}_D^{\text{sa}}$  has real dimension  $2D^2$ . Therefore among the elements  $(|\psi_j\rangle\langle\psi_j|, |\varphi_j\rangle\langle\varphi_j|)$  of  $\mathcal{M}_D^{\text{sa}} \times \mathcal{M}_D^{\text{sa}}$  we can find a nontrivial linear relation

$$\sum_{j \in J} c_j (|\psi_j\rangle\langle\psi_j|, |\varphi_j\rangle\langle\varphi_j|) = 0. \quad (38)$$

Define subsets  $K, L$  of  $J$  by  $K = \{k \in J : c_k > 0\}$  and  $L = \{l \in J : c_l < 0\}$ . We can then rewrite this as

$$\sum_{k \in K} c_k (|\psi_k\rangle\langle\psi_k|, |\varphi_k\rangle\langle\varphi_k|) = \sum_{l \in L} (-c_l) (|\psi_l\rangle\langle\psi_l|, |\varphi_l\rangle\langle\varphi_l|) \quad (39)$$

so that the coefficients  $c_k$  and  $-c_l$  are strictly positive. Without loss of generality, we may assume that

$$\sum_{k \in K} c_k d(|\psi_k\rangle, |\varphi_k\rangle)^p \geq \sum_{l \in L} (-c_l) d(|\psi_l\rangle, |\varphi_l\rangle)^p. \quad (40)$$

We will aim to replace a portion of the transport plan corresponding to the left-hand side, with a portion corresponding to the right-hand side.

Let  $m = \min_{k \in K} \left\{ \frac{q_k}{c_k} \right\}$ , and let  $k'$  be a minimiser. We can then form a new transport plan

$$Q' = \{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}_{j \notin K \cup L} \cup \{(q_k - mc_k, |\psi_k\rangle, |\varphi_k\rangle)\}_{k \in K} \cup \{(q_l - mc_l, |\psi_l\rangle, |\varphi_l\rangle)\}_{l \in L} \quad (41)$$

replacing  $m$  times the left hand side of (39) with  $m$  times the right hand side.  $k'$  attains the minimum in the definition of  $m$  so any multiple of  $(|\psi_{k'}\rangle, |\varphi_{k'}\rangle)$  is removed from the plan. The linear relation means that the resulting plan is still a transport plan between  $\rho$  and  $\sigma$ , and (40) means that the cost is not increased. Hence we can find a transport plan between  $\rho$  and  $\sigma$  with fewer elements, without increasing the transport cost.

We may then optimise the transport cost over all transport plans of size at most  $2D^2$ . This set is compact and the  $p^{\text{th}}$ -order cost (13) of a transport plan is a continuous function of the transport plan  $Q$  for  $d$  continuous, so the infimum is attained.  $\square$

The existence of an optimal transport plan will be particularly useful later when looking at examples, applications, and further properties.

Another key property of this  $W_p^d$  is continuity, which we can prove provided that  $d$  is continuous. This will be necessary for a coherent definition of a dual in Sec. IV A.

**Proposition 17.** *Suppose  $d$  is continuous on  $\mathbb{P}\mathcal{H}$  and let  $1 \leq p < \infty$ . Then  $W_p^d$  is uniformly continuous.*

*Proof.* The proof is quite technical and not particularly instructive, so has been placed in Appendix D1 for the convenience of the reader.  $\square$

For  $p = 1$  specifically, we furthermore have joint convexity.

**Proposition 18.**  *$W_1^d$  is jointly convex.*

*Proof.* Suppose  $\rho_1, \sigma_1, \rho_2$ , and  $\sigma_2$  are quantum states, and let  $r_1 + r_2 = 1, r_i \geq 0$ . Let  $Q_1 = \{(q_{1,j}, |\psi_{1,j}\rangle, |\varphi_{1,j}\rangle)\}_j$  be any transport plan between  $\rho_1$  and  $\sigma_1$ , and  $Q_2 = \{(q_{2,k}, |\psi_{2,k}\rangle, |\varphi_{2,k}\rangle)\}_k$  any transport plan between  $\rho_2$  and  $\sigma_2$ . Then  $Q = r_1 Q_1 \cup r_2 Q_2 := \{(r_1 q_{1,j}, |\psi_{1,j}\rangle, |\varphi_{1,j}\rangle)\}_j \cup \{(r_2 q_{2,k}, |\psi_{2,k}\rangle, |\varphi_{2,k}\rangle)\}_k$  is a transport plan between  $r_1 \rho_1 + r_2 \rho_2$  and  $r_1 \sigma_1 + r_2 \sigma_2$ .

Then we have

$$T_1^d(Q) = \sum_j r_1 q_{1,j} d(|\psi_{1,j}\rangle, |\varphi_{1,j}\rangle) + \sum_k r_2 q_{2,k} d(|\psi_{2,k}\rangle, |\varphi_{2,k}\rangle) = r_1 T_1^d(Q_1) + r_2 T_1^d(Q_2). \quad (42)$$

Taking the infimum over  $Q_1$  and  $Q_2$  shows that  $W_1^d(r_1 \rho_1 + r_2 \rho_2, r_1 \sigma_1 + r_2 \sigma_2) \leq r_1 W_1^d(\rho_1, \sigma_1) + r_2 W_1^d(\rho_2, \sigma_2)$ .  $\square$

## A. Dual picture

We can now take a look at the dual picture for the first-order transport distance, with some regularity conditions on the underlying metric  $d$  which allow the dual to be well-defined. As we will see later, this will then allow us to define a version of the Wasserstein distance for  $p = 1$  that satisfies the triangle inequality and inherits many of the properties of the original  $W_1^d$ .

**Definition 19.** *Let  $d$  be a metric on  $\mathbb{P}\mathcal{H}$ . Suppose  $d$  is continuous and that the 2-norm is Lipschitz with respect to  $d$ . We define the **dual constant of a self-adjoint operator  $O$**  as*

$$L_d(O) = \sup_{\rho \neq \sigma} \frac{\text{Tr}[O(\rho - \sigma)]}{W_1^d(\rho, \sigma)}. \quad (43)$$

We refer to this as the  $d$ -Lipschitz constant. Usually, in the classical case, the Lipschitz constant of a function with respect to a metric is defined by taking the supremum only with respect to point masses, not probability distributions. As we see below in Proposition 20, we can also take w.l.o.g. the supremum only with respect to pure states and only define it with mixed states for convenience.

**Proposition 20.** *Let  $d$  be a metric on  $\mathbb{P}\mathcal{H}$ . Suppose  $d$  is continuous and that the 2-norm is Lipschitz with respect to  $d$ . Then*

$$L_d(O) = \sup_{|\psi\rangle \neq |\varphi\rangle} \frac{\text{Tr}[O(|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|)]}{d(|\psi\rangle, |\varphi\rangle)}. \quad (44)$$

*Proof.* For any  $\rho$  and  $\sigma$ , let  $Q = \{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}$  be an optimal transport plan between them. Then

$$L_d(O) = \sup_{\rho \neq \sigma} \frac{\text{Tr}[O(\rho - \sigma)]}{W_1^d(\rho, \sigma)} \quad (45)$$

$$= \sup_{\rho \neq \sigma} \frac{\sum_j q_j \text{Tr}[O(|\psi_j\rangle\langle\psi_j| - |\varphi_j\rangle\langle\varphi_j|)]}{\sum_j q_j d(|\psi_j\rangle, |\varphi_j\rangle)} \quad (46)$$

$$\leq \sup_{\rho \neq \sigma} \max_j \frac{\text{Tr}[O(|\psi_j\rangle\langle\psi_j| - |\varphi_j\rangle\langle\varphi_j|)]}{d(|\psi_j\rangle, |\varphi_j\rangle)} \quad (47)$$

$$\leq \sup_{|\psi\rangle \neq |\varphi\rangle} \frac{\text{Tr}[O(|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|)]}{d(|\psi\rangle, |\varphi\rangle)} \quad (48)$$

$$= \sup_{|\psi\rangle \neq |\varphi\rangle} \frac{\text{Tr}[O(|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|)]}{W_1^d(|\psi\rangle\langle\psi|, |\varphi\rangle\langle\varphi|)} \leq L_d(O) \quad (49)$$

and so this is a chain of equalities.  $\square$

Importantly, this means that this  $L_d$  is a function of the metric  $d$  and is independent of our definition of  $W_p^d$ . It also means that our choice of  $p = 1$  in the definition is arbitrary: defining  $L_{d,p}(O) = \sup_{\rho \neq \sigma} \text{Tr}[O(\rho - \sigma)]/W_p^d(\rho, \sigma)$  gives the same quantity as  $L_d(O)$ . It is also important to note that under the regularity conditions already established on  $d$ , this quantity is a norm.

**Proposition 21.** *Let  $d$  be a continuous metric on  $\mathbb{P}\mathcal{H}$  such that the 2-norm is Lipschitz with respect to  $d$ . Then  $L_d(O)$  is a norm on the space of traceless self-adjoint operators.*

*Proof.* For finiteness, we use  $\text{Tr}[O(\rho - \sigma)] \leq 2 \|O\|_\infty \|\rho - \sigma\|_1$  together with Proposition 12.

To show nondegeneracy, suppose  $O$  is nonzero and let  $|\psi\rangle, |\varphi\rangle$  be eigenstates of  $O$  with positive and negative eigenvalues respectively, which must exist as  $O$  is traceless. Then  $\rho = |\psi\rangle\langle\psi|, \sigma = |\varphi\rangle\langle\varphi|$  gives  $\text{Tr}[O(\rho - \sigma)]/W_1^d(\rho, \sigma) > 0$ .

For the other norm properties, clearly  $L_d(\lambda O) = |\lambda|L_d(O)$ . And suppose we have Hermitian self-adjoint operators  $O_1$  and  $O_2$ . Let the supremum in  $L_d(O_1 + O_2)$  be achieved by  $\rho$  and  $\sigma$ , then

$$L_d(O_1 + O_2) = \text{Tr}[(O_1 + O_2)(\rho - \sigma)]/W_1^d(\rho, \sigma) = \text{Tr}[O_1(\rho - \sigma)]/W_1^d(\rho, \sigma) + \text{Tr}[O_2(\rho - \sigma)]/W_1^d(\rho, \sigma) \leq L_d(O_1) + L_d(O_2) \quad (50)$$

which proves the triangle inequality for  $L_d$ .  $\square$

We can then dualise one more time and consider the norm

$$\|\rho - \sigma\|_{DW_1^d} = \sup_{L_d(O) \leq 1} \text{Tr}[O(\rho - \sigma)]. \quad (51)$$

**Proposition 22.** *Let  $\|\cdot\|_{DW_1^d}$  be defined by  $\|X\|_{DW_1^d} = \sup_{L_d(O) \leq 1} \text{Tr}[OX]$  on the space of traceless Hermitian operators.*

*Then this is a norm, and on quantum states  $\rho, \sigma$  we have*

$$W_1^d(\rho, \sigma) \geq \|\rho - \sigma\|_{DW_1^d}. \quad (52)$$

*Proof.* For the norm, it is clear that when  $X = 0$  we have  $\|X\|_{DW_1^d}$  equal to zero. The fact that  $\|\lambda X\|_{DW_1^d} = |\lambda| \|X\|_{DW_1^d}$  is clear from the definition, and the triangle inequality holds as

$$\|X_1 + X_2\|_{DW_1^d} = \sup_{L_d(O) \leq 1} \text{Tr}[O(X_1 + X_2)] \leq \sup_{L_d(O_1) \leq 1} \text{Tr}[O_1 X_1] + \sup_{L_d(O_2) \leq 1} \text{Tr}[O_2 X_2] = \|X_1\|_{DW_1^d} + \|X_2\|_{DW_1^d}. \quad (53)$$

For nondegeneracy, take  $O$  to be the projector onto the positive part of  $X$  normalised to  $L_d(O) = 1$ , which gives  $\text{Tr}[OX] > 0$ .

On states  $\rho, \sigma$ , let  $O$  be any operator with  $L_d(O) \leq 1$ . Then

$$1 \geq L_d(O) = \sup_{\rho' \neq \sigma'} \frac{\text{Tr}[O(\rho' - \sigma')]}{W_1^d(\rho', \sigma')} \geq \frac{\text{Tr}[O(\rho - \sigma)]}{W_1^d(\rho, \sigma)} \quad (54)$$

and so  $\text{Tr}[O(\rho - \sigma)] \leq W_1^d(\rho, \sigma)$ . Taking the supremum over  $O$  gives  $\|\rho - \sigma\|_{DW_1^d} \leq W_1^d(\rho, \sigma)$ .  $\square$

The inequality  $W_1^d(\rho, \sigma) \geq \|\rho - \sigma\|_{DW_1^d}$  is important in our understanding of these quantities. It is as yet unclear whether or not equality holds in this equation, and establishing the conditions for equality is an important open problem, not least because this would allow us to recover the triangle inequality for  $W_1^d$ . There are some simple necessary conditions for equality in this equation, namely that  $W_1^d$  depends only on  $\rho - \sigma$ , and that it scales like a norm.

However, we can consider the case where there exists a metric  $\|\cdot\|_d$  such that  $d(|\psi\rangle, |\varphi\rangle) = \||\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|\|_d$ . Replacing  $\|\cdot\|_2$  with  $\|\cdot\|_d$  in the proof of Proposition 12, and using  $d(|\psi\rangle, |\varphi\rangle) = \||\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|\|_d$ , we get that  $W_1^d(\rho, \sigma) \geq \|\rho - \sigma\|_d$ . This allows us to recover even more properties of  $\|\cdot\|_{DW_1^d}$ :

**Proposition 23.** *Suppose that there exists norm  $\|\cdot\|_d$  such that  $d(|\psi\rangle, |\varphi\rangle) = \||\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|\|_d$ . Then:*

1.  $W_1^d(\rho, \sigma) \geq \|\rho - \sigma\|_{DW_1^d} \geq \|\rho - \sigma\|_d$ .
2. When  $\rho$  and  $\sigma$  are pure, this becomes an equality.
3. For all  $1 \leq q \leq \infty$ , we have  $W_q^d = W_q^{DW_1^d}$ .

*Proof.* As discussed above, we know that  $\|\rho - \sigma\|_d \leq W_1^d(\rho, \sigma)$ . Letting  $\|\cdot\|_D$  be the dual to  $\|\cdot\|_d$  on the space of traceless Hermitian operators, we have then that  $\|O\|_D \geq L_d(O)$ . Dualising once more, and noting that the double dual of a norm is the norm itself, we know for all  $X$  that  $\|X\|_d \leq \|X\|_{DW_1^d}$ . Combining this with Proposition 22 gives the chain

$$W_1^d(\rho, \sigma) \geq \|\rho - \sigma\|_{DW_1^d} \geq \|\rho - \sigma\|_d. \quad (55)$$

If  $\rho, \sigma$  are pure then by Proposition 11 we have  $W_1^d(\rho, \sigma) = \|\rho - \sigma\|_d$ , and so the whole chain (55) is an equality. It follows that for  $|\psi\rangle, |\varphi\rangle$ , we have

$$d(|\psi\rangle, |\varphi\rangle) = \||\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|\|_{DW_1^d}. \quad (56)$$

This means in turn that for all  $1 \leq q \leq \infty$ , we have  $W_q^d = W_q^{DW_1^d}$ .  $\square$

We present this norm here, not as a replacement for  $W_p^d$ , but because the two complement each other nicely. This method of defining  $\|\cdot\|_{DW_1^d}$  via a supremum of a trace of the difference of two states over Lipschitz observables mirrors exactly the Kantorovich-Rubinstein theorem from classical optimal transport [Vil03, p. 34]. In taking the double dual, we gain an easy proof of the triangle inequality, albeit at the expense of flexibility of order  $p$  and of natural interpretation in terms of transport plans and couplings. We have seen here that  $W_p^d$  and  $\|\cdot\|_{DW_1^d}$  are closely related, particularly when  $d$  is induced by a norm. We will see later in Sec. VA and Sec. VB that in many cases  $\|\cdot\|_{DW_1^d}$  essentially recovers the original norm  $\|\cdot\|_d$ .

## V. SPECIAL INSTANCES

### A. $W_1^H$ distance on $n$ -qudit systems

[PMTL21] introduced a quantum Wasserstein distance of order 1 which generalises the Hamming distance on the discrete hypercube. This is defined on Hilbert space  $\mathcal{H} = (\mathbb{C}^d)^{\otimes n}$ . The distance defined is normed, and we notate it here by  $\|\rho - \sigma\|_{W_1^H}$ .

$\|\cdot\|_{W_1^H}$  has the interesting property that it recovers the classical first-order Wasserstein distance  $\mathcal{W}_1^H$  on the Hamming cube, for states that are diagonal in the computational basis. That is, for  $r$  and  $s$  probability distributions on  $\{0, 1, \dots, d-1\}^n$ , and states  $\rho = \sum_{x \in \{0, 1, \dots, d-1\}^n} r(x)|x\rangle\langle x|$  and  $\sigma = \sum_{y \in \{0, 1, \dots, d-1\}^n} |y\rangle\langle y|$  we have

$$\|\rho - \sigma\|_{W_1^H} = \mathcal{W}_1^H(r, s). \quad (57)$$

Furthermore, its formulation mirrors the Kantorovich-Rubinstein theorem with the definition of the quantum Lipschitz constant [PMTL21, Definition 8]:

$$\|O\|_L = \max\{\text{Tr}[O(\rho - \sigma)] : \|\rho - \sigma\|_{W_1^H} \leq 1\}. \quad (58)$$

It then induces a metric  $d_H$  on  $\mathbb{P}\mathcal{H}$ , given by  $d(|\psi\rangle, |\varphi\rangle) = \|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|\|_{W_1^H}$ , from which we can define a  $p^{\text{th}}$  order Wasserstein distance  $W_p^H$  as above. For the special case  $p = 1$ , we will write  $W_{p=1}^H$  to avoid confusion.

We might expect that property in equation (57) extends to the  $W_p^H$  distance: that is, that for classical states  $\rho$  and  $\sigma$  defined by  $r$  and  $s$  as above, that

$$W_p^H(\rho, \sigma) = \mathcal{W}_p^H(r, s). \quad (59)$$

However, in this case, we recover some interesting differences between the classical and quantum definitions of the  $p$ -Wasserstein distances, by taking ‘quantum shortcuts’ in our transport plans.

For  $p = 1$ , equality occurs in (59): an optimal classical coupling  $\gamma$  between  $r$  and  $s$  gives us the transport plan  $\{(\gamma(x, y), |x\rangle, |y\rangle)\}_{x, y \in \{0, 1, \dots, d-1\}^n}$  which has transport cost  $\mathcal{W}_1^H(r, s)$ , and we know that  $W_{p=1}^H(\rho, \sigma) \geq \|\rho - \sigma\|_{W_1^H} = \mathcal{W}_1^H(r, s)$  from Proposition 12 above and Proposition 6 of [PMTL21].

However, for  $p > 1$ , we can find quantum ‘shortcuts’ between classical states. Indeed, consider the case  $n = d = 2$  and the states  $\rho = |00\rangle\langle 00|$ ,  $\sigma = \frac{\mathbb{I}^{\otimes 2}}{4}$ . Classically, the distributions  $\delta_{00}$  and the uniform distribution have a  $\mathcal{W}_\infty^H$  distance of 2. However, consider the quantum transport plan

$$\left\{ \left( \frac{1}{4}, |00\rangle, |\varphi^{\pm\pm}\rangle \right) \right\} \quad (60)$$

for the standard 2-qubit Bell states

$$\begin{aligned} |\varphi^{++}\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle) & |\varphi^{+-}\rangle &= \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle) \\ |\varphi^{-+}\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) & |\varphi^{--}\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \end{aligned} \quad (61)$$

This corresponds to the separable coupling

$$\tau = \sum_{\pm\pm} \frac{1}{4} |00\rangle\langle 00| \otimes |\varphi^{\pm\pm}\rangle\langle\varphi^{\pm\pm}| \quad (62)$$

of  $\rho$  and  $\sigma$ . Proposition 2 of [PMTL21] shows that both

$$\| |00\rangle\langle 00| - |\varphi^{+\pm}\rangle\langle\varphi^{+\pm}| \|_{W_1^H} \leq \sqrt{2} \quad \text{and} \quad \| |00\rangle\langle 00| - |\varphi^{-\pm}\rangle\langle\varphi^{-\pm}| \|_{W_1^H} \leq \frac{\sqrt{5} + 3}{4}. \quad (63)$$

This in turn gives us  $W_\infty^H(\rho, \sigma) \leq \max\left\{\sqrt{2}, \frac{\sqrt{5}+3}{4}\right\} = \sqrt{2}$ .

However, from Proposition 14 we see that  $W_p^H$  does inherit the invariance properties of  $\|\cdot\|_{W_1^H}$ , namely invariance under local unitaries and qubit swaps.

We also can relate the double-dual norm  $\|\cdot\|_{DW_1^H}$  to the norm  $\|\cdot\|_{W_1^H}$  as follows.

**Proposition 24.** *Let  $\rho, \sigma$  be states on  $\mathcal{H} = (\mathbb{C}^d)^{\otimes n}$ . Then*

$$2 \|\rho - \sigma\|_{W_1^H} \geq \|\rho - \sigma\|_{DW_1^H} \geq \|\rho - \sigma\|_{W_1^H}. \quad (64)$$

*Proof.* The lower bound comes from equation (55). For the upper bound, we refer to the dual  $\|O\|_L$ , and show that  $\|O\|_L \leq 2L_d(O)$ . Taking the dual of this equation will give the upper bound required.

We have from [PMTL21, Proposition 15], that

$$2 \max_{1 \leq i \leq n} \|O - \text{Tr}_i O \otimes \mathbb{I}_i\|_\infty \geq \|O\|_L. \quad (65)$$

So we will show that  $L_d(O) \geq \max_{1 \leq i \leq n} \|O - \text{Tr}_i O \otimes \mathbb{I}_i\|_\infty$ .

Fix  $i$ , and let  $|\psi\rangle$  be an eigenvector of  $O - \text{Tr}_i O \otimes \mathbb{I}_i$  with an eigenvalue which is maximal in absolute value, assuming without loss of generality that this is positive. Let  $\mu_{\text{Haar}}$  be the Haar measure on the unitary group  $\mathcal{U}(d)$  acting on the  $i^{\text{th}}$  qudit. Writing  $U_i$  for a unitary on the  $i^{\text{th}}$  qubit,  $\mathbb{I}_i$  for the identity on the  $i^{\text{th}}$  qubit, and  $\mathbb{I}_i$  for the identity acting on all except the  $i^{\text{th}}$  qubit, we note that

$$\mathbb{E}_{U_i \sim \mu_{\text{Haar}}} \text{Tr}[(O - \text{Tr}_i O \otimes \mathbb{I}_i) U_i \otimes \mathbb{I}_i |\psi\rangle\langle\psi| U_i^\dagger \otimes \mathbb{I}_i] = \text{Tr}[(O - \text{Tr}_i O \otimes \mathbb{I}_i) \text{Tr}_i |\psi\rangle\langle\psi| \otimes \mathbb{I}_i / d] = 0. \quad (66)$$

Therefore taking any  $U_i \in \mathcal{U}(d)$  such that  $U_i |\psi\rangle$  has  $\text{Tr}[(O - \text{Tr}_i O \otimes \mathbb{I}_i) U_i \otimes \mathbb{I}_i |\psi\rangle\langle\psi| U_i^\dagger \otimes \mathbb{I}_i] < 0$ , let this  $U_i \otimes \mathbb{I}_i |\psi\rangle$  be  $|\varphi\rangle$ . Note that  $\text{Tr}_i[|\psi\rangle\langle\psi|] = \text{Tr}_i[|\varphi\rangle\langle\varphi|]$ . This gives

$$\frac{\text{Tr}[O(|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|)]}{\| |\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi| \|_{W_1^H}} \geq \frac{\text{Tr}[O(|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|)]}{1} \quad (67)$$

$$= \text{Tr}[O(|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|)] + \text{Tr}[\text{Tr}_i O (\text{Tr}_i |\psi\rangle\langle\psi| - \text{Tr}_i |\varphi\rangle\langle\varphi|)] \quad (68)$$

$$= \text{Tr}[(O - \text{Tr}_i O \otimes \mathbb{I}_i)(|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|)] \quad (69)$$

$$\geq \|O - \text{Tr}_i O \otimes \mathbb{I}_i\|_\infty \quad (70)$$

which concludes the proof.  $\square$

## B. Trace distance

In this section, we consider the case where  $d$  is induced by the trace distance (that is, half the trace norm). For pure states  $|\psi\rangle, |\varphi\rangle$ , we have

$$d(|\psi\rangle, |\varphi\rangle) = \frac{1}{2} \| |\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi| \|_1 = \sqrt{1 - |\langle\psi|\varphi\rangle|^2}. \quad (71)$$

The trace distance, when applied to pure states on a  $D$ -dimensional space, is a direct analogue of the discrete metric on a space with  $D$  elements. This means that it is the simplest case to consider in terms of optimal transport. The trace distance on mixed states can also be considered as a quantum generalisation of the total variation distance  $d_{TV}(\mu, \nu) = \sum_{i=1}^D |\mu(i) - \nu(i)|$ , which is the classical  $W_1$  distance on this discrete space.

We write the  $p^{\text{th}}$ -order transport cost associated with this distance as  $T_p^1$  and the associated quantum Wasserstein distance as  $W_p^1$ . We note from Proposition 2 of [PT21] that this agrees with  $W_p^H$  in the case of a single qudit. From this we inherit all the properties of  $W_p^H$ , notably Proposition 24 which gives us  $\|\rho - \sigma\|_1 \geq \|\rho - \sigma\|_{DW_1^1} \geq \frac{1}{2} \|\rho - \sigma\|_1$ . However, we can go one step further.

**Proposition 25.** *Let  $\rho, \sigma$  be states on  $\mathbb{C}^d$ . Then*

$$\|\rho - \sigma\|_{DW_1^1} = \frac{1}{2} \|\rho - \sigma\|_1. \quad (72)$$

*Proof.* That  $\|\rho - \sigma\|_{DW_1^1} \geq \frac{1}{2} \|\rho - \sigma\|_1$  is a direct consequence of Proposition 12. For the other direction, we once again consider the dual. The double dual of the 1-norm is itself, and so to show inequality in the other direction we need only show for any traceless Hermitian operator  $O$  that

$$\sup_{\rho \neq \sigma} \frac{\text{Tr}[O(\rho - \sigma)]}{\frac{1}{2} \|\rho - \sigma\|_1} \leq L_1(O) \quad (73)$$

as taking the dual of this equation would give the inequality in the other direction.

For any  $\rho \neq \sigma$ , let  $\rho - \sigma = \rho' - \sigma'$  for  $\rho', \sigma'$  positive semidefinite operators with  $\rho' \perp \sigma'$ . Then write  $\rho' = \sum_j \mu_j |\psi_j\rangle\langle\psi_j|$  and  $\sigma' = \sum_k \nu_k |\varphi_k\rangle\langle\varphi_k|$  in spectral decompositions. Let  $\gamma$  be a classical coupling of the measures  $\mu$  and  $\nu$ . It then follows that

$$\frac{1}{2} \|\rho - \sigma\|_1 = \frac{1}{2} \sum_{j,k} \gamma_{j,k} \| |\psi_j\rangle\langle\psi_j| - |\varphi_k\rangle\langle\varphi_k| \|_1 \quad (74)$$

and so

$$\frac{\text{Tr}[O(\rho - \sigma)]}{\frac{1}{2} \|\rho - \sigma\|_1} = \frac{\sum_{j,k} \gamma_{j,k} \text{Tr}[O(|\psi_j\rangle\langle\psi_j| - |\varphi_k\rangle\langle\varphi_k|)]}{\sum_{j,k} \gamma_{j,k} \| |\psi_j\rangle\langle\psi_j| - |\varphi_k\rangle\langle\varphi_k| \|_1} \leq \sup_{|\psi\rangle \neq |\varphi\rangle} \frac{\text{Tr}[O(|\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi|)]}{\| |\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi| \|_1} = L_1(O) \quad (75)$$

which concludes the proof.  $\square$



### C. Complexity geometry

A distance  $d(I, U)$  giving lower bounds for the complexity of synthesising a unitary  $U \in \mathcal{SU}(2^n)$  from a universal one- and two-qubit gate set was defined in [Nie06] and refined in [DN08, NDGD06]. This distance  $d$  on  $\mathcal{SU}(2^n)$  is a geodesic distance of a Riemannian manifold, where the Riemannian metric is chosen such that local travel is fast in directions corresponding to multiplication by low-weight unitaries, and slow in directions corresponding to multiplication by high-weight unitaries.

This idea of expressing quantum gate complexity in terms of Riemannian geometry has seen renewed interest in recent years, from applications in black hole thermodynamics [BRS<sup>+</sup>16, Hel23] to rigid bodies [BS19] and the complexity of typical unitaries [Bro23]. However, this metric is originally defined as a distance between unitaries, with the complexity of unitary expressed in terms of its distance from the identity. This extends naturally to distances between pure states as the lowest complexity of a unitary which transforms one into the other. Our optimal transport formulation allows for a natural extension of this metric to mixed states, in a way that can be considered as quantifying the lowest possible complexity of transforming one mixed state into another. A related approach in [Rua21] extends a variation of this complexity geometry metric, one in which multiplication by a unitary is independent of weight, to mixed states using purification methods described in [AHS19].

Formally, [Nie06] defines a right-invariant Riemannian metric  $g$  on  $\mathcal{SU}(2^n)$  given by the following inner product on  $T_I \mathcal{SU}(2^n)$ . A vector  $X$  in the tangent space  $T_U \mathcal{SU}(2^n)$  to  $\mathcal{SU}(2^n)$  at  $U$  is identified with its Hamiltonian representation  $H$ , given by  $X = \left[ \frac{d}{dt} e^{-iHt} U \right]_{t=0}$ .  $H$  can be decomposed as  $H_P + H_Q$ , where  $H_P$  is a linear combination of Pauli matrices of weight at most 2, and  $H_Q$  is a linear combination of Pauli matrices of weight at least 3. Defining operations  $\mathcal{P}$  and  $\mathcal{Q}$  by  $\mathcal{P}(H) = H_P$  and  $\mathcal{Q}(H) = H_Q$ , the inner product on  $T_U \mathcal{SU}(2^n)$  is then defined by

$$\langle H, J \rangle = \frac{\text{Tr}(H\mathcal{P}(J)) + q\text{Tr}(H\mathcal{Q}(J))}{2^n} \quad (76)$$

where  $q > 4^n$  is a penalty parameter. The length  $\sqrt{\langle H, H \rangle}$  will then be of order 1 for 2-local Hamiltonians, and of order  $q$  otherwise.  $q > 4^n$  is chosen such that for any geodesic, the associated Hamiltonian path has an approximately low-weight decomposition.

The length of a curve  $U(t)$  defined by evolution  $\dot{U}(t) = -iH(t)U(t)$  is then defined as standard by

$$\int \sqrt{\langle H(t), H(t) \rangle} dt \quad (77)$$

and the distance  $d(I, U)$  is simply the geodesic distance on this Riemannian manifold.

The main purpose of  $d$  is to find a geometric interpretation of gate complexity, and [DN08, Equation 3] gives bounds for  $d$  in terms of gate complexity. Let  $G(U)$  be the exact gate complexity of  $U$ , i.e. the minimal number of one- and two-qubit gates required to synthesise  $U$  exactly. For  $\epsilon \geq 0$ , let  $G(U, \epsilon)$  be the minimal number of one- and two-qubit gates required to synthesise a gate  $V$  such that  $\|U - V\|_\infty \leq \epsilon$ , also known as the  $\epsilon$ -approximate gate complexity. We then have bounds

$$\frac{\kappa G(U, \epsilon)^{1/3} \epsilon^{2/3}}{n^2} \leq d(I, U) \leq G(U) \quad (78)$$

for some constant  $\kappa > 0$ .

With these unitaries acting on the  $n$ -qubit space  $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$ , we can define a metric  $d_C$  on  $\mathbb{P}\mathcal{H}$  by

$$d_C(|\psi\rangle, |\varphi\rangle) = \min \{d(I, U) : U \in \mathcal{SU}(2^n), U|\psi\rangle = |\varphi\rangle\}. \quad (79)$$

The metric properties of  $d_C$  come directly from the metric properties and right-invariance of  $d$ . Operationally, this gives a lower bound for the minimum circuit complexity required to synthesise  $|\varphi\rangle$  from  $|\psi\rangle$ . Indeed,

$$\frac{\kappa(\min\{G(U, \epsilon) : U|\psi\rangle = |\varphi\rangle\})^{1/3} \epsilon^{2/3}}{n^2} \leq d_C(|\psi\rangle, |\varphi\rangle) \leq \min\{G(U) : U|\psi\rangle = |\varphi\rangle\}. \quad (80)$$

In order to say anything useful about the quantum Wasserstein distance induced by this metric  $d_C$ , we must demonstrate some basic continuity properties. Continuity of  $d_C$  is inherent from the fact that  $d$  is a geodesic distance on a Riemannian manifold and Hölder continuity of the 2-norm with respect to  $d_C$  comes from the following proposition.

**Proposition 26.** *Let  $U \in SU(2^n)$ . Then*

$$d(I, U) \geq 2^{-n/2} \|U - I\|_2. \quad (81)$$

*Proof.* Suppose  $U(t)$  is a geodesic curve in  $SU(2^n)$  with  $U(t) = I$  and  $U(T) = U$ , generated by Hamiltonian  $H(t)$  satisfying  $\dot{U}(t) = -iH(t)U(t)$ . Then for any  $N$ , we have

$$\|U - I\|_2 \leq \sum_{j=0}^{N-1} \|U((j+1)T/N) - U(jT/N)\|_2 \quad (82)$$

$$\leq \sum_{j=0}^{N-1} \|i(T/N)H(jT/N)U(jT/N) + o(T/N)\|_2 \quad (83)$$

$$\rightarrow \int_0^T \|H(t)\|_2 dt \quad \text{as } N \rightarrow \infty \quad (84)$$

$$\leq 2^{n/2} \int_0^T \sqrt{\langle H(t), H(t) \rangle} dt \quad (85)$$

using the inequality  $2^{-n/2} \|H\|_2 \leq \sqrt{\langle H, H \rangle}$  in the last line. The required regularity to bound  $o(T/N)$  uniformly comes from the smoothness of the metric.

Taking the infimum over such curves gives  $d(I, U) \geq 2^{-n/2} \|U - I\|_2$ .  $\square$

**Corollary 27.** *Let  $|\psi\rangle, |\varphi\rangle \in \mathbb{P}\mathcal{H}$ . Then*

$$2^{(n+1)/2} d_C(|\psi\rangle, |\varphi\rangle) \geq \| |\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi| \|_2. \quad (86)$$

*Proof.* Let  $U \in SU(2^n)$  have  $U|\psi\rangle = |\varphi\rangle$ . Then

$$\|U - I\|_2^2 = \text{Tr}[(U - I)^\dagger(U - I)] \quad (87)$$

$$\geq \langle\psi|(U - I)^\dagger(U - I)|\psi\rangle \quad (88)$$

$$\geq 2(1 - |\langle\psi|\varphi\rangle|). \quad (89)$$

Using the formula  $\| |\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi| \|_2^2 = 2(1 - |\langle\psi|\varphi\rangle|)^2$ , we get

$$\|U - I\|_2^2 \geq 2 \left( 1 - \sqrt{1 - \frac{1}{2} \| |\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi| \|_2^2} \right) \quad (90)$$

$$\geq \frac{1}{2} \| |\psi\rangle\langle\psi| - |\varphi\rangle\langle\varphi| \|_2^2. \quad (91)$$

Combining this with Proposition 26 gives the result.  $\square$

It follows from Proposition 12 that all  $W_p^C$  defined from this  $d_C$  are nondegenerate. This gives a natural extension of the ideas of state complexity to mixed states, to which we can apply results such as Proposition 33 on cq sources.

Looking at  $\rho$  and  $\sigma$  in their eigenbases, we can give a concrete interpretation of these values. Indeed, let

$$\rho = \sum_{b \in \{0,1\}^n} r_b |\psi_b\rangle\langle\psi_b| \quad \sigma = \sum_{c \in \{0,1\}^n} s_c |\varphi_c\rangle\langle\varphi_c| \quad (92)$$

for  $r$  and  $s$  some classical probability distributions on  $\{0,1\}^n$ . Letting  $U$  be any unitary such that all  $U|\psi_b\rangle = |b\rangle$ ,  $V$  any unitary such that all  $V|\varphi_c\rangle = |c\rangle$ , and  $q$  be an optimal  $p^{\text{th}}$ -order classical coupling of the distributions  $r$  and  $s$ , we can consider transport plan

$$Q = \{(q_{bc}, |\psi_b\rangle, |\varphi_c\rangle)\}_{b,c \in \{0,1\}^n} \quad (93)$$

which has a first-order transport cost of at most  $C(U) + C(V) + \mathcal{W}_1^H(r, s)$ . This allows us to conclude that

$$W_1^C(\rho, \sigma) \leq C(U) + C(V) + \mathcal{W}_1^H(r, s). \quad (94)$$

This splits the quantum transport distance arising from complexity geometry into two parts: the classical transport cost between the states, and their quantum complexity as a whole.

## VI. APPLICATIONS

### A. Results for random quantum states

To understand these quantities in general, it is useful to look at how they behave on random quantum states. We will look at both the versions stemming from  $\|\cdot\|_{W_1^d}$  and from complexity geometry.

We look at a few regimes in the definition of ‘random’ states. For random pure states, we generate  $|\psi\rangle$  according to the uniform measure on the unit sphere in  $\mathcal{H}$ , and take  $\rho = |\psi\rangle\langle\psi|$ . For mixed states, we adjoin an auxiliary system  $\mathcal{A}$  of dimension  $s$ , generate a random pure state  $|\psi\rangle$  on  $\mathcal{H} \otimes \mathcal{A}$ , then take  $\rho = \text{Tr}_{\mathcal{A}}|\psi\rangle\langle\psi|$ . The distribution of  $\rho$  depends entirely on the values of  $s$  and  $\dim\mathcal{H}$  chosen.

Note that for the two versions studied, the underlying space  $\mathcal{H}$  is a qudit space  $\mathcal{H} = (\mathbb{C}^d)^{\otimes n}$ . It is convenient, in this case, to write  $s = d^m$ , as this allows us to consider the qudit ratio  $c = \frac{m}{n}$  between the auxiliary and base systems. Note that while  $s$  is always an integer,  $m$  need not be, i.e. we will also consider auxiliary dimensions that are not a power of  $d$ . We can then consider the regime  $c < 1$  as ‘low rank’, and regime  $c > 1$  as ‘high rank’.

For mixed states in the high-rank regime, we see exponential decay in the expected  $W_1^d$  distance between two i.i.d. states, no matter the underlying metric  $d$ . This is summarised in the following proposition. Note that while it is phrased for qudit systems, it applies for any  $\mathcal{H}, \mathcal{A}$  where  $c = \frac{\log \dim \mathcal{A}}{\log \dim \mathcal{H}}$  and  $d^n = \dim \mathcal{H}$ . We write  $\text{diam}_d(\mathbb{P}\mathcal{H})$  for the diameter of  $\mathbb{P}\mathcal{H}$  under metric  $d$ .

**Proposition 28.** *Let  $\mathcal{H} = (\mathbb{C}^d)^{\otimes n}$  with i.i.d. random mixed states  $\rho, \sigma$  generated by a auxiliary system of  $\mathcal{A}$  of dimension  $s = d^m$ . Let  $c = \frac{m}{n}$ , and suppose  $c > 1$ . Then for any  $\beta > 0$ , we have*

$$\mathbb{P} \left[ W_1^d(\rho, \sigma) \geq \beta d^{-(c-3)n/2} \text{diam}(\mathbb{P}\mathcal{H}) \right] \leq \frac{1}{\beta^2}. \quad (95)$$

*Proof.* For random  $\rho, \sigma$  generated from large auxiliary systems, we generally expect both to be close to maximally mixed. And so letting the minimum eigenvalue among  $\rho$  and  $\sigma$  be  $\frac{1}{d^n} - \delta$ , we can split up  $\rho$  into parts  $\rho - (\frac{1}{d^n} - \delta) \mathbb{I}$  and  $(\frac{1}{d^n} - \delta) \mathbb{I}$ , both of which are positive semidefinite. We can do the same for  $\sigma$ . We can then transport  $(\frac{1}{d^n} - \delta) \mathbb{I}$  onto  $(\frac{1}{d^n} - \delta) \mathbb{I}$  at zero cost, and transport  $\rho - (\frac{1}{d^n} - \delta) \mathbb{I}$  onto  $\sigma - (\frac{1}{d^n} - \delta) \mathbb{I}$  via any partial transport plan, at a maximum cost of  $\text{Tr} \left[ \rho - (\frac{1}{d^n} - \delta) \mathbb{I} \right] \text{diam}_d(\mathbb{P}\mathcal{H}) = \delta d^n \text{diam}_d(\mathbb{P}\mathcal{H})$ . We will show that this is most likely very small.

Focusing on  $\rho$ , we know from [SR95] that

$$\mathbb{E}[S(\rho)] \geq n \log d - \frac{1}{2} d^{-(c-1)n}. \quad (96)$$

Knowing also that  $S(\rho) \leq n \log d$ , and using the top-down Markov inequality, we get that for any  $\alpha > 0$  we have

$$\mathbb{P} \left[ S(\rho) \geq n \log d - \frac{\alpha}{2} d^{-(c-1)n} \right] \geq 1 - \frac{1}{\alpha}. \quad (97)$$

Using then that  $D(\rho || \frac{I}{d^n}) = n \log d - S(\rho)$ , and the quantum Pinsker’s inequality, we have

$$\mathbb{P} \left[ \left\| \rho - \frac{I}{d^n} \right\|_1 \leq \sqrt{\frac{\alpha}{2}} d^{-(c-1)n/2} \right] \geq 1 - \frac{1}{\alpha} \quad (98)$$

and so

$$\mathbb{P} \left[ \left\| \rho - \frac{I}{d^n} \right\|_{\infty} \leq \sqrt{\frac{\alpha}{2}} d^{-(c-1)n/2} \right] \geq 1 - \frac{1}{\alpha}. \quad (99)$$

Reintroducing  $\sigma$ , we then get that

$$\mathbb{P} \left[ \max \left\{ \left\| \rho - \frac{I}{d^n} \right\|_{\infty}, \left\| \sigma - \frac{I}{d^n} \right\|_{\infty} \right\} \leq \sqrt{\frac{\alpha}{2}} d^{-(c-1)n/2} \right] \geq \left( 1 - \frac{1}{\alpha} \right)^2 \geq 1 - \frac{2}{\alpha}. \quad (100)$$

Note that for any  $\rho, \sigma$  with  $\max \left\{ \left\| \rho - \frac{I}{d^n} \right\|_{\infty}, \left\| \sigma - \frac{I}{d^n} \right\|_{\infty} \right\} \leq \sqrt{\frac{\alpha}{2}} d^{-(c-1)n/2}$ , we can take  $\delta = \sqrt{\frac{\alpha}{2}} d^{-(c-1)n/2}$ . Then setting  $\beta = \sqrt{\alpha/2}$ , and applying the transport plan described above, we have

$$\mathbb{P} \left[ W_1^d(\rho, \sigma) \geq \sqrt{\frac{\alpha}{2}} d^{-(c-1)n/2} \cdot d^n \text{diam}_d(\mathbb{P}\mathcal{H}) \right] \leq \frac{2}{\alpha} \quad (101)$$

and so

$$\mathbb{P} \left[ W_1^d(\rho, \sigma) \geq \beta d^{-(c-3)n/2} \text{diam}_d(\mathbb{P}\mathcal{H}) \right] \leq \frac{1}{\beta^2}. \quad (102)$$

□

This result can be easily applied to the two underlying distances mentioned above. For qudit ratios  $c > 3 + \frac{2}{n} \log_d \text{diam}_d(\mathbb{P}\mathcal{H})$  we can define  $\beta$  by, for any  $\lambda \in (0, 1)$ , value

$$\log_d \beta = \lambda \left( c - 3 - \frac{2}{n} \log_d \text{diam}_d(\mathbb{P}\mathcal{H}) \right) \frac{n}{2} \quad (103)$$

to show that the probability of an exponentially small deviation falls exponentially as the number  $n$  of qudits increases.

For the  $W_1^H$  case, we know  $\text{diam}_d(\mathbb{P}\mathcal{H}) = n$ , and so this exponential decay applies for qubit ratio  $c > 3$  and large enough  $n$ . Applying this to the expectation gives, taking  $\lambda = 1/3$  for an optimal decay rate,

$$\mathbb{E}_{\rho, \sigma} [W_1^H(\rho, \sigma)] \leq \left( 1 - \frac{1}{\beta^2} \right) \beta d^{-(c-3)n/2} \text{diam}_d(\mathbb{P}\mathcal{H}) + \frac{1}{\beta^2} \text{diam}_d(\mathbb{P}\mathcal{H}) \quad (104)$$

$$\leq n^{1-\lambda} \exp_d \left( -\frac{1}{2}(1-\lambda)(c-3)n \right) + \exp_d n^{1+2\lambda} (\lambda(c-3)n) \quad (105)$$

$$= \exp_d \left( -\frac{1}{3}(c-3)n + \frac{2}{3} \log_d n \right) + \exp_d \left( -\frac{1}{3}(c-3)n + \frac{5}{3} \log_d n \right) \quad (106)$$

$$= \left( n^{2/3} + n^{5/3} \right) \exp_d \left( -\frac{1}{3}(c-3)n \right) \quad (107)$$

For the  $W_1^C$  case, any  $n$ -qudit gate can be synthesised in at most  $2^n(2^n - 1)$  one- and two-qubit gates [NC10], and so the metric space  $\mathbb{P}\mathcal{H}$  has diameter at most  $2^{2n}$ . It then follows that for any qudit ratio  $c > 7$ , the probability of an exponentially large deviation becomes exponentially small.

Applying equation (95) to the expectation gives, taking  $\lambda = \frac{c-3}{3(c-7)}$  for an optimal decay rate,

$$\mathbb{E}_{\rho, \sigma} [W_1^C(\rho, \sigma)] \leq \left( 1 - \frac{1}{\beta^2} \right) \beta 2^{-(c-3)n/2} \text{diam}_d(\mathbb{P}\mathcal{H}) + \frac{1}{\beta^2} \text{diam}_d(\mathbb{P}\mathcal{H}) \quad (108)$$

$$\leq 2^{-(1-\lambda)(c-3)n/2} 2^{(1-\lambda)2n} + 2^{-\lambda(c-3)n} 2^{(1+2\lambda)2n} \quad (109)$$

$$= 2^{-(1-\lambda)(c-7)n/2} + 2^{-(\lambda(c-7)-2)n} \quad (110)$$

$$= 2 \cdot 2^{(c-9)n/3} \quad (111)$$

giving exponential decay in expectation for qubit ratios  $c > 9$ .

For the low-rank setting, we look first at the  $W_1^H$  distance. There are two lines of intuition here. The first is that  $W_1^H$  generalises the Hamming distance, and the Hamming distance quantifies the local distinguishability of  $d$ -nary strings. If this property propagated to the quantum setting, we'd expect  $W_1^H$  to be small on average as random pure states are generally locally indistinguishable. The second is that the average Hamming distance between two  $d$ -nary strings of length  $n$  is  $n(1 - 1/d)$ , and so we might also expect the average  $W_1^H$  distance between random pure strings to grow linearly with the number of qudits.

Let  $\mathcal{H} = (\mathbb{C}^d)^{\otimes n}$  and let  $m = \log_d s$ , noting again that, while  $s$  is an integer,  $m$  need not be. In the case  $m < n$ , we can apply Theorem 9.1 of [PT23] to lower bound the expected distance between two low-rank random mixed states. This result was noted independently in [PKP23].

**Proposition 29.** *Let  $\rho, \sigma$  be two i.i.d. random mixed states on  $\mathcal{H} = (\mathbb{C}^d)^{\otimes n}$  generated using an auxiliary system of dimension  $s = d^m$  for  $m < n$ . Write  $c = \frac{m}{n}$ . Then*

$$\mathbb{E}_{\rho, \sigma} [W_{p=1}^H(\rho, \sigma)] \geq \lambda_c n \quad (112)$$

where  $\lambda_c$  satisfies  $(1 - c) \log d = h_2(\lambda) + \lambda \log(d^2 - 1)$  for  $h_2$  the binary entropy.

*Proof.* First note from Proposition 12 that  $W_{p=1}^H(\rho, \sigma) \geq \|\rho - \sigma\|_{W_1^H}$ , and so we prove that  $\mathbb{E}_{\rho, \sigma} \left[ \|\rho - \sigma\|_{W_1^H} \right] \geq \lambda n$ .

Fix  $\rho$ , and note that averaging over  $\sigma$  and using convexity of the norm we have

$$\mathbb{E}_\sigma \left[ \|\rho - \sigma\|_{W_1^H} \right] \geq \|\rho - \mathbb{E}_\sigma \sigma\|_{W_1^H} \quad (113)$$

$$= \left\| \rho - \frac{\mathbb{I}_d^{\otimes n}}{d^n} \right\|_{W_1^H}. \quad (114)$$

Applying Theorem 9.1 of [PT23] then gives, for  $S$  the von Neumann entropy of a state,

$$(1-c) \log d \leq \frac{1}{n} \left| S(\rho) - S\left(\frac{\mathbb{I}_d^{\otimes n}}{d^n}\right) \right| \leq h_2 \left( \frac{\|\rho - \mathbb{I}_d^{\otimes n}/d^n\|_{W_1^H}}{n} \right) + \frac{\|\rho - \mathbb{I}_d^{\otimes n}/d^n\|_{W_1^H}}{n} \log(d^2 - 1). \quad (115)$$

Noting then that the function  $g(t) = h_2(t) + t \log(d^2 - 1)$  takes the value  $(1-c) \log d$  at exactly one value  $\lambda \in [0, 1]$ , and that for  $t < \lambda$  we have  $g(t) < g(\lambda)$  and for  $t > \lambda$  we have  $g(t) > g(\lambda)$ , we conclude that  $\|\rho - \mathbb{I}_d^{\otimes n}/d^n\|_{W_1^H} > \lambda n$ . Averaging over  $\rho$  gives the result.  $\square$

For  $\rho, \sigma$  random pure states, we simply take the case  $m = 0$ . In general, this shows that the expected  $W_{p=1}^H$  distance between two random states generated using small auxiliary systems grows linearly with the number  $n$  of qubits.

Turning our attention to the  $W_1^C$  distance generated from complexity geometry on  $\mathbb{P}((\mathbb{C}^2)^{\otimes n})$ , we see a similar picture for pure states. As noted earlier, for the approximate gate complexity  $G(U, \epsilon)$  and the gate complexity  $G(U)$ , we have the bound

$$\frac{\kappa G(U, \epsilon)^{1/3} \epsilon^{2/3}}{n^2} \leq d(I, U) \leq G(U) \quad (116)$$

for some constant  $\kappa > 0$ .

For pure states we also know that  $W_p^C(|\psi\rangle\langle\psi|, |\varphi\rangle\langle\varphi|) = d_C(|\psi\rangle, |\varphi\rangle)$ . And so to show the behaviour of  $W_p^C$  distances on pure states, we look at  $d_C$ .

**Lemma 30.** *Let  $\mathcal{H} = (\mathbb{C}^2)^{\otimes n}$  be an  $n$ -qudit space, and let  $\mathcal{S} \subseteq SU(4)$  be a finite universal gate set with inverses. Letting  $G_{\mathcal{S}}(U, \epsilon)$  be the  $\epsilon$ -approximate gate complexity of  $U$  from set  $\mathcal{S}$  viewed as a set of gates on 2 qubits, and  $G(U, \epsilon)$  the  $\epsilon$ -approximate gate complexity of  $U$  using any one- or two-qubit gates, we have*

$$G(U, \epsilon) \text{poly}(\log(G(U, \epsilon)) + \log(\epsilon^{-1})) \geq G_{\mathcal{S}}(U, 2\epsilon) \quad (117)$$

*Proof.* Let  $V_1, \dots, V_{G(U, \epsilon)}$  be any circuit of one- and two-qubit gates to synthesise  $V$  such that  $\|U - V\|_\infty \leq \epsilon$ . Using Solovay-Kitaev, each of these can be approximated to within error  $\epsilon/G(U, \epsilon)$  in  $\text{poly}(\log(G(U, \epsilon)/\epsilon))$  gates from  $\mathcal{S}$ . Compounding errors linearly, these form a circuit of length  $G(U, \epsilon) \text{poly}(\log(G(U, \epsilon)) + \log(\epsilon^{-1}))$  of gates from  $\mathcal{S}$  which synthesises  $U$  to within operator norm  $2\epsilon$ .  $\square$

**Lemma 31.** *Let  $\mathcal{S} \subseteq SU(4)$  be a finite universal gate set with inverses. Fix  $|\psi\rangle$ . Sampling  $|\varphi\rangle$  from the Haar measure on  $\mathbb{P}\mathcal{H}$ , let  $U_{|\psi\rangle \rightarrow |\varphi\rangle}^{\text{opt}} \in SU(2^n)$  have  $U_{|\psi\rangle \rightarrow |\varphi\rangle}^{\text{opt}} |\psi\rangle = |\varphi\rangle$  and suppose it has minimum  $\epsilon$ -approximate complexity among all such unitaries in  $SU(2^n)$ . We have that for all  $\delta$ ,*

$$\mathbb{P}_{|\varphi\rangle} \left[ G_{\mathcal{S}}(U_{|\psi\rangle \rightarrow |\varphi\rangle}^{\text{opt}}, 2\epsilon) \leq 2^{(1-\delta)n} \right] \leq e^{-\Omega(2^n \log((2\epsilon)^{-1}))} \quad (118)$$

*Proof.* There are  $|\mathcal{S}|^{2^{(1-\delta)n}}$  circuits of length  $2^{(1-\delta)n}$  made from gates in  $|\mathcal{S}|$ , and  $\mathbb{P}\mathcal{H}$  has real dimension  $2^{n+1} - 2$ . Therefore there are  $e^{\Omega(2^n \log((2\epsilon)^{-1}))}$   $2\epsilon$ -balls in  $\mathbb{P}\mathcal{H}$ . It follows then that the  $2\epsilon$ -balls around outputs of length- $2^{(1-\delta)n}$  circuits cover a proportion  $e^{\mathcal{O}(2^{(1-\delta)n} \log |\mathcal{S}|) - \Omega(2^n \log((2\epsilon)^{-1}))} \leq e^{-\Omega(2^n \log((2\epsilon)^{-1}))}$  of possible output states in  $\mathbb{P}\mathcal{H}$ .  $\square$

Combining these two propositions with equation (78) gives the result.

**Corollary 32.** *Fix state  $|\psi\rangle$  on  $n$  qubits, and let  $|\varphi\rangle$  be sampled from the Haar measure on  $\mathbb{P}\mathcal{H}$ . For all  $\delta > 0$ ,*

$$\mathbb{P}_{|\varphi\rangle} \left[ d(|\psi\rangle, |\varphi\rangle) \leq \epsilon^{2/3} n^{-1} \kappa \left( \frac{2^{(1-\delta)n}}{\text{poly}(n, \log \epsilon^{-1})} \right)^{1/3} \right] \leq e^{-\Omega(2^n \log((2\epsilon)^{-1}))}. \quad (119)$$

*Proof.* The proof is technical and not particularly instructive, so has been placed in Appendix D 2.  $\square$

In other words, the chance of two Haar-random pure states on  $n$  qubits being less than exponentially far apart in the complexity geometry distance becomes exponentially small as  $n$  tends towards infinity.

## B. Operational interpretation in terms of classical-quantum sources

In this section, we show that the  $W_p^d$  distances have an operational significance for distances between classical-quantum (cq) states and classical-quantum (cq) sources. Indeed, let  $R$  and  $S$  be two cq sources, each controlled by a classical random variable  $X$  on  $\{1, \dots, N\}$  with probabilities  $p_i$ . On input  $i$ , let  $R$  output  $|\psi_i\rangle\langle\psi_i|$  and  $S$  output  $|\varphi_i\rangle\langle\varphi_i|$ . Let the output have dimension  $D$ . These sources can be simulated by measuring the first (classical) register of the following cq states in the standard basis:

$$\tilde{\rho} = \sum_{i=1}^N p_i |i\rangle\langle i| \otimes |\psi_i\rangle\langle\psi_i| \quad \tilde{\sigma} = \sum_{i=1}^N p_i |i\rangle\langle i| \otimes |\varphi_i\rangle\langle\varphi_i|. \quad (120)$$

Letting then  $\rho = \sum_{i=1}^N p_i |\psi_i\rangle\langle\psi_i|$  and  $\sigma = \sum_{i=1}^N p_i |\varphi_i\rangle\langle\varphi_i|$ , these  $\rho$  and  $\sigma$  are the expected outputs of  $R$  and  $S$  respectively. The  $W_1^d$  distance provides a lower bound between the expected distance between the outputs. Broadly speaking, we interpret the distance as the cost of moving between  $R$  and  $S$ .

**Proposition 33.** *Let  $R$  and  $S$  be cq sources with expected outputs  $\rho$  and  $\sigma$  respectively of dimension  $D$ , and let  $1 \leq p < \infty$ . Given access to the output register and classical control register, the expected distance  $d$  between the outputs  $r$  and  $s$  satisfies*

$$\mathbb{E}_X [d(r, s)^p] \geq W_p^d(\rho, \sigma)^p \quad (121)$$

and this bound is sharp.

*Proof.* For the lower bound, consider quantum transport plan  $Q = \{(p_i, |\psi_i\rangle, |\varphi_i\rangle)\}_{i=1}^N$  between  $\rho$  and  $\sigma$ . The  $p^{\text{th}}$ -order cost of this transport plan is

$$T_p^d(Q) = \sum_{i=1}^N p_i d(|\psi_i\rangle, |\varphi_i\rangle)^p = \mathbb{E}_X [d(r, s)^p] \quad (122)$$

which is lower bounded by the optimal  $p^{\text{th}}$ -order quantum transport cost  $W_p^d(\rho, \sigma)$ .

For sharpness, let  $Q = \{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}_j$  be any transport plan between  $\rho$  and  $\sigma$ . The sources

$$R = \sum_{j \in J} q_j |j\rangle\langle j| \otimes |\psi_j\rangle\langle\psi_j| \quad S = \sum_{j \in J} q_j |j\rangle\langle j| \otimes |\varphi_j\rangle\langle\varphi_j| \quad (123)$$

controlled by random variable  $Y$  taking values in  $J$  with probabilities  $q_j$  then have  $p^{\text{th}}$  moment

$$\mathbb{E}_Y [d(r, s)^p] = \sum_{j \in J} q_j d(|\psi_j\rangle, |\varphi_j\rangle)^p. \quad (124)$$

Taking the infimum over all transport plans gives sharpness. □

We also get from Proposition 16 that when  $d$  is continuous, we can take the first register to have size at most  $2D^2$  in the equality case.

In the case where  $d$  is the complexity geometry metric  $d_C$ , this means that  $W_p^C$  effectively quantifies the  $p^{\text{th}}$  moment of the gate complexity of transforming one source into another, post-output. Indeed, for sources  $R$  and  $S$  as above, and  $U_{|\psi\rangle \rightarrow |\varphi\rangle}^{\text{opt}} \in \mathcal{SU}(2^n)$  a unitary with  $U_{|\psi\rangle \rightarrow |\varphi\rangle}^{\text{opt}} |\psi\rangle = |\varphi\rangle$ , and minimal complexity among all such  $U$ , we know that

$$\mathbb{E}_X [G(U_{r \rightarrow s}^{\text{opt}})^p] \geq W_p^C(\rho, \sigma)^p. \quad (125)$$

Similarly, the  $W_\infty^d$  distance gives a lower bound for the highest possible value of  $d(r, s)$ . It follows from the definition of  $W_\infty^d$  that

$$\max_i d(|\psi_i\rangle, |\varphi_i\rangle) \geq W_\infty^d(\rho, \sigma) \quad (126)$$

and taking the infimum of the left-hand side over  $\mathcal{Q}(\rho, \sigma)$  shows that the bound is sharp. Operationally, for the  $W_\infty^C$  distance, this means  $W_\infty^C(\rho, \sigma)$  is a lower bound for the worst-case scenario cost of transforming  $R$  into  $S$ , post-output.

### C. Hypercontractivity and noise

In the hierarchy of  $W_p^d$  in order  $p$ , we saw in equation (20) that if  $p_1 < p_2$  then  $W_{p_1}^d(\rho, \sigma) \leq W_{p_2}^d(\rho, \sigma)$ . This hierarchy mirrors the hierarchy in the standard  $L^p$  norms, for which the notion of hypercontractivity [Bon70, Bis11, KLLM21] has been used in various ways to quantify the noise of an operation [KLLM21, O'D14]. Broadly speaking, an operator  $T$  on a space of functions is hypercontractive if, for some  $p_2 > p_1$ , we have for all functions  $f$  that  $\|Tf\|_{p_2} \leq \|f\|_{p_1}$ . Hypercontractivity and the noise of an operator are most closely linked in the hypercontractivity theorem [Bon70, Chapter 7], which demonstrates the hypercontractive properties of the standard Boolean noise operator.

We will show that this idea carries over to the quantum  $W_p^d$  distances, and that the ratio  $\frac{W_{p_1}^d(\rho, \sigma)}{W_{p_2}^d(N(\rho), N(\sigma))}$  can be considered as a measure of noise in the channel  $N$ . In this setting, the ‘standard’ noise channels are the replacement channel  $R_{\delta, x}$ , given by

$$R_{\delta, x}(\rho) = (1 - \delta)\rho + \delta|x\rangle\langle x| \quad (127)$$

and the depolarising channel  $S_\delta$  given by

$$S_\delta(\rho) = (1 - \delta)\rho + \delta\mathbb{I}/D \quad (128)$$

where  $D = \dim \mathcal{H}$ .

**Proposition 34.** *Let  $\rho, \sigma$  be two quantum states on  $\mathcal{H}$  and let  $1 \leq p_1 < \infty$ , and suppose  $W_{p_1}^d(\rho, \sigma) = M$ . For  $p_2 > p_1$ , let  $1 - \delta \leq (M/\text{diam}_d(\mathbb{P}\mathcal{H}))^{p_2 - p_1}$ . Then the replacement channel  $R_{\delta, x}$  and the depolarising channel  $S_\delta(\rho)$  have*

$$W_{p_2}^d(R_{\delta, x}(\rho), R_{\delta, x}(\sigma)) \leq W_{p_1}^d(\rho, \sigma) \quad (129)$$

and

$$W_{p_2}^d(S_\delta(\rho), S_\delta(\sigma)) \leq W_{p_1}^d(\rho, \sigma). \quad (130)$$

*Proof.* Let  $Q = \{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\}_j$  be an optimal  $p_1^{\text{th}}$ -order transport plan from  $\rho$  to  $\sigma$ , and let

$$Q' = (1 - \delta)Q \cup \{(\delta, |x\rangle, |x\rangle)\} \quad \text{for channel } R_{\delta, x} \quad (131)$$

or

$$Q' = (1 - \delta)Q \cup \{(\delta/D, |i\rangle, |i\rangle)\}_{i=1}^D \quad \text{for channel } S_\delta \quad (132)$$

for  $|1\rangle, \dots, |D\rangle$  an orthonormal basis of  $\mathcal{H}$ . These are transport plans from  $R_{\delta, x}(\rho)$  to  $R_{\delta, x}(\sigma)$  and from  $S_\delta(\rho)$  to  $S_\delta(\sigma)$  respectively. In both cases,

$$T_{p_2}^d(Q') = \left( (1 - \delta) \sum_j q_j d(|\psi_j\rangle, |\varphi_j\rangle)^{p_2} \right)^{1/p_2} = (1 - \delta)^{1/p_2} T_{p_2}^d(Q)^{1/p_2} \leq \left( \frac{M}{\text{diam}_d(\mathbb{P}\mathcal{H})} \right)^{1 - p_1/p_2} T_{p_2}^d(Q)^{1/p_2}. \quad (133)$$

So it remains to show that

$$T_{p_1}^d(Q)^{1/p_1} \geq \left( \frac{M}{\text{diam}_d(\mathbb{P}\mathcal{H})} \right)^{1 - p_1/p_2} T_{p_2}^d(Q)^{1/p_2}. \quad (134)$$

Given quantities  $\{A_j\}_j$  subject to constraints

$$\sum_j q_j A_j^{p_1} = M^{p_1} \quad (135)$$

$$0 \leq A_j \leq \text{diam}_d(\mathbb{P}\mathcal{H}), \quad (136)$$

the maximum value of  $\sum_j q_j A_j^q$  is achieved when all  $A_j$  are either  $\text{diam}_d(\mathbb{P}\mathcal{H})$  or 0, with values  $q_1 = (M/\text{diam}_d(\mathbb{P}\mathcal{H}))^{p_1}$  and  $q_2 = 1 - q_1$ . This gives

$$T_{p_2}^d(Q) \leq (M/\text{diam}_d(\mathbb{P}\mathcal{H}))^{p_1} \text{diam}_d(\mathbb{P}\mathcal{H})^{p_2} \quad (137)$$

and therefore that

$$\frac{T_{p_1}^d(Q)^{1/p_1}}{T_{p_2}^d(Q)^{1/p_2}} \geq \frac{M}{\text{diam}_d(\mathbb{P}\mathcal{H})} \left( \frac{\text{diam}_d(\mathbb{P}\mathcal{H})}{M} \right)^{p_1/p_2} = \left( \frac{M}{\text{diam}_d(\mathbb{P}\mathcal{H})} \right)^{1-p_1/p_2}. \quad (138)$$

□

We note from the condition  $1 - \delta \leq (M/\text{diam}_d(\mathbb{P}\mathcal{H}))^{p_2-p_1}$  that this result is applicable only when  $W_{p_1}^d$  is close to  $\text{diam}_d(\mathbb{P}\mathcal{H})$  or when  $p_2 - p_1$  is small. Otherwise, we would require  $\delta$  so large that the channels are no longer of practical use. Our results on random states from Sec. VIA demonstrate that this is indeed a relevant case, as for random low-rank states,  $W_p^H$  and  $W_p^C$  are generally high.

Particularly in the case of complexity geometry, this shows that channel noise reduces complexity. These results also demonstrate the value of considering arbitrary  $p$  in our construction of the  $W_p^d$  distances. Such consideration is not possible without being able to relate Wasserstein distances of different orders to one another. In general, for arbitrary  $p_1, p_2$ , this shows that  $\frac{W_{p_1}^d(\rho, \sigma)}{W_{p_2}^d(N(\rho), N(\sigma))}$  can be well considered as a measure of noise in the channel  $N$ .

## VII. CONCLUSION

In this work, we have introduced a novel definition of the quantum Wasserstein distance by combining the coupling method and a metric on the set of pure states. This novel definition successfully captures the essence of the classical Wasserstein distance. A significant aspect of our approach is its inherent adaptability, effortlessly incorporating established metrics on quantum states such as trace distance and naturally extending pure-state metrics, for instance, Nielsen's complexity metric, to cater to mixed states.

Furthermore, we established various properties of this new definition. While we acknowledge that these properties are not exhaustive, they nevertheless offer advantages compared to other recent generalisations, such as the fact that one definition can cover several examples in the literature in a unified way. A significant challenge remains: establishing the triangle inequality in its generality. Our findings, though, hint at the possibility that under suitable conditions the dual approach yields a proof of the triangle inequality.

Our exploration of specific cases reveals the  $W_1^1$  distance as a potentially powerful tool for bounding the trace distance between quantum states, drawing parallels with classical approaches for determining total variation distance and mixing time bounds. Additionally, our work enriches the understanding of the complexity geometry of quantum states, offering a new lens through which to view and quantify the complexity of transformations within quantum ensembles.

Our examination of the behaviour of the Wasserstein distance under random quantum states unveils various phase transitions. These results, derived from entropic inequalities and continuity bounds, debunk some existing speculations (e.g. that  $\|\cdot\|_{W_1^H}$  captures local distinguishability) while affirming others (the complexity of small subsystems of random quantum states is low).

In conclusion, our research represents a significant stride forward in the pursuit of understanding optimal transport in quantum mechanics. The novel quantum Wasserstein distance that we have proposed holds great promise, not only as an analytical tool but also as a medium for further exploration and discovery in quantum computation and information. While our work has paved the way, many challenges and open problems remain, especially when it comes to finding new applications of the methods laid out here.

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## Appendix A: Comparison to other proposed definitions of a quantum Wasserstein distance

Until now, finding a coherent way to define a quantum optimal transport cost, regardless of the underlying metric on the Hilbert space, has proved elusive. Some definitions (such as in [PT21], [CM14] and [GMP15]) work well for specific orders  $p$ , and specific underlying metrics. A further definition was proposed recently in [CYL<sup>+</sup>19] using standard quantum couplings and using projection onto the asymmetric subspace as a cost function, with the motivation of mimicking the definition of total variation distance as the Wasserstein distance corresponding to the trivial metric.

Originally, [CYL<sup>+</sup>19] defined a second-order Wasserstein semi-distance  $W$  on states on  $\mathcal{H} = \mathbb{C}^d$  as follows. Letting  $\mathbb{F}|a\rangle \otimes |b\rangle = |b\rangle \otimes |a\rangle$  define the flip operator on  $\mathcal{H} \otimes \mathcal{H}$ , we can then define the symmetric projector  $P_{\text{sym}}(d)$  as the projector onto the 1-eigenspace of  $\mathbb{F}$ , and  $P_{\text{asym}}(d)$  the projector onto its  $(-1)$ -eigenspace. Note  $P_{\text{sym}}(d) + P_{\text{asym}}(d) = \mathbb{I}_{\mathbb{C}^d \otimes \mathbb{C}^d}$ .

They then define the quantum optimal transport cost

$$T(\rho, \sigma) = \min_{\tau_{AB} \in \mathcal{D}(\mathbb{C}^d \otimes \mathbb{C}^d), \tau_A = \rho, \tau_B = \sigma} \text{Tr}[\tau_{AB} P_{\text{asym}}(d)] \quad (\text{A1})$$

and  $W(\rho, \sigma) = \sqrt{T(\rho, \sigma)}$ . This definition was further studied in [FECZ22] and [CEFZ23], and refined in [MH22] to give data processing. It gives a 2-Wasserstein semi-distance which is equivalent to the trace distance.

[MH22] then showed that this original definition does not satisfy a data-processing inequality, so it does not mirror the original trace distance in this regard. The definition in Eq. (A1) was then refined to give the data processing inequality by considering a complete version:

$$T_s(\rho, \sigma) = T(\rho \otimes \mathbb{I}/2, \sigma \otimes \mathbb{I}/2) \quad (\text{A2})$$

and  $W_s(\rho, \sigma) = \sqrt{T_s(\rho, \sigma)}$ . Note that in general, the complete version of a quantity requires an optimisation over auxiliary systems of arbitrary size, however [MH22] shows that the maximally mixed state of one qubit suffices.

There are two main differences between this path to obtaining a generalisation of the Wasserstein distance and ours. First, in this path, the cost of transforming one state into another is given by the expectation value of an observable on the bipartite system. In our case, we depart from a metric on the set of point masses/pure states. Although the metric version is in direct analogy with the classical version, optimising over the expectation value of an observable certainly has a more operational interpretation. Second, in the definition of Eq. (A1) we see that we indeed optimise over all couplings, including separable ones. In our definition, we only optimise over separable ones, which gives the definition in Eq. (A1) a more quantum flavor. Furthermore, computing Eq. (A1) corresponds to an SDP, so it can be computed efficiently in the dimension, whereas it is unclear if we can efficiently compute our version in general. However, one of the main motivations for our work was to obtain a unified way of obtaining various versions of  $W_p$  present in the literature, including the definition of [PMTL21]. However, it appears that approaches like that of Eq. (A1) cannot mimic the behaviour of the Wasserstein distance of de Palma et al. Consider, for example, the potential extension to an  $n$ -qudit space given by

$$T(\rho, \sigma) = \min \left\{ \text{Tr} \left[ \tau_{AB} \left( \sum_{i=1}^n P_{i,\text{asym}}(d) \right) \right] : \tau_{AB} \in \mathcal{D} \left( (\mathbb{C}^d)^{\otimes n} \otimes (\mathbb{C}^d)^{\otimes n} \right) : \tau_A = \rho, \tau_B = \sigma \right\} \quad (\text{A3})$$

where  $P_{i,\text{asym}}(d)$  is the projection onto the asymmetric subspace of the  $i^{\text{th}}$  qudits (and is the identity on the other qudits). In stabilising, it makes little difference whether we stabilise each qudit individually with its own copy of  $\mathbb{I}/2$  or share one, so we stabilise this definition to

$$T_s(\rho, \sigma) = \min \left\{ \text{Tr} \left[ \tau_{AB} \left( \sum_{i=1}^n P_{i,\text{asym}}(d \otimes 2) \right) \right] : \right. \quad (\text{A4})$$

$$\left. \tau_{AB} \in \mathcal{D} \left( (\mathbb{C}^d \otimes \mathbb{C}^2)^{\otimes n} \otimes (\mathbb{C}^d \otimes \mathbb{C}^2)^{\otimes n} \right), \tau_A = \rho \otimes (\mathbb{I}/2)^{\otimes n}, \tau_B = \sigma \otimes (\mathbb{I}/2)^{\otimes n} \right\} \quad (\text{A5})$$

and  $W_s(\rho, \sigma) = \sqrt{T_s(\rho, \sigma)}$ .

We'll show, however, that any such type of generalisation leads to some states  $\rho$  with  $T_s(\rho, \rho) > 0$ . Take, in this example,  $n = d = 2$  and  $\rho$  to be a Bell state  $|\psi^+\rangle\langle\psi^+|$ . As  $\rho$  is pure, the set of possible couplings  $\tau$  is very limited. In the non-stabilised definition,  $\tau$  can only be  $|\psi^+\rangle\langle\psi^+| \otimes |\psi^+\rangle\langle\psi^+|$ . In the stabilised definition,  $\tau$  must have form  $|\psi^+\rangle\langle\psi^+| \otimes |\psi^+\rangle\langle\psi^+| \otimes \omega$  for some coupling  $\omega$  of  $\mathbb{I}^{\otimes 2}/4$  and  $\mathbb{I}^{\otimes 2}/4$ .

However, when looking at applying  $P_{\text{asym}}$  to the individual qubits, we note that as the Bell state has qubit marginals  $\mathbb{I}/2$ , we will have nonzero transport cost from  $\rho$  to itself. Indeed in the non-stabilised case,

$$T(\rho, \sigma) = \sum_{i=1}^2 \text{Tr} [|\psi^+\rangle\langle\psi^+| \otimes |\psi^+\rangle\langle\psi^+| (P_{i,\text{asym}}(2))] \quad (\text{A6})$$

$$= 2 \text{Tr} \left[ \left( \frac{\mathbb{I}}{2} \otimes \frac{\mathbb{I}}{2} \right) P_{\text{asym}}(2) \right] \quad (\text{A7})$$

$$= \frac{1}{2} \text{Tr} [P_{\text{asym}}(2)] = \frac{1}{2}. \quad (\text{A8})$$

In the stabilised case, we still have for any  $\tau$ , that

$$\mathrm{Tr} \left[ \tau_{AB} \left( \sum_{i=1}^2 P_{i,\mathrm{asym}}(2 \otimes 2) \right) \right] \quad (\text{A9})$$

$$= \sum_{i=1}^2 \mathrm{Tr} [ |\psi^+\rangle\langle\psi^+| \otimes |\psi^+\rangle\langle\psi^+| \otimes \omega (P_{i,\mathrm{asym}}(2 \otimes 2)) ] \quad (\text{A10})$$

$$= \sum_{i=1}^2 \mathrm{Tr} \left[ \left( \frac{\mathbb{I}}{2} \otimes \frac{\mathbb{I}}{2} \otimes \omega_i \right) P_{\mathrm{asym}}(2 \otimes 2) \right] \quad (\text{A11})$$

$$= \sum_{i=1}^2 \mathrm{Tr} \left[ \left( \frac{\mathbb{I}}{2} \otimes \frac{\mathbb{I}}{2} \otimes \omega_i \right) (P_{\mathrm{asym}}(2) \otimes P_{\mathrm{sym}}(2) + P_{\mathrm{sym}}(2) \otimes P_{\mathrm{asym}}(2)) \right] \quad (\text{A12})$$

$$= \sum_{i=1}^2 \frac{1}{4} \mathrm{Tr} [\omega_i P_{\mathrm{sym}}(2)] + \frac{3}{4} \mathrm{Tr} [\omega_i P_{\mathrm{asym}}(2)] \quad (\text{A13})$$

$$\geq \sum_{i=1}^2 \frac{1}{4} (\mathrm{Tr} [\omega_i P_{\mathrm{sym}}(2)] + \mathrm{Tr} [\omega_i P_{\mathrm{asym}}(2)]) = \sum_{i=1}^2 \frac{1}{4} \mathrm{Tr} [\omega_i] = \frac{1}{2} \quad (\text{A14})$$

where in line (A11),  $\omega_i$  is a coupling of  $\mathbb{I}/2$  with itself, on the  $i^{\mathrm{th}}$  stabilising qubits.

We see from the details of this example that, no matter whether or not we stabilise using many qubits or a single qubit, and no matter the size of the space, any attempt to put a  $P_{\mathrm{asym}}$  projector on a subspace of  $\mathcal{H}$  will result in highly entangled pure states, those which have marginals close to maximally mixed on subspaces where  $P_{\mathrm{asym}}$  is placed, having nonzero self-distance. This is largely because the coupling of a pure state with itself is forced to be the product of the state with itself, and because the identity on  $\mathbb{C}^d \otimes \mathbb{C}^d$  has a nonzero asymmetric and a nonzero symmetric component. Thus, it appears that a version of the Wasserstein distance that is not based on a single observable, like ours, is more suited to obtain generalisations of quantities like the one of de Palma et al.

## Appendix B: Development of the proposed definition

### 1. Definition of a transport plan

During the development of this proposal, many different ways of defining a transport plan were considered. They all had different versions of the conditions

$$\sum_j q_j |\psi_j\rangle\langle\psi_j| = \rho, \sum_j q_j |\varphi_j\rangle\langle\varphi_j| = \sigma, q_j > 0. \quad (\text{B1})$$

As in the definition of the  $W_1$  norm in [PMTL21], a first proposal was simply the condition

$$\sum_j q_j (|\psi_j\rangle\langle\psi_j| - |\varphi_j\rangle\langle\varphi_j|) = \rho - \sigma, q_j > 0. \quad (\text{B2})$$

It quickly becomes clear, that using a transport plan of this form containing telescoping sums, could lead to the degeneracy of  $W_p^d$  when  $p > 1$ . The main stumbling block here centred on the unboundedness of  $\sum_j q_j$ .

Two proposals for restricting  $\sum_j q_j$  were then considered, the first being

$$\sum_j q_j = 1 \quad (\text{B3})$$

and the second

$$\sum_j q_j = \frac{1}{2} \|\rho - \sigma\|_1. \quad (\text{B4})$$

Both of these were discounted when considering the transport plans that were allowed under these regimes, and their impact on the norm  $W_\infty^H$ .

For transport plans of the form (B3), consider the  $W_\infty^H$  distance on  $\mathcal{H} = (\mathbb{C}^3)^{\otimes 2}$ , and the states  $\rho = \frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|22\rangle\langle 22|$ ,  $\sigma = \frac{1}{2}|11\rangle\langle 11| + \frac{1}{2}|22\rangle\langle 22|$ . Classically, the infinite-order transport distance between the measures  $\mu = \frac{1}{2}\delta_{00} + \frac{1}{2}\delta_{22}$  and  $\nu = \frac{1}{2}\delta_{11} + \frac{1}{2}\delta_{22}$  on the Hamming cube  $\{0, 1, 2\}^2$  is 2. With the definition from (B3) however, we could define a transport plan

$$Q = \left\{ \left( \frac{1}{2}, |00\rangle, |01\rangle \right), \left( \frac{1}{2}, |01\rangle, |11\rangle \right) \right\} \quad (\text{B5})$$

with a maximum  $d(|\psi_j\rangle, |\varphi_j\rangle)$  of 1. Though as in (60) we are perfectly happy that the  $W_\infty^H$  distance might not match Ornstein's  $\bar{d}$ -distance for classical measures, it certainly should not differ because of a transport plan of a classical nature such as this one.

The picture for condition (B4) is very similar. Consider  $W_\infty^H$  on  $\mathcal{H} = (\mathbb{C}^2)^{\otimes 2}$ , with states  $\rho = \frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|01\rangle\langle 01|$ ,  $\sigma = \frac{1}{2}|01\rangle\langle 01| + \frac{1}{2}|11\rangle\langle 11|$ . Classically, these have an infinite-order transport distance of 1 on the Hamming cube  $\{0, 1\}^2$ . However, because  $\frac{1}{2}\|\rho - \sigma\|_1$  is small in this case, the only permitted transport plan is

$$Q = \left\{ \left( \frac{1}{2}, |00\rangle, |11\rangle \right) \right\} \quad (\text{B6})$$

with a maximum  $d(|\psi_j\rangle, |\varphi_j\rangle)$  of 2. The condition (B4) does not permit quantum versions of the standard classical transport plans, and so this definition of a transport plan seems strictly worse than the one we propose in this work.

## 2. Entangled couplings and transport plans

The main reason we need to restrict to separable couplings is the fact that it is not obvious at first how to attribute a distance to an entangled state starting from a distance on  $\mathbb{P}\mathcal{H}$  and then attribute a transportation cost to transport plans that include entangled pure states and satisfy the marginal constraints.

One possibility is as follows: given a state  $|\psi\rangle$  in  $\mathbb{P}(\mathcal{H} \otimes \mathcal{H})$  and  $SD(|\psi\rangle)$  the set of Schmidt decompositions of  $|\psi\rangle$ , we define  $d(|\psi\rangle)$  as:

$$d(|\psi\rangle) = \inf_{\sum_i \sqrt{p_i} |\phi_1\rangle \otimes |\phi_2\rangle \in SD(|\psi\rangle)} \sum_i p_i d(|\phi_1\rangle, |\phi_2\rangle). \quad (\text{B7})$$

It is then easy to see that we recover the original distance when considering product states. However, it is also easy to see that, at least for the case  $p = 1$ , enlarging the set of possible states to include entangled states offers no advantage. Indeed, given any Schmidt decomposition of an entangled  $|\psi\rangle = \sum_i \sqrt{p_i} |\phi_1\rangle \otimes |\phi_2\rangle$ , adding instead  $\{(p_i, |\phi_1\rangle, |\phi_2\rangle)\}_i$  to the transport plan will give the same cost and still satisfy the marginal constraints. Thus, at least for this possible generalisation of the distance to entangled states, there is no advantage in considering entangled couplings.

## Appendix C: Towards the triangle inequality

As with many other attempts to generalise the classical Wasserstein distances to the quantum setting, the triangle inequality eludes us. The central barrier to the triangle inequality is the quantum marginal problem: even in the case where we do not require our couplings to be separable, there is no coherent way to build a coupling  $\tau_{13}$  from coupling  $\tau_{12}$  of  $\rho_1$  and  $\rho_2$  and coupling  $\tau_{23}$  of  $\rho_2$  and  $\rho_3$ .

All known proofs of the triangle inequality for the classical  $\mathcal{W}_p$  distances rely on this idea: given a coupling  $\gamma_{12}$  of measures  $\mu_1$  and  $\mu_2$ , and coupling  $\gamma_{23}$  of  $\mu_2$  and  $\mu_3$ , we can find measure  $\gamma_{123}$  with (1, 2)-marginal  $\gamma_{12}$  and (2, 3)-marginal  $\gamma_{23}$ . We can then take the (1, 3)-marginal  $\gamma_{13}$  of this overarching measure, and show that [CD08]

$$T_p(\gamma_{13})^{1/p} \leq T_p(\gamma_{12})^{1/p} + T_p(\gamma_{23})^{1/p} \quad (\text{C1})$$

via Minkowski's inequality. Without an equivalent  $\tau_{123}$  in the quantum setting from which to form coupling  $\tau_{13}$ , there is as of yet no clear path to a triangle inequality.

For the case  $p = 1$ , we can focus on the case where  $\|\rho - \sigma\|_{DW_1^d} = W_1^d(\rho, \sigma)$ , as  $\|\cdot\|_{DW_1^d}$  does satisfy the triangle inequality. As mentioned in Sec. IV A, this remains a key open problem of our work.

## Appendix D: Auxiliary proofs

### 1. Proof of Proposition 17 on the continuity of $W_p^d$

**Proposition 17.** *Suppose  $d$  is continuous on  $\mathbb{P}\mathcal{H}$  and let  $1 \leq p < \infty$ . Then  $W_p^d$  is uniformly continuous.*

*Proof.* Take  $\epsilon > 0$ . Let  $\rho, \sigma, \rho', \sigma'$  be states on  $\mathbb{P}\mathcal{H}$  with  $\|\rho - \rho'\|_\infty \leq \delta$  and  $\|\sigma - \sigma'\|_\infty \leq \delta$ , for some  $\delta$  to be chosen later. For any transport plan from  $\rho$  to  $\sigma$ , we will form a transport plan from  $\rho'$  to  $\sigma'$  with a similar cost. Note that as  $\mathcal{H}$  is finite-dimensional,  $\mathbb{P}\mathcal{H}$  is compact and so  $d$  is uniformly continuous.

Let  $c \gg 1$  (also to be chosen later, but note scale  $1 \gg c\delta$ ) and let  $S_{\rho'}, S_{\sigma'}$  respectively be the span of the eigenvectors of  $\rho', \sigma'$  whose eigenvalues are at least  $c\delta$ . Let  $\Pi_{\rho'}, \Pi_{\sigma'}$  be the projectors onto  $S_{\rho'}, S_{\sigma'}$  respectively.

Let

$$Q = \{(q_j, |\psi_j\rangle, |\varphi_j\rangle)\} \quad (D1)$$

be any  $p^{\text{th}}$ -order transport plan from  $\rho$  to  $\sigma$ . Define then  $|\psi_j\rangle = |\psi_j^{\rho'}\rangle + |\psi_j^\perp\rangle$  where  $|\psi_j^{\rho'}\rangle = \Pi_{\rho'}|\psi_j\rangle$  and  $|\psi_j^\perp\rangle$  is perpendicular to  $S_{\rho'}$ . Define  $|\varphi_j^{\sigma'}\rangle$  and  $|\varphi_j^\perp\rangle$  analogously.

We can then begin to define a transport plan from  $\rho'$  to  $\sigma'$ . Let

$$\tilde{\rho} = \Pi_{\rho'}\rho\Pi_{\rho'} = \sum_j q_j |\psi_j^{\rho'}\rangle \langle \psi_j^{\rho'}| \quad (D2)$$

and define  $\tilde{\sigma}$  analogously. Note that  $\|\Pi_{\rho'}(\rho - \rho')\Pi_{\rho'}\|_\infty \leq \|\rho - \rho'\|_\infty < \delta$ . Therefore

$$\tilde{\rho} \leq \Pi_{\rho'}\rho\Pi_{\rho'} + \delta\mathbb{I}_{S_{\rho'}} \leq \left(1 + \frac{1}{c}\right) \Pi_{\rho'}\rho\Pi_{\rho'} \leq \left(1 + \frac{1}{c}\right) \rho' \quad (D3)$$

and so  $\frac{c}{c+1}\tilde{\rho} \leq \rho'$ .

The same holds for  $\sigma$ , so  $\frac{c}{c+1}\tilde{\sigma} \leq \sigma'$ .

We may then begin to build our new transport plan starting with the partial transport plan

$$Q_1 = \left\{ \left( q'_j, \frac{|\psi_j^{\rho'}\rangle}{\sqrt{\langle \psi_j^{\rho'} | \psi_j^{\rho'} \rangle}}, \frac{|\varphi_j^{\sigma'}\rangle}{\sqrt{\langle \varphi_j^{\sigma'} | \varphi_j^{\sigma'} \rangle}} \right) \right\} \quad (D4)$$

where  $q'_j = \frac{c}{c+1}q_j \min\{\langle \psi_j^{\rho'} | \psi_j^{\rho'} \rangle, \langle \varphi_j^{\sigma'} | \varphi_j^{\sigma'} \rangle\}$ . Note then that

$$\rho' \geq \frac{c}{c+1}\tilde{\rho} \geq \sum_j q'_j \frac{|\psi_j^{\rho'}\rangle \langle \psi_j^{\rho'}|}{\langle \psi_j^{\rho'} | \psi_j^{\rho'} \rangle} \quad \text{and} \quad \sigma' \geq \frac{c}{c+1}\tilde{\sigma} \geq \sum_j q'_j \frac{|\varphi_j^{\sigma'}\rangle \langle \varphi_j^{\sigma'}|}{\langle \varphi_j^{\sigma'} | \varphi_j^{\sigma'} \rangle}. \quad (D5)$$

We can then transport the positive semidefinite operator  $\rho' - \sum_j q'_j \frac{|\psi_j^{\rho'}\rangle \langle \psi_j^{\rho'}|}{\langle \psi_j^{\rho'} | \psi_j^{\rho'} \rangle}$  onto  $\sigma' - \sum_j q'_j \frac{|\varphi_j^{\sigma'}\rangle \langle \varphi_j^{\sigma'}|}{\langle \varphi_j^{\sigma'} | \varphi_j^{\sigma'} \rangle}$  via any partial transport plan. Let these transport plan elements form set  $Q_2$ . It follows that  $Q_1 \cup Q_2$  is a transport plan from  $\rho'$  to  $\sigma'$ .

We can now attempt bounding the cost of this transport plan. We will show that  $Q_2$  has a very small cost and that  $Q_1$  has a cost very close to  $T_p^d(Q)$ . Starting with the  $Q_2$  part, we know that

$$T_p^d(Q_2) \leq \text{Tr} \left[ \rho' - \sum_j q'_j \frac{|\psi_j^{\rho'}\rangle \langle \psi_j^{\rho'}|}{\langle \psi_j^{\rho'} | \psi_j^{\rho'} \rangle} \right] \text{diam}_d(\mathbb{P}\mathcal{H})^d. \quad (D6)$$

We will show that this trace part is very small. Indeed

$$\mathrm{Tr} \left[ \rho' - \sum_j q'_j \frac{|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|}{\langle\psi_j^{\rho'}|\psi_j^{\rho'}\rangle} \right] = \left\| \rho' - \sum_j q'_j \frac{|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|}{\langle\psi_j^{\rho'}|\psi_j^{\rho'}\rangle} \right\|_1 \quad (\text{D7})$$

$$\leq \|\rho - \rho'\|_1 + \left\| \rho - \sum_j q'_j \frac{|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|}{\langle\psi_j^{\rho'}|\psi_j^{\rho'}\rangle} \right\|_1 \quad (\text{D8})$$

$$\leq \delta \dim \mathcal{H} + \left\| \rho - \sum_j q'_j \frac{|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|}{\langle\psi_j^{\rho'}|\psi_j^{\rho'}\rangle} \right\|_1 \quad (\text{D9})$$

Choose  $M > 0$  (again to be determined later), and select  $L > 0$  such that whenever  $\mathrm{Tr}|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}| \geq 1 - L$  and  $\mathrm{Tr}|\varphi_j^{\sigma'}\rangle\langle\varphi_j^{\sigma'}| \geq 1 - L$  we have  $d(|\psi_j^{\rho'}\rangle, |\varphi_j^{\sigma'}\rangle)^p < d(|\psi_j\rangle, |\varphi_j\rangle)^p + M$ . This is possible by uniform continuity of  $d$ . We then split the set of  $j$  into those for which the projections onto  $S_{\rho'}$  and  $S_{\sigma'}$  are large, and those for which they are not.

Let

$$\mathcal{J} = \left\{ j : \mathrm{Tr}|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|, \mathrm{Tr}|\varphi_j^{\sigma'}\rangle\langle\varphi_j^{\sigma'}| > 1 - L \right\}. \quad (\text{D10})$$

and we can split up these 1-norm terms into  $j \in \mathcal{J}$  and  $j \notin \mathcal{J}$ . For  $j \in \mathcal{J}$ , we have

$$\left\| q_j |\psi_j\rangle\langle\psi_j| - q'_j \frac{|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|}{\mathrm{Tr}|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|} \right\|_1 \leq q_j \left\| |\psi_j\rangle\langle\psi_j| - \frac{|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|}{\mathrm{Tr}|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|} \right\|_1 + |q_j - q'_j| \quad (\text{D11})$$

$$\leq 2q_j \sqrt{L} + \left( L + \frac{1}{c+1} \right) q_j = \left( 2\sqrt{L} + L + \frac{1}{c+1} \right) q_j \quad (\text{D12})$$

and for  $j \notin \mathcal{J}$ , we have  $\left\| q_j |\psi_j\rangle\langle\psi_j| - q'_j \frac{|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|}{\mathrm{Tr}|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|} \right\|_1 \leq 2q_j$ . In order to bound  $\sum_{j \notin \mathcal{J}} q_j$ , let  $\{|\alpha\rangle\}_\alpha$  be some orthonormal basis for the orthogonal complement of  $S_{\rho'}$ . We have

$$\|\rho - \rho'\|_\infty \dim \mathcal{H} \geq \sum_\alpha \langle \alpha | \rho - \rho' | \alpha \rangle \geq \mathrm{Tr} \left[ \sum_j q_j (|\psi_j^\perp\rangle\langle\psi_j^\perp| + |\varphi_j^\perp\rangle\langle\varphi_j^\perp|) \right] - c\delta \dim \mathcal{H}. \quad (\text{D13})$$

The same applies to  $\sigma$ . Hence

$$\sum_{j \notin \mathcal{J}} q_j \leq \frac{1}{L} \sum_{j \notin \mathcal{J}} q_j \mathrm{Tr} [ |\psi_j^\perp\rangle\langle\psi_j^\perp| + |\varphi_j^\perp\rangle\langle\varphi_j^\perp| ] \quad (\text{D14})$$

$$\leq \frac{1}{L} \mathrm{Tr} \left[ \sum_j q_j (|\psi_j^\perp\rangle\langle\psi_j^\perp| + |\varphi_j^\perp\rangle\langle\varphi_j^\perp|) \right] \quad (\text{D15})$$

$$\leq \frac{1}{L} \dim \mathcal{H} (\|\rho - \rho'\|_\infty + \|\sigma - \sigma'\|_\infty + 2c\delta) \quad (\text{D16})$$

$$\leq \frac{2\delta(c+1)}{L} \dim \mathcal{H}. \quad (\text{D17})$$

This gives us

$$\left\| \rho - \sum_j q'_j \frac{|\psi_j^{\rho'}\rangle\langle\psi_j^{\rho'}|}{\langle\psi_j^{\rho'}|\psi_j^{\rho'}\rangle} \right\|_1 \leq 2\sqrt{L} + L + \frac{1}{c+1} + \frac{4\delta(c+1)}{L} \dim \mathcal{H}. \quad (\text{D18})$$

By symmetry this holds for  $\sigma$ , and so substituting into equation (D9) and then (D6) gives

$$T_p^d(Q_2) \leq \left( \delta \dim \mathcal{H} + 2\sqrt{L} + L + \frac{1}{c} + \frac{4\delta(c+1)}{L} \dim \mathcal{H} \right) \mathrm{diam}_d(\mathbb{P}\mathcal{H})^p. \quad (\text{D19})$$

This bounds  $T_p^d(Q_2)$  above.

For the bounding of  $Q_1$ , we have

$$T_p^d(Q_1) = \sum_j q'_j d(|\psi_j^{\rho'}\rangle, |\varphi_j^{\sigma'}\rangle)^p \quad (\text{D20})$$

$$= \sum_{j \in \mathcal{J}} q'_j d(|\psi_j^{\rho'}\rangle, |\varphi_j^{\sigma'}\rangle)^p + \sum_{j \notin \mathcal{J}} q'_j d(|\psi_j^{\rho'}\rangle, |\varphi_j^{\sigma'}\rangle)^p \quad (\text{D21})$$

$$\leq \sum_{j \in \mathcal{J}} q_j d(|\psi_j\rangle, |\varphi_j\rangle)^p + M + \frac{2\delta}{L} \dim \mathcal{H} \cdot \text{diam}_d(\mathbb{P}\mathcal{H})^p \quad (\text{D22})$$

$$\leq T_p^d(Q) + M + \frac{2\delta}{L} \dim \mathcal{H} \cdot \text{diam}_d(\mathbb{P}\mathcal{H})^p. \quad (\text{D23})$$

It follows then that

$$T_p^d(Q_1 \cup Q_2) \leq T_p^d(Q) + M + \left( \frac{(4c+6)\delta}{L} \dim \mathcal{H} + \delta \dim \mathcal{H} + 2\sqrt{L} + L + \frac{1}{c+1} \right) \text{diam}_d(\mathbb{P}\mathcal{H})^p. \quad (\text{D24})$$

And so choosing  $M < \frac{1}{4}\epsilon$ ,  $L$  sufficiently small such that the continuity condition for  $M$  is satisfied and such that  $2\sqrt{L} + L \leq \frac{\epsilon}{4 \text{diam}_d(\mathbb{P}\mathcal{H})^p}$ ,  $c = \frac{4 \text{diam}_d(\mathbb{P}\mathcal{H})^p}{\epsilon}$ , and then choosing  $\delta < \frac{\epsilon}{4(1+(4c+6)/L) \dim \mathcal{H} \text{diam}_d(\mathbb{P}\mathcal{H})^p}$  gives  $T_p^d(Q_1 \cup Q_2) \leq T_p^d(Q) + \epsilon$ . Thus we have a transport plan for  $\rho'$  to  $\sigma'$  with cost at most  $\epsilon$  more than the transport cost of plan  $Q$  between  $\rho$  and  $\sigma$ .

Taking the infimum over all such transport plans  $Q$ , we see that whenever  $\|\rho - \rho'\|_\infty < \delta$  and  $\|\sigma - \sigma'\|_\infty < \delta$ , we have

$$\inf_{Q' \in \mathcal{Q}(\rho', \sigma')} T_p^d(Q') \leq \epsilon + \inf_{Q \in \mathcal{Q}(\rho, \sigma)} T_p^d(Q). \quad (\text{D25})$$

It follows that  $W_p^d$  is uniformly continuous.  $\square$

## 2. Proof of Corollary 32 on the approximate gate complexity of random pure states

**Corollary 32.** Fix state  $|\psi\rangle$  on  $n$  qubits, and let  $|\varphi\rangle$  be sampled from the Haar measure on  $\mathbb{P}\mathcal{H}$ .

$$\mathbb{P}_{|\varphi\rangle} \left[ d(|\psi\rangle, |\varphi\rangle) \leq \epsilon^{2/3} n^{-1} \kappa \left( \frac{2^{(1-\delta)n}}{\text{poly}(n, \log \epsilon^{-1})} \right)^{1/3} \right] \leq e^{\Omega(2^n \log((2\epsilon)^{-1}))}. \quad (\text{D26})$$

*Proof.* Using equation (78) and the above, we have

$$d(|\psi\rangle, |\varphi\rangle) \geq \min_{U \in \text{SU}(2^n), U|\psi\rangle = |\varphi\rangle} \kappa G(U, \epsilon)^{1/3} \epsilon^{2/3} n^{-2} \quad (\text{D27})$$

$$\geq \min_{U \in \text{SU}(2^n), U|\psi\rangle = |\varphi\rangle} \kappa \left( \frac{G_S(U, 2\epsilon)}{\text{poly}(\log(G(U, \epsilon)) + \log(\epsilon^{-1}))} \right)^{1/3} \epsilon^{2/3} n^{-2} \quad (\text{D28})$$

$$\geq \min_{U \in \text{SU}(2^n), U|\psi\rangle = |\varphi\rangle} \kappa \left( \frac{G_S(U, 2\epsilon)}{\text{poly}(n, \log(\epsilon^{-1}))} \right)^{1/3} \epsilon^{2/3} n^{-2}. \quad (\text{D29})$$

It follows that

$$\mathbb{P}_{|\varphi\rangle} \left[ d(|\psi\rangle, |\varphi\rangle) \leq \epsilon^{2/3} n^{-1} \kappa \left( \frac{2^{(1-\delta)n}}{\text{poly}(n, \log \epsilon^{-1})} \right)^{1/3} \right] \quad (\text{D30})$$

$$\leq \mathbb{P}_{|\varphi\rangle} \left[ \min_{U \in \text{SU}(2^n), U|\psi\rangle = |\varphi\rangle} \kappa \left( \frac{G_S(U, 2\epsilon)}{\text{poly}(n, \log(\epsilon^{-1}))} \right)^{1/3} \epsilon^{2/3} n^{-2} \leq \epsilon^{2/3} n^{-2} \kappa \left( \frac{2^{(1-\delta)n}}{\text{poly}(n, \log \epsilon^{-1})} \right)^{1/3} \right] \quad (\text{D31})$$

$$= \mathbb{P}_{|\varphi\rangle} [G_S(U_{|\psi\rangle \rightarrow |\varphi\rangle}^{\text{opt}}, 2\epsilon) \leq 2^{(1-\delta)n}] \quad (\text{D32})$$

$$\leq e^{\Omega(2^n \log((2\epsilon)^{-1}))} \quad (\text{D33})$$

as claimed.  $\square$