

# EXTENDING QUANTUM DETAILED BALANCE THROUGH OPTIMAL TRANSPORT

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ABSTRACT. We develop a general approach to setting up and studying classes of quantum dynamical systems close to and structurally similar to systems having specified properties, in particular detailed balance. This is done in terms of transport plans and Wasserstein distances between systems on possibly different observable algebras.

*Keywords:* quantum optimal transport; transport plans; Wasserstein distance; detailed balance; nonequilibrium; dynamical systems

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## 1. INTRODUCTION

The goal of this paper is to develop a natural framework in which one can study extensions (including weaker forms) of quantum detailed balance conditions, with the aim of ultimately providing classes of systems with non-equilibrium steady states, having structural similarities to systems satisfying conventional detailed balance conditions. Put differently, we establish a new approach to deviation from detailed balance, even in the classical case. Our approach is via optimal transport.

One of the paper's main objectives is to develop a point of view that shows why the bimodule approach to noncommutative optimal transport, as developed in [38, 39], fits perfectly with dynamical systems possessing steady states, and thus provides a framework for their analysis. At the same time this theory of optimal transport is developed further, as motivated by our goal above.

As has often been pointed out (see for example [2, 3, 4, 21, 44]), to study non-equilibrium successfully, it is of great value to restrict to classes of non-equilibrium states with sufficient structure to be of interest, but still amenable to analysis. Our approach promises to provide classes of systems structurally close to systems satisfying detailed balance, which should ensure that they have enough structure to build a theory around them, and still be relevant to physical situations.

The essence of our framework is to extend detailed balance conditions by considering balance between two systems, in the sense of [41], making use of couplings of the states of the two systems. However, couplings can also be interpreted in terms of transport. Optimal transport, through Wasserstein distances between systems, can then give a quantitative version of the theory in [41], quantifying how far the two systems are from one another. In particular, if one of the two systems is a simple or well understood system satisfying some detailed balance condition, this setup can be used to define extensions of this condition in the other system. Essentially, some properties of one system are carried over to the other in a very structured and quantifiable way. This can be done even if the two systems have different observable algebras, although one would prefer some natural physical relation between certain observables of the two systems. Such a relation is in fact built into the Wasserstein distance, with the mentioned observables acting as coordinates in the respective systems.

We use a transport plan approach to quadratic Wasserstein distances between systems (extending Wasserstein distances between states) developed in [38, 39], though we need to extend it to systems on different observable algebras. It should be noted that while these distances may be actual metrics, they are more generally only pseudometrics and can even lack symmetry. The term "distance" is therefore used in this generalized sense. The triangle inequality will always hold, though. This

is essential for obtaining certain bounds on deviation from detailed balance in Subsection 8.1.

There are other approaches to quantum Wasserstein distances, at least between states (rather than systems) on the same algebra, some key papers being [16, 22, 24, 28, 32, 52, 70], along with many others. Many of these use a dynamical (see [14]) rather than transport plan approach.

However, the approach in [38, 39] appears most appropriate to fit with [41], due to its bimodule setup and level of generality. Indeed, the approach in [38, 39] was developed in large part with this goal in mind. In particular, it will be seen that the asymmetry inherent to the bimodule approach to transport plans, is natural from the perspective of refining or extending concepts regarding systems.

Optimal transport and Wasserstein distance between classical dynamical systems do not appear to have been studied anywhere near as extensively as between measures, but there have been some papers on the topic, the first of these appearing to be [59]. Even aside from the quantum setup of this paper, though, the goals and approach in those papers are quite different from ours.

In the literature one can find other approaches to extend quantum detailed balance to non-equilibrium situations, or to study the deviation from detailed balance, including via entropy production. See for example [2, 3, 4, 17, 18, 21, 42, 43, 44, 66]. Our work is an alternative, and we believe complementary, approach. This paper will not attempt to connect our approach to those mentioned above or to entropy production. We leave this for future work. However, we note that by following very different routes than ours, the papers [10, 31, 68] did connect entropy production to optimal transport and Wasserstein distance.

Although our main motivation is to extend quantum detailed balance properties, it appears that our approach is new in the classical case as well, and may have application there. Moreover, our framework is not restricted only to extending detailed balance. Although the latter appears to be a very natural application of the balance and optimal transport approach, it should apply to other properties of systems with invariant states as well. For example ergodic properties.

Our approach will be formulated in terms of von Neumann algebras, with unital completely positive (u.c.p.) maps serving as the dynamics of open systems, although for reasons to be explained, merely unital positive (u.p.) maps will also be allowed. This places the results of Tomita-Takesaki theory at our disposal, along with the related theory of bimodules (or correspondences in the sense of Connes), which are indispensable for the technical underpinnings of the general theory. In addition, this von Neumann algebra setting is conceptually very clear, for example in terms of comparison to the classical case. This

combination of conceptual clarity along with powerful technical tools, is the reason we use the theory of von Neumann algebras as the basic setting.

We nevertheless strive to make the essential ideas accessible to those not well versed in von Neumann algebras, by also expressing or illustrating many of the key points in special cases, using examples in terms of  $n \times n$  matrix algebras or classical Markov chains on finite sets.

**1.1. A reader's guide.** The reader can get an elementary overview of our ideas, goals and approach, along with some motivation and intuition, from Section 4, while Examples 2.1 and 7.4 together with most of Subsection 3.2 form an entry point to the more general framework, but for the simple case of  $n \times n$  matrix algebras. The bulk of the paper can then be read as if written for the latter special case, though much of the technical proofs in Sections 7 and 8 will not be clear from this point of view.

Section 2 reviews the basic elements needed in our mathematical framework in terms of von Neumann algebras, but we also express the key points in finite dimensions, requiring only some linear algebra. In Section 3 we give a conceptual exposition of the approach introduced in this paper, including an outline of Wasserstein distance. Subsequently Sections 4 and 6 treat simple examples to clarify the approach and to illustrate how extended or refined detailed balance conditions are obtained. Section 4 has been written in such a way that it should for the most part be accessible without reading the previous sections. Prior to Section 6, a specific form of quantum detailed balance, namely standard quantum detailed balance with respect to a reversing operation, is reviewed in Section 5, along with brief general remarks on quantum detailed balance. In order to do this, the notion of KMS duals needs to be discussed as well. The latter also plays a role in the general theory of Wasserstein distances. While Section 5 logically belongs before Section 6, the latter is accessible without having read Section 5.

The sections mentioned in the previous paragraph essentially set out, motivate and illustrate our approach to analyzing systems via (optimal) transport to and from other (typically simpler) systems. What is still needed is the theoretical underpinning for a basic tool of the theory, namely Wasserstein distance, which the next two sections are devoted to. In Section 7 we give the general definition and derive the basic metric properties of Wasserstein distances between systems on possibly different von Neumann algebras.

Further properties of Wasserstein distances are then investigated in Section 8, along with their consequences. Symmetries of Wasserstein distances obtained in Subsection 8.1, along with the triangle inequality, show how the Wasserstein distance of a system from a possibly simpler (say classical) system satisfying detailed balance, can bound how

far the system is from satisfying detailed balance. This is one of the central conclusions of the paper, and is summarized in Corollary 8.6. Next, keep in mind that a Wasserstein distance can be an asymmetric pseudometric. In particular, zero distance between two systems does not mean that they are the same. Subsection 8.2 investigates how zero Wasserstein distance between two systems relates to common structure in the two systems.

The paper concludes with a short synopsis together with a brief discussion of further work and possibilities in Section 9.

## 2. BASIC CONCEPTS

Here we provide and review relevant concepts and technical definitions used in subsequent sections. Some of these definitions, in particular that of systems, only appear in a special form in this section, with more general versions being treated in Section 7. This is done for clarity and to emphasize the core ideas. For example, here we focus on the case of discrete time.

**2.1. Preliminary definitions, conventions and notations.** Throughout the paper,  $A$ ,  $B$  and  $C$  denote  $\sigma$ -finite von Neumann algebras in standard form, except when stated otherwise. See [9, 29, 51] for the original papers on standard forms, and [19, Section 2.5.4] for a very good treatment. We denote identity operators on Hilbert spaces by 1. In particular, the unit  $1_A$  of a von Neumann algebra  $A$ , represented on a Hilbert space  $H_A$ , will usually be denoted by 1. Denote the set of faithful normal states on  $A$  by  $\mathfrak{F}(A)$ . The normal states are exactly those given by density matrices (see [19, Theorem 2.4.21]).

By the universality of a certain natural positive cone  $\mathcal{P}_A \subset H_A$  associated to  $A$ , the modular conjugation associated to all  $\mu \in \mathfrak{F}(A)$  is the same and will be denoted  $J_A$ . It is an anti-unitary operator in  $H_A$  with  $J_A^2 = 1$ , and we can define the linear map

$$j_A := J_A(\cdot)^* J_A : \mathcal{B}(H_A) \rightarrow \mathcal{B}(H_A)$$

on the bounded linear operators  $\mathcal{B}(H_A)$ , i.e.,  $j_A(a) := J_A a^* J_A$  for every bounded linear  $a : H_A \rightarrow H_A$ . Then  $j_A$  is easily seen to be an anti- $*$ -automorphism. I.e.,  $j_A$  is linear, bijective and  $j_A(a^*) = j_A(a)^*$ , but  $j_A(ab) = j_A(b)j_A(a)$  for all  $a, b \in \mathcal{B}(H_A)$ . From this we can define

$$\mu' = \mu \circ j_A \in \mathfrak{F}(A')$$

on the commutant  $A'$  of  $A$  for every  $\mu \in \mathfrak{F}(A)$ , i.e.,  $\mu'(a') = \mu(j_A(a'))$  for all  $a' \in A'$ . Since every  $\mu \in \mathfrak{F}(A)$  is given by a (unique) cyclic and separating vector  $\Lambda_\mu \in \mathcal{P}_A$  for  $A$ , through

$$\mu(a) = \langle \Lambda_\mu, a \Lambda_\mu \rangle$$

for all  $a \in A$  in terms of  $H_A$ 's inner product, we can represent  $\mu'$  by

$$\mu'(a') = \langle \Lambda_\mu, a' \Lambda_\mu \rangle$$

for all  $a' \in A'$ .

**Example 2.1.** This example briefly recounts a standard form for the von Neumann algebra  $M_n$  of  $n \times n$  complex matrices. First note that any faithful state (necessarily normal in finite dimensions) on  $M_n$  is given by  $\mu(a) = \text{Tr}(\rho_\mu a)$  for all  $a \in M_n$ , where  $\rho_\mu \in M_n$  is some density matrix whose eigenvalues are strictly positive. However, in the general theory we don't use this representation directly. We rather use a standard form, one formulation of which is as follows. Write

$$H_A = \mathbb{C}^n \otimes_s \mathbb{C}^n = M_n,$$

where elementary tensors in  $H_A$  are written in the form  $x \otimes_s y := xy^\top$  in terms of usual matrix multiplication, for column vectors  $x, y \in \mathbb{C}^n$  and with the row vector  $y^\top$  being the transpose of  $y$ . The inner product of  $H_A$  is

$$\langle X, Y \rangle := \text{Tr}(X^*Y)$$

where  $X^* = X^\dagger$  is the usual adjoint of the matrix  $X \in M_n$ . We represent  $M_n$  on  $H_A$  as

$$A = M_n \otimes_s 1_n$$

with  $1_n$  the  $n \times n$  identity matrix. Here we use the notation  $\otimes_s$  to represent the tensor product  $M_n \otimes M_n$  on  $H_A = M_n$  via

$$(a \otimes_s b)X := aXb^\top$$

for all  $a, b \in M_n$ . An alternative but equivalent representation is the ‘‘usual’’ tensor product  $H_A = \mathbb{C}^n \otimes \mathbb{C}^n$  taken as the Kronecker product, but  $\otimes_s$  emphasizes the bimodule structure inherent to our setting and it is more convenient for certain purposes, as will be seen in Example 3.1. (Also see [40, Section 2].)

In this representation we use the notation  $\pi(a) := a \otimes_s 1_n$  and  $\pi'(b) = 1_n \otimes_s b$  for  $a, b \in M_n$ , in terms of which we have

$$\mu(\pi(a)) = \text{Tr}(\rho_\mu a) = \langle \Lambda_\mu, \pi(a)\Lambda_\mu \rangle$$

for all  $a \in M_n$ , where

$$\Lambda_\mu := \rho_\mu^{1/2} \in H_A.$$

Furthermore,  $A$ 's commutant is

$$A' = 1_n \otimes_s M_n,$$

while  $J_A$  is given by

$$J_A \pi(a)\Lambda_\mu = \pi'((a^*)^\top)\Lambda_\mu$$

(which is indeed independent of the faithful state  $\mu$ ) and one has

$$j_A(\pi(a)) = \pi'(a^\top) \quad \text{and} \quad j_A(\pi'(a)) = \pi(a^\top)$$

for  $a \in M_n$ . Note that this means that

$$\mu'(\pi'(a)) = \mu(\pi(a^\top)) = \text{Tr}(\rho_\mu a^\top) = \text{Tr}(\rho_\mu^\top a)$$

for every  $a \in M_n$ . It is easily shown that  $\pi(a^*) = \pi(a)^*$  and  $\pi'(a^*) = \pi'(a)^*$ , i.e.,  $\langle X, \pi(a)Y \rangle = \langle \pi(a^*)X, Y \rangle$ , and similarly for  $\pi'$ . The natural positive cone is defined (see [19, Definition 2.5.25]) to be

$$\mathcal{P}_A = \{\pi(a)j_A(\pi(a)^*)1_n : a \in M_n\} = \{aa^* : a \in M_n\},$$

the trace one elements of which give exactly all the density matrices in  $M_n$ , with  $1_n$  essentially serving as a “reference” element of  $H_A$ .

Keeping these points in mind, one can fairly easily specialize the general von Neumann algebraic setting above to  $M_n$ .

To conclude this example, note that when using the usual tensor product  $\otimes$  instead of  $\otimes_s$ , all the above still goes through, as they are simply different representations of the tensor product, but the resulting representation of  $\Lambda_\mu$  becomes less convenient for our purposes.

**Remark 2.2.** Strictly speaking, everything we have done so far continues to work even if the state  $\mu$  is not faithful (as  $\mathcal{P}_A$  includes all normal states). However, certain duals (see Definition 2.3) are going to play a central role in our work. Their definition requires cyclic vectors for  $A$  in  $\mathcal{P}_A$ , and these are necessarily also separating for  $A$ , making the corresponding states on  $A$  faithful. Hence our focus on faithful states.

Dynamical maps in this paper will be unital positive linear maps (u.p. maps, for short) between von Neumann algebras. In quantum physics one is generally interested in unital completely positive linear maps (u.c.p. maps), but our mathematical framework (and indeed that of [39]) works for u.p. maps. In addition, for certain kinds of detailed balance, we want to be able to view reversing operations, which are not completely positive in the noncommutative case, as a form of dynamics as well (see Sections 5 and 7). We therefore need to cover maps which are merely positive, in our framework. A key notion for us will be that of a dual of a dynamical map. A form general enough for this paper, is as follows.

**Definition 2.3.** Given a u.p. map  $E : A \rightarrow B$  satisfying  $\nu \circ E = \mu$  for some  $\mu \in \mathfrak{F}(A)$  and  $\nu \in \mathfrak{F}(B)$ , its *dual* (w.r.t.  $\mu$  and  $\nu$ )

$$E' : B' \rightarrow A'$$

is defined by

$$\langle \Lambda_\mu, aE'(b')\Lambda_\mu \rangle = \langle \Lambda_\nu, E(a)b'\Lambda_\nu \rangle$$

for all  $a \in A$  and  $b' \in B'$ .

Note that according to [1, Proposition 3.1],  $E'$  exists, and it is a u.p. map satisfying  $\mu' \circ E' = \nu'$ . Under the given assumptions, the maps  $E$  and  $E'$  are necessarily normal, i.e.,  $\sigma$ -weakly continuous. If  $E$  is u.c.p., then so is  $E'$ . The reader can refer to [1] for the theory behind such duals, also summarized in [41, Section 2]. We do not include  $\mu$  and  $\nu$  in the notation for the dual, as it will always be clear from context, and would make the notation unnecessarily cumbersome.

We also point out that unitality and invariance can be viewed as dual properties, in the following sense: Assume that two linear maps  $E : A \rightarrow B$  and  $F : B' \rightarrow A'$  satisfy

$$\langle \Lambda_\mu, aF(b')\Lambda_\mu \rangle = \langle \Lambda_\nu, E(a)b'\Lambda_\nu \rangle$$

for all  $a \in A$  and  $b' \in B'$ . If  $\nu \circ E = \mu$ , then setting  $b' = 1$ , we see that  $F(1) = 1$ , since  $\Lambda_\mu$  is cyclic and separating. The converse is trivial. Similarly for  $\mu \circ F = \nu$  versus  $E(1) = 1$ , by the fact that  $\Lambda_\nu$  is cyclic and separating for  $B$  in terms of its Hilbert space.

The main mathematical object of concern in this paper is a system. A *system*  $\mathbf{A}$  is defined as

$$\mathbf{A} = (A, \alpha, \mu)$$

with  $A$  a von Neumann algebra (as above),  $\alpha : A \rightarrow A$  a u.p. map, and  $\mu \in \mathfrak{F}(A)$  such that  $\mu \circ \alpha = \mu$ .

The *dual* of a system  $\mathbf{A}$  is defined as the system

$$\mathbf{A}' = (A', \alpha', \mu').$$

These notations will be used as a conventions in the rest of the paper, along with

$$\mathbf{B} = (B, \beta, \nu)$$

for a system on  $B$ . In Section 7, however, the definition of a system will be generalized.

**2.2. Transport plans between systems.** The main method of studying systems in this paper is through transport between systems. Given two systems  $\mathbf{A}$  and  $\mathbf{B}$ , a *transport plan*  $\omega$  from  $\mathbf{A}$  to  $\mathbf{B}$  is a state  $\omega$  on the algebraic tensor product  $A \odot B'$  such that

$$(1) \quad \omega(a \otimes 1) = \mu(a) \quad \text{and} \quad \omega(1 \otimes b') = \nu'(b')$$

and

$$(2) \quad \omega(\alpha(a) \otimes b') = \omega(a \otimes \beta'(b'))$$

for all  $a \in A$  and  $b' \in B'$ . We express this by the notation

$$\mathbf{A}\omega\mathbf{B}$$

and denote the set of all such transport plans  $\omega$  by

$$T(\mathbf{A}, \mathbf{B}).$$

The notion  $\mathbf{A}\omega\mathbf{B}$  was introduced in [41] under the name ‘‘balance’’ as an extension of certain detailed balance conditions. The latter would be formulated in terms of  $B = A$ , with  $\beta$  being some variation on the dual  $\alpha'$  of  $\alpha$ , while  $\omega$  is a specific state; this will be reviewed in Section 5. At the same time it extends the notion of a joining in ergodic theory, which allows one to study certain qualitative and structural aspects of dynamical systems, essentially by comparing different systems (see [47] for the classical theory, and [35, 36, 37, 11, 12, 13] for a



noncommutative version). Both these points are relevant in this paper as well. However, we take the (optimal) transport point of view in this paper, hence we refer to  $\mathbf{A}\omega\mathbf{B}$  as transport from  $\mathbf{A}$  to  $\mathbf{B}$ , rather than as balance. A special case of this was used in [38], specifically for modular dynamics (from Tomita-Takesaki theory), to obtain symmetry of Wasserstein metrics on states.

If the state  $\omega$  is only required to satisfy the coupling property (1), then it is called a *transport plan*  $\omega$  from  $\mu$  to  $\nu$ . The set of all of these is denoted by

$$T(\mu, \nu).$$

This is in fact a fairly direct extension of classical transport plans, a nice discussion of which, including why it is thought of as transport, can be found in the introduction to [69]. There a transport plan  $\pi$  from one probability measure  $\mu$  (on a space  $X$ ) to another  $\nu$  (on a space  $Y$ ) is simply a coupling of the two measures, i.e.,  $\pi(U \times Y) = \mu(U)$  and  $\pi(X \times V) = \nu(V)$ , with the following interpretation:  $\pi(U \times V)$  is the “amount” of probability transported from  $U \subset X$  to  $V \subset Y$ .

The reason for involving the dual of a system, in particular the commutant of the von Neumann algebra, is to alleviate obstacles due to noncommutativity. This is what ultimately allows one to obtain the usual metric properties for Wasserstein distances, specifically the triangle inequality and zero distance between a system and itself. It is at the core of the bimodule approach to Wasserstein distances, and serves as the key to the mathematical foundation of this paper.

It is well known in quantum physics, in particular in the context of quantum information, that a transport plan  $\omega$  corresponds to a u.c.p. map i.e., a channel,  $E_\omega : A \rightarrow B$ , although the terminology “transport plan” is not standard in this context, nor the interpretation as transport (as an analogy to the classical case). See in particular [26] for the finite dimensional case, as is typically used in quantum information. A general form of this correspondence was discussed and used in [11, 41], making use of [1]. In the context of transport plans, this of course means that a transport plan can be represented as a u.c.p. map, as has been pointed out by [33]. In this way a transport plan can indeed be viewed as a dynamical map from one system to another, in the conventional quantum mechanical sense. The relevant technical details will be presented in Section 7. In the classical setting the correspondence between couplings of probability measures and Markov operators was studied in a special case (for couplings of a measure with itself) in [20], and more generally in [57, 15], though it does not appear to be widely used in classical optimal transport.

### 3. CONCEPTUAL EXPOSITION

In this section we describe the basic conceptual approach of this paper, including a preliminary discussion of Wasserstein distance without

proofs. This also provides the basics on Wasserstein distance needed in the examples studied in the subsequent sections. The general theory of Wasserstein distance will be taken up in Section 7. The key ideas of this section are illustrated in a simple classical case in Section 4, which the reader can read before this section with minimal loss in continuity.

**3.1. Extending dynamical properties by optimal transport.** Given a property which a system may have or may not have, we aim to define an extended or generalized version of this property for a system  $\mathbf{A}$ , by requiring  $\mathbf{A}$  to satisfy

$$\mathbf{A}\omega\mathbf{B}$$

for some system  $\mathbf{B}$  which does satisfy the original property. In particular, our goal is to define extensions of detailed balance conditions in this way. Keep in mind that when  $\omega$  is a product state,  $\mathbf{A}\omega\mathbf{B}$  is trivial. To ensure that the condition  $\mathbf{A}\omega\mathbf{B}$  is nontrivial and indeed as strong as possible, we are going to frame this approach as an optimal transport problem. Wasserstein distances will deliver optimal transport plans, which in our approach are viewed as the strongest cases of the condition  $\mathbf{A}\omega\mathbf{B}$ . This optimization and Wasserstein distances will be discussed in more detail in the next subsection.

Of course, one may as well instead consider

$$\mathbf{B}\psi\mathbf{A},$$

which gives an alternative way to extend properties from  $\mathbf{B}$  to  $\mathbf{A}$ , by viewing it as an optimal transport problem from  $\mathbf{B}$  to  $\mathbf{A}$ . The two points of view are complementary, but not equivalent. It will indeed be seen later on that the Wasserstein distances involved are not necessarily symmetric.

We are going to motivate this transport plan interpretation by viewing it as a refinement of the transfer of probabilities in  $\mathbf{A}$  itself during each step in its discrete time evolution.

First notice that the two basic properties satisfied by the completely positive map  $\alpha$ , namely invariance  $\mu \circ \alpha$  and unitality, which are dual to one another, can respectively be expressed as  $\mathbf{A}\omega\mathbf{B}$  and  $\mathbf{B}\psi\mathbf{A}$ , if  $\mathbf{B}$  is taken as a 1-point system. By the latter terminology we mean that  $B = \mathbb{C}$ . In terms of the algebraic tensor product  $A \odot B'$ , one then necessarily has

$$\omega = \mu \odot \nu' \quad \text{and} \quad \psi = \nu \odot \mu',$$

which means that  $\mathbf{A}\omega\mathbf{B}$  merely says

$$\mu \circ \alpha(a)b' = \omega(\alpha(a) \otimes b') = \omega(a \otimes \beta'(b')) = \mu(a)b'$$

for all  $a \in A$  and  $b' \in B' = \mathbb{C}$ , i.e.,  $\mu \circ \alpha = \mu$ , while  $\mathbf{B}\psi\mathbf{A}$  similarly expresses  $\mu' \circ \alpha' = \mu'$ , which is dual (and equivalent) to  $\alpha(1) = 1$ .

In terms of transport between  $\mathbf{A}$  and  $\mathbf{B}$ , this means that transport from  $\mathbf{A}$  to a single point expresses state invariance, while transport from a single point to  $\mathbf{A}$  expresses unitality of  $\alpha$ . In the classical case

where  $\mathbf{A}$  consists of a finite number of points, one can in fact identify the 1-point system as an arbitrary point in  $\mathbf{A}$ , as will be seen in the next section.

By replacing the 1-point system by a general  $\mathbf{B}$ , we in effect lift transfer of probabilities to or from a single point, to a more general form of transport to or from  $\mathbf{B}$ . The condition  $\mathbf{A}\omega\mathbf{B}$  then refines state invariance, while  $\mathbf{B}\psi\mathbf{A}$  refines unitality. This refinement of these two dual properties each places further restrictions on  $\mathbf{A}$ , determined by the properties of  $\mathbf{B}$ .

By enforcing optimal transport through a Wasserstein distance, these refinements are made as strong as possible, quantifying how strongly the properties of  $\mathbf{B}$  are reflected in  $\mathbf{A}$ . This can then be used to explore generalized versions of properties of  $\mathbf{B}$  in an arbitrary system  $\mathbf{A}$ .

When  $\mathbf{A}$  and  $\mathbf{B}$  are systems on the same observable algebra, and the Wasserstein distance is a (typically asymmetric) metric, then the extreme case of zero distance means that  $\mathbf{A} = \mathbf{B}$ , i.e.,  $\mathbf{A}$  has all of  $\mathbf{B}$ 's properties. Other cases are typically weaker versions of this extreme case, which can for example provide weakened forms of detailed balance in  $\mathbf{A}$ .

Placing restrictions on a system  $\mathbf{A}$  through (optimal) transport to or from a “model system”  $\mathbf{B}$  is natural, as such conditions generalize probability transfer between individual points in a classical system. When  $\mathbf{B}$  is assumed to satisfy some form of detailed balance, this provides a way to formulate extensions of this detailed balance condition in  $\mathbf{A}$ . As this is done in a very structured way, it has the potential to provide classes of systems having sufficient structure to include natural, yet mathematically accessible, non-equilibrium systems.

Note that as  $\mathbf{A}\omega\mathbf{B}$  and  $\mathbf{B}\psi\mathbf{A}$  relate to two different properties of  $\mathbf{A}$ , namely  $\mu\alpha = \mu$  and  $\alpha(1) = 1$  respectively, we would not expect perfect symmetry between the two situations, even classically. This is indeed what is found. In particular, our Wasserstein distances typically turn out to be asymmetric, since the two directions (the distance from  $\mathbf{A}$  to  $\mathbf{B}$  versus from  $\mathbf{B}$  to  $\mathbf{A}$ ) relate to different (though dual) aspects of dynamics.

For simplicity, in the examples of this paper the case where  $\mathbf{B}$  is a classical system on a finite set of points will be emphasized. On the one hand this simplifies calculations involved, but it also simplifies and clarifies how to identify detailed balance type properties consequently appearing in  $\mathbf{A}$ .

**3.2. Wasserstein distances.** We intend to define a Wasserstein distance from  $\mathbf{A}$  to  $\mathbf{B}$  in analogy to quadratic Wasserstein distance between probability measures on  $\mathbb{R}^d$ , while also taking the dynamics into account. Due to the dynamics and noncommutativity, such distances are typically not symmetric, i.e., the distance from  $\mathbf{B}$  to  $\mathbf{A}$  may differ

than that from  $\mathbf{A}$  to  $\mathbf{B}$ . In Section 7 it will be seen that one can define refined versions of these Wasserstein distances, including symmetric versions. In this section, however, only the most basic form will be outlined in a special case. The general development of the theory is postponed until Section 7.

We assume that  $\mathbf{A}$  and  $\mathbf{B}$  are equipped with “ $d$ -dimensional coordinate systems” expressed as

$$k = (k_1, \dots, k_d) \quad \text{and} \quad l = (l_1, \dots, l_d)$$

respectively, where  $k_i \in A$  and  $l_i \in B$  for  $i = 1, \dots, d$ . Here we do not place any restrictions on the choice of  $k$  and  $l$ , for example,  $l_1 = l_2$  is allowed.

When we confine ourselves to the case of finite dimensional or abelian von Neumann algebras, then these coordinate systems define a cost  $I(\omega)$  for any transport plan  $\omega \in T(\mathbf{A}, \mathbf{B})$  from  $\mathbf{A}$  to  $\mathbf{B}$  by

$$(3) \quad I(\omega) = \omega \left( \sum_{i=1}^d |k_i \otimes 1 - 1 \otimes (S_\nu l_i^* S_\nu)|^2 \right)$$

in analogy to the classical transport cost for a transport plan  $\pi$  between two measures on the same subset  $X$  of  $\mathbb{R}^d$

$$(4) \quad I(\pi) = \int_{X \times X} \|x - y\|^2 d\pi(x, y)$$

in terms of the Euclidean norm on  $\mathbb{R}^d$ . Wasserstein distance is obtained as the minimum of the square root of the cost.

Note, however, the inclusion of the conjugate linear operator  $S_\nu : H_B \rightarrow H_B$  from Tomita-Takesaki theory, defined by

$$S_\nu b \Lambda_\nu := b^* \Lambda_\nu.$$

The inclusion of this operator ensures that we get the usual metric properties, in particular the triangle inequality and zero distance between a system and itself. For more general von Neumann algebras,  $S_\nu$  can be unbounded, leading to technical complications which we can circumvent in Section 7 by an alternative approach containing (3) as special case. For the examples discussed in Sections 4 and 6, the formulation (3) will be sufficient though. In addition it gives a bird’s-eye view of both the similarities and the differences between the classical and noncommutative cases.

In relation to the latter point, notice that for abelian  $B$ , finite dimensional or not, one has  $S_\nu b^* S_\nu = b$  for all  $b \in B$ . In this way the classical cost (4) can be recovered as a special case of the form in (3), at least for a bounded subset  $X$  of  $\mathbb{R}^d$ .

Of course, as opposed to the case of Wasserstein distance between measures on the same space  $X$ , (3) is also set up to provide costs and

consequently distances between systems on different von Neumann algebras. This is of central importance to our aims, allowing one to analyze a system by comparing it to simpler or well understood systems, including those on other algebras.

The Wasserstein distance from  $\mathbf{A}$  to  $\mathbf{B}$  corresponding to the chosen coordinate systems, is defined as

$$(5) \quad W(\mathbf{A}, \mathbf{B}) := \inf_{\omega \in T(\mathbf{A}, \mathbf{B})} I(\omega)^{1/2}.$$

This infimum is reached, as will be seen in Section 7, therefore optimal transport plans (i.e., plans with minimum cost) always exist. The key point in this definition, though, is that the infimum is over the set of all transport plans from  $\mathbf{A}$  to  $\mathbf{B}$ , making this Wasserstein distance a natural way to obtain optimal forms of the transport conditions in the previous subsection.

To apply this in practice and particular examples, one should keep in mind that the  $k$  and  $l$  appearing in a Wasserstein distance are viewed as “coordinates” measuring particular aspects of  $\mathbf{A}$  and  $\mathbf{B}$  respectively. In particular, they may be chosen to be relevant observables in  $\mathbf{A}$  and  $\mathbf{B}$ . In addition, for every  $p$  one can aim to choose  $k_p$  and  $l_p$  to measure corresponding quantities in  $\mathbf{A}$  and  $\mathbf{B}$ , say spin in some direction of a particular spin site in each, in order for the difference between  $k_p$  and  $l_p$  in (3) to have a sensible physical meaning.

A cardinal point regarding (3) is that zero cost between a quantum system and itself can always be attained by using a maximally entangled state as the transport plan. This is why we have

$$W(\mathbf{A}, \mathbf{A}) = 0$$

as one would expect of a distance function. This appears to be a simple point, but it is subtler than one may initially expect. The key aspect of this is illustrated as part of the next example.

**Example 3.1.** Consider the standard form of  $M_n$  as described in Example 2.1. Note that we can identify  $A \odot A'$  with  $M_n \otimes_s M_n$  and  $\pi(a) \otimes \pi'(b)$  with  $a \otimes_s b$ . To see that our setup indeed leads to  $W(\mathbf{A}, \mathbf{A}) = 0$  for the von Neumann algebra  $M_n$ , consider the entangled state  $\omega = \delta_\mu$  of  $\mu$  and  $\mu'$ , defined on  $A \odot A'$  by

$$\delta_\mu(a \otimes_s b) := \langle \Lambda_\mu, (a \otimes_s b) \Lambda_\mu \rangle = \text{Tr}(\rho_\mu^{1/2} a \rho_\mu^{1/2} b^\top)$$

for  $a, b \in M_n$ . This is a pure state, since the vector  $\Lambda_\mu \in H_A$  is a pure state of the composite system, reducing to  $\mu$  and  $\mu'$  respectively, and in this sense we view  $\delta_\mu$  as a maximally entangled state of  $\mu$  and  $\mu'$ . (When  $\rho_\mu$  is diagonal with diagonal entries  $p_1, \dots, p_n$ , we in fact have the conventional and well known representation  $\sum_{i=1}^n \sqrt{p_i} e_i \otimes e_i$  of  $\Lambda_\mu$ , but our standard form above is more convenient below for the general case.)

Note that for  $a, b \in M_n$  we have

$$S_\mu^* \pi(a)^* S_\mu \pi(b) \Lambda_\mu = \pi'((\rho_\mu^{-1/2} a \rho_\mu^{1/2})^\top) \pi(b) \Lambda_\mu,$$

hence  $S_\mu^* \pi(a)^* S_\mu = \pi'((\rho_\mu^{-1/2} a \rho_\mu^{1/2})^\top) \in A'$ , which is the first key point of this example. Furthermore,  $S_\nu \pi(a^*) S_\nu \Lambda_\mu = \pi(a) \Lambda_\mu$ , therefore

$$\delta_\mu(|\pi(a) - S_\nu \pi(a^*) S_\nu|^2) = 0.$$

Hence  $\delta_\mu \in T(\mu, \mu)$  is a transport plan having zero cost. This is what makes  $W(\mathbf{A}, \mathbf{A}) = 0$  possible, concluding this example.

Our general theory of Wasserstein distances and their basic metric properties, including  $W(\mathbf{A}, \mathbf{A}) = 0$  and the triangle inequality, will be treated in Section 7. In some other approaches to Wasserstein distances via transport plans (in the special case of states, rather than systems), the property  $W(\mu, \mu) = 0$  and the usual triangle inequality are not obtained. For example [49] and [33], even though the latter follows a similar approach to cost as this paper. It should be noted that these papers nevertheless manage to make progress on their applications, and indeed [46] has pointed out that a lack of the usual metric properties is actually of value in certain contexts. A nice discussion and enlightening illustrations of the obstacles to metric properties for quantum Wasserstein distances via transport plans can be found in [6].

For our purposes though, it is most natural to have the triangle inequality (see for example its use in Corollary 8.6) and  $W(\mathbf{A}, \mathbf{A}) = 0$ . On the other hand, asymmetry of a Wasserstein distance has a natural place in our theory, as already hinted in Subsection 3.1. This will also be seen in the next section. The bimodule setup for Wasserstein metrics indeed provide symmetric and asymmetric Wasserstein distances, depending on the restrictions we place on the transport plans, as has been discussed in [38, 39] and will be seen in Section 7.

#### 4. A SIMPLE CLASSICAL EXAMPLE

We now clarify the approach in the previous section further by illustrating it with classical systems, each on a finite number of points. In this case the transfer of probabilities are easy to follow, making the setup in Subsection 3.1 particularly transparent.

**4.1. The setting.** Represent the von Neumann algebra  $A$  of complex-valued functions on  $m$  points as  $A = \mathbb{C}^m$ , viewed as column matrices. Then  $A$  is an algebra with involution (and indeed an abelian von Neumann algebra) by using entry-wise operations; for example the involution is given by taking the complex conjugate of each entry. We label the points  $1, \dots, m$ . A standard form of  $A$  is obtained by representing the entries of  $a \in A$  along the diagonal of an  $m \times m$  matrix acting on  $H_A = \mathbb{C}^m$ , or simply letting  $A$  act entry-wise on  $H_A$ , so essentially we

have  $A$  in standard form (with  $A' = A$  and  $j_A : A \rightarrow A$  the identity map, hence not relevant in this section). Similarly, for  $B$  on  $n$  points.

We consider Markov chains on these  $m$  and  $n$  point sets, respectively given by the  $m \times m$  and  $n \times n$  transition matrices

$$\alpha = [\alpha_{pq}] \quad \text{and} \quad \beta = [\beta_{rs}],$$

where

$$(6) \quad \alpha_{pq} \geq 0 \quad \text{and} \quad \sum_{q=1}^m \alpha_{pq} = 1,$$

and similarly for  $\beta$ . Note that  $\alpha_{pq}$  is the probability for a transition to occur from point  $p$  to point  $q$ .

The states  $\mu$  and  $\nu$  on  $A$  and  $B$  respectively, are represented as row matrices

$$\mu = [ \mu_1 \quad \cdots \quad \mu_m ] \quad \text{and} \quad \nu = [ \nu_1 \quad \cdots \quad \nu_n ],$$

with  $\mu_p > 0$  and  $\mu_1 + \dots + \mu_m = 1$  and correspondingly for  $\nu$ . These are assumed to be invariant,

$$\mu\alpha = \mu \quad \text{and} \quad \nu\beta = \nu,$$

in terms of usual matrix multiplication, i.e.,  $\mu \circ \alpha = \mu\alpha$ . Correspondingly  $\alpha$  acts on  $A$  through usual matrix multiplication,  $\alpha(a) = \alpha a$ , hence we have a system  $\mathbf{A} = (A, \alpha, \mu)$ .

The system  $\mathbf{B} = (B, \beta, \nu)$  is said to be in *detailed balance*, when

$$\nu_r \beta_{rs} = \nu_s \beta_{sr},$$

for all  $r, s = 1, \dots, n$ , i.e., the transfer of probability from point  $r$  to point  $s$ , is the same as from  $s$  to  $r$ . This is a strictly stronger property than invariance, except for  $n = 2$ , in which case the two properties are equivalent.

In the current representation, the dual (from Subsection 2.1) of  $\mathbf{A}$  is the system  $\mathbf{A}' = (A, \alpha', \mu)$  with  $\alpha'$  given by

$$\alpha'_{pq} = \frac{\mu_q}{\mu_p} \alpha_{qp}$$

for all  $p, q = 1, \dots, m$ . This tells us that  $\mathbf{A}'$  is the time-reversal of  $\mathbf{A}$ . Detailed balance of  $\mathbf{B}$  can thus be expressed as  $\beta' = \beta$ , i.e.,

$$\mathbf{B}' = \mathbf{B}.$$

**4.2. Extending probability transfer to or from a point.** The total transfer of probability from the whole of  $\mathbf{A}$  to a single point  $q$  in  $\mathbf{A}$ , can be written as

$$(7) \quad \sum_{p=1}^m \mu_p \alpha_{pq} = \mu_q,$$

which simply expresses the invariance  $\mu\alpha = \mu$ . In Subsection 3.1 we pointed out that  $\mathbf{A}\omega\mathbf{B}$  generalizes this condition, being viewed as probability transfer from  $\mathbf{A}$  to  $\mathbf{B}$ , instead of from  $\mathbf{A}$  to a single point in  $\mathbf{A}$ . We interpreted  $\mathbf{A}\omega\mathbf{B}$  as a refinement of  $\mu\alpha = \mu$ . This will now be seen concretely for the current classical systems. (We now write  $\otimes$ , instead of  $\odot$  as in Subsection 3.1, since in finite dimensions we do not need to distinguish between algebraic tensor products and completions thereof.)

Using the Kronecker product convention

$$\mu \otimes \nu = [ \mu\nu_1 \quad \cdots \quad \mu\nu_n ],$$

a transport plan  $\omega$  from  $\mu$  to  $\nu$  can be represented as

$$\omega = [ \omega_{11} \quad \cdots \quad \omega_{m1} \quad \cdots \quad \omega_{1n} \quad \cdots \quad \omega_{mn} ],$$

with  $\omega_{pr} \geq 0$ , in terms of which the conditions

$$\sum_{r=1}^n \omega_{pr} = \mu_p \quad \text{and} \quad \sum_{p=1}^m \omega_{pr} = \nu_r$$

express the coupling properties of  $\omega$ . Note that in this finite context, the transport plan  $\omega$  says exactly that the portion  $\omega_{pr}$  of the probability  $\mu_p$  of point  $p$  in  $\mathbf{A}$ , is transported to point  $r$  in  $\mathbf{B}$ , with the coupling conditions above expressing the total transport from  $p$  and to  $r$  respectively.

Then

$$\omega(\alpha(a) \otimes b) = \omega \begin{bmatrix} \alpha(a)b_1 \\ \vdots \\ \alpha(a)b_n \end{bmatrix} = \sum_{p,q,r} \omega_{pr} \alpha_{pq} a_q b_r,$$

and similarly

$$\omega(a \otimes \beta'(b)) = \sum_{q,r,s} \omega_{qs} a_q \beta'_{sr} b_r.$$

For  $\omega$  to be a transport plan from  $\mathbf{A}$  to  $\mathbf{B}$ , written  $\mathbf{A}\omega\mathbf{B}$  or  $\omega \in T(\mathbf{A}, \mathbf{B})$ , requires the further condition  $\omega(\alpha(a) \otimes b) = \omega(a \otimes \beta'(b))$ , expressed by

$$(8) \quad \sum_{p=1}^m \omega_{pr} \alpha_{pq} = \sum_{s=1}^n \omega_{qs} \beta'_{sr} = \sum_{s=1}^n \omega_{qs} \frac{\nu_r}{\nu_s} \beta_{rs},$$

which when summed over  $r$  gives exactly (7). Hence (8) is clearly a refinement of (7).

Essentially the probability  $\mu_p$  of  $p$  in  $\mathbf{A}$  is split into  $n$  ‘‘compartments’’ having probabilities  $\omega_{p1}, \dots, \omega_{pn}$  respectively, with the transition probability  $\alpha_{pq}$  to  $q$  in  $\mathbf{A}$  then acting on each of these compartments. The sum of the probabilities transported from the  $r$ ’th compartment of each of  $\mathbf{A}$ ’s points to  $q$  by  $\alpha$ , is then required to be given by the total transport by  $\beta'$  from  $q$ ’s compartments to point  $r$  in  $\mathbf{B}$ .



Paraphrasing this: the transport from  $r$  to  $q$  by  $\alpha$ , is equal to the transport from  $q$  to  $r$  by  $\beta'$ . The analogy with detailed balance is clear. Keep in mind that we are particularly interested in the case where  $\beta' = \beta$ , i.e., where  $\mathbf{B}$  is in detailed balance.

In this way  $\alpha$  is required in some measure to adhere to rules laid down by  $\beta$ . In the one extreme case where  $\omega = \mu \otimes \nu$ , no restrictions are placed on  $\alpha$  by  $\mathbf{A}\omega\mathbf{B}$ . In the other extreme, with  $(A, \mu) = (B, \nu)$  and  $\omega$  the diagonal measure associated to  $\mu$ , i.e.,  $\omega_{pp} = \mu_p$  while  $\omega_{pq} = 0$  for  $p \neq q$ , the condition  $\mathbf{A}\omega\mathbf{B}$  forces  $\alpha = \beta$ . The role of a Wasserstein distance  $W(\mathbf{A}, \mathbf{B})$  is to optimize this to determine how much of, or to what extent,  $\mathbf{B}$ 's behaviour is reflected in that of  $\mathbf{A}$ .

Analogously for the transfer of probability from a single point  $p$  in  $\mathbf{A}$  to the whole of  $\mathbf{A}$ , versus  $\mathbf{B}\psi\mathbf{A}$ . The latter acts as a refinement of the dual property  $\alpha(1_m) = 1_m$  with  $1_m$  the column with 1 as all  $m$  entries, i.e.,  $\mu\alpha' = \mu$  (or  $\mu' \circ \alpha' = \mu'$  in the general abstract notation), instead of  $\mu\alpha = \mu$ . As above,  $\mathbf{B}\psi\mathbf{A}$  is expressed by

$$(9) \quad \sum_{r=1}^n \psi_{rp} \beta_{rs} = \sum_{q=1}^m \psi_{sq} \alpha'_{qp} = \sum_{q=1}^m \psi_{sq} \frac{\mu_p}{\mu_q} \alpha_{pq},$$

the sum over  $s$  of which gives the transfer of probability from a single point  $p$  in  $\mathbf{A}$  to the whole of  $\mathbf{A}$ ,

$$\sum_{q=1}^m \mu_p \alpha_{pq} = \mu_p,$$

which indeed simply expresses  $\alpha(1_m) = 1_m$ . In the paraphrased form as above, (9) says that the transport from  $p$  to  $s$  by  $\beta$ , is equal to the transport from  $s$  to  $p$  by  $\alpha'$ . Again this requires  $\mathbf{A}$  to adhere in some degree to some aspects of  $\mathbf{B}$ 's behaviour, the extent of which will be measured by the Wasserstein distance  $W(\mathbf{B}, \mathbf{A})$ .

To clarify the connection to the case  $\mathbf{A}\omega\mathbf{B}$ , we can without loss of generality use the dual transport plan  $\omega'$ , which in this context (the general case to be treated in Section 8) is simply the reverse of a transport plan  $\omega$  from  $\mathbf{A}$  to  $\mathbf{B}$ , namely

$$\omega' = \left[ \begin{array}{cccc} \omega'_{11} & \cdots & \omega'_{n1} & \cdots \\ & & \omega'_{1m} & \cdots \\ & & & \omega'_{nm} \end{array} \right],$$

where  $\omega'_{rp} = \omega_{pr}$ , with  $\mathbf{B}\omega'\mathbf{A}$  therefore expressed by

$$\sum_{q=1}^m \omega_{qs} \frac{\mu_p}{\mu_q} \alpha_{pq} = \sum_{r=1}^n \omega_{pr} \beta_{rs}.$$

Note that there is an asymmetry between  $\mathbf{A}\omega\mathbf{B}$  and  $\mathbf{B}\omega'\mathbf{A}$ . This boils down to  $\mathbf{A}\omega\mathbf{B}$  being equivalent to  $\mathbf{B}'\omega'\mathbf{A}'$ , as is easily checked, rather than to  $\mathbf{B}\omega'\mathbf{A}$ . The set of transport plans  $T(\mathbf{B}, \mathbf{A})$  need not consist of the reversals of the transport plans  $T(\mathbf{A}, \mathbf{B})$ . In particular, the optimal transport plan from  $\mathbf{B}$  to  $\mathbf{A}$  need not be the reverse (i.e.,

the dual) of the optimal transport plan from  $\mathbf{A}$  to  $\mathbf{B}$ . Consequently, we can typically expect  $W(\mathbf{A}, \mathbf{B}) \neq W(\mathbf{B}, \mathbf{A})$ . If both  $\mathbf{A}$  and  $\mathbf{B}$  satisfy detailed balance, then  $\mathbf{A}\omega\mathbf{B}$  and  $\mathbf{B}\omega'\mathbf{A}$  are equivalent, which will ensure  $W(\mathbf{A}, \mathbf{B}) = W(\mathbf{B}, \mathbf{A})$ .

**4.3. An explicit example.** In order to do explicit calculations easily, we consider an example for the case  $m = 4$  and  $n = 2$ . This example also illustrates how an appropriate Wasserstein distance can be chosen, and the low dimensions allow us to find a simple formula for it, which in turn sheds light on its role.

Let both the systems  $\mathbf{A}$  and  $\mathbf{B}$  be given by Markov chains as in the previous subsection, where we take  $\mathbf{A}$  to be the composite of two 2-point systems, while  $\mathbf{B}$  is a 2-point system. In the case of  $\mathbf{A}$ , the indices in  $\alpha_{pq}$  refer to the points of its 4-point set  $\{1, 2\} \times \{1, 2\}$  labeled as follows in terms of the original 2-point set  $\{1, 2\}$ :

$$\begin{aligned} 1 &\equiv (1, 1), & 2 &\equiv (2, 1) \\ 3 &\equiv (1, 2), & 4 &\equiv (2, 2) \end{aligned}$$

For  $\mathbf{B}$  on the other hand, we adapt the notation for the transition matrix as follows:

$$\beta = \begin{bmatrix} \tilde{r} & r \\ s & \tilde{s} \end{bmatrix}$$

with  $0 \leq r, s \leq 1$ , and

$$\tilde{r} = 1 - r \quad \text{and} \quad \tilde{s} = 1 - s.$$

Recall that due to  $\nu\beta = \nu$ ,  $\mathbf{B}$  necessarily satisfies detailed balance, namely

$$\nu_1 r = \nu_2 s.$$

We interpret  $\mathbf{A}$  as a system consisting of two classical spins, and  $\mathbf{B}$  as a single classical spin. Natural ‘‘coordinates’’, measuring these spin values are therefore

$$k_1 = \frac{1}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \otimes 1_2 \quad \text{and} \quad k_2 = 1_2 \otimes \frac{1}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

for  $\mathbf{A}$ , where  $1_2$  is the column with 1 as both entries, and

$$(10) \quad l = l_1 = l_2 = \frac{1}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

for  $\mathbf{B}$ . This will define the Wasserstein distances from  $\mathbf{A}$  to  $\mathbf{B}$ , and from  $\mathbf{B}$  to  $\mathbf{A}$ ; see Subsection 3.2.

We assume that the cost  $\omega c_{AB}$  for a transport plan  $\omega \in T(\mathbf{A}, \mathbf{B})$  is given as in (3) by the *cost matrix*

$$c_{AB} = |k_1 \otimes 1_2 - 1_4 \otimes l|^2$$

from systems on  $A$  to systems on  $B$  (here  $S_\nu l^* S_\nu = l$ , since  $B$  is abelian), which in transposed form (for typographical convenience) is

$$c_{AB}^\top = (0, 1, 0, 1, 1, 0, 1, 0).$$

(In this subsection we often write row matrices as tuples to clearly delineate the entries). This measures the square of the difference in the value of the “first” spin in  $\mathbf{A}$  and the spin in  $\mathbf{B}$ . Lower cost should therefore correspond to transitions from the set  $\{1, 3\}$  to the set  $\{2, 4\}$  and vice versa in  $\mathbf{A}$ , in order to conform to transitions between 1 and 2 in  $\mathbf{B}$ .

A convenient parametrization of the set  $T(\mu, \nu)$  of transport plans  $\omega$  from  $\mu$  to  $\nu$  for this cost matrix, is

$$\omega = (\mu_1 - \gamma_1, \gamma_2, \mu_3 - \gamma_3, \gamma_4, \gamma_1, \mu_2 - \gamma_2, \gamma_3, \mu_4 - \gamma_4),$$

where  $0 \leq \gamma_i \leq \mu_i$  for  $i = 1, 2, 3, 4$ , and

$$\mu_1 - \gamma_1 + \gamma_2 + \mu_3 - \gamma_3 + \gamma_4 = \nu_1.$$

This is convenient, since then the cost of the transport plan is then given by

$$\omega c_{AB} = \gamma_1 + \gamma_2 + \gamma_3 + \gamma_4,$$

the minimum of which over all  $\omega \in T(\mathbf{A}, \mathbf{B})$  is the squared Wasserstein distance  $W(\mathbf{A}, \mathbf{B})^2$ .

Any  $\omega \in T(\mathbf{A}, \mathbf{B})$  is described by the further conditions

$$(\mu_1\alpha_{12} + \mu_3\alpha_{32}) + (-\gamma_1\alpha_{12} + \gamma_2\alpha_{22} - \gamma_3\alpha_{32} + \gamma_4\alpha_{42}) = \mu_2s + \gamma_2(\bar{r} - s)$$

$$(\mu_1\alpha_{14} + \mu_3\alpha_{34}) + (-\gamma_1\alpha_{14} + \gamma_2\alpha_{24} - \gamma_3\alpha_{34} + \gamma_4\alpha_{44}) = \mu_4s + \gamma_4(\bar{r} - s)$$

and

$$(\mu_2\alpha_{21} + \mu_4\alpha_{41}) + (\gamma_1\alpha_{11} - \gamma_2\alpha_{21} + \gamma_3\alpha_{31} - \gamma_4\alpha_{41}) = \mu_1r + \gamma_1(\bar{r} - s)$$

$$(\mu_2\alpha_{23} + \mu_4\alpha_{43}) + (\gamma_1\alpha_{13} - \gamma_2\alpha_{23} + \gamma_3\alpha_{33} - \gamma_4\alpha_{43}) = \mu_3r + \gamma_3(\bar{r} - s),$$

which we now view as an extended or generalized detailed balance condition. Due to the invariance  $\mu\alpha = \mu$ , there are other equivalent ways of stating these conditions, however, the form above emphasizes transitions in  $\mathbf{A}$  from the set  $\{1, 3\}$  to the set  $\{2, 4\}$  in the first two conditions, and vice versa in the last two. This generalized detailed balance condition is trivial when  $\omega = \mu \otimes \nu$ , though, and is therefore not of much use as it stands. We need to quantify how strong it is, which is where the cost and Wasserstein distance come into play.

In particular, zero cost  $\omega c_{AB} = 0$  corresponds to the conditions

$$(11) \quad \mu_1\alpha_{12} + \mu_3\alpha_{32} = \mu_2s, \quad \mu_1\alpha_{14} + \mu_3\alpha_{34} = \mu_4s$$

and

$$(12) \quad \mu_2\alpha_{21} + \mu_4\alpha_{41} = \mu_1r, \quad \mu_2\alpha_{23} + \mu_4\alpha_{43} = \mu_3r,$$

which in our picture therefore give the form of the generalized detailed balance condition in  $\mathbf{A}$  closest (in terms of our chosen cost) to the detailed balance in  $\mathbf{B}$ . We note that these conditions are indeed satisfied by a multitude of systems  $\mathbf{A}$  and  $\mathbf{B}$ , hence zero cost can indeed be reached, in this case for the uniquely determined transport plan

$$\omega = (\mu_1, 0, \mu_3, 0, 0, \mu_2, 0, \mu_4).$$

It is also clear that in this example  $\mathbf{B}$  is uniquely determined by  $\mathbf{A}$  when  $\omega_{c_{AB}} = 0$ . In particular,  $\mu_1 + \mu_3 = \nu_1$ .

In the latter, we obviously have  $W(\mathbf{A}, \mathbf{B}) = 0$ . However, more generally for any  $\mathbf{A}$  and  $\mathbf{B}$  in this example,  $W$  gives us bounds on how far the generalized detailed balance condition is from the optimal form (11) and (12). To see this, a simple definition of the deviation from this optimal form can for example be taken as

$$f = |\mu_1\alpha_{12} + \mu_3\alpha_{32} - \mu_2s| + |\mu_1\alpha_{14} + \mu_3\alpha_{34} - \mu_4s| \\ + |\mu_2\alpha_{21} + \mu_4\alpha_{41} - \mu_1r| + |\mu_2\alpha_{23} + \mu_4\alpha_{43} - \mu_3r|,$$

from which we clearly see that

$$f \leq 4(1 + |\tilde{r} - s|)W(\mathbf{A}, \mathbf{B})^2 \\ = \begin{cases} 4(\tilde{r} + \tilde{s})W(\mathbf{A}, \mathbf{B})^2 & \text{if } r + s \leq 1 \\ 4(r + s)W(\mathbf{A}, \mathbf{B})^2 & \text{if } r + s \geq 1. \end{cases}$$

For the special case

$$r + s = 1$$

this bound takes the simple form

$$f \leq 4W(\mathbf{A}, \mathbf{B})^2.$$

Because of the signs in front of the  $\gamma_i$ 's in the conditions for  $\omega \in T(\mathbf{A}, \mathbf{B})$  above, this is not necessarily a very tight bound, though. A version of all this for each of the individual terms in  $f$  can also be written down.

Perfectly analogous results are obtained for transport from  $\mathbf{B}$  to  $\mathbf{A}$ , in terms of  $\alpha'$  instead of  $\alpha$ , and  $W(\mathbf{B}, \mathbf{A})$  instead of  $W(\mathbf{A}, \mathbf{B})$ . We note that  $\mathbf{B}\omega'\mathbf{A}$  can also be expressed via  $\mathbf{A}'\omega\mathbf{B}'$  (see Section 8).

To be clear, the cost matrix from  $B$  to  $A$  is obtained by simply swapping the roles of  $A$  and  $B$ . That is,

$$c_{BA} = |l \otimes 1_4 - 1_2 \otimes k_1|^2,$$

while the parametrization of the set  $T(\nu, \mu)$  of transport plans  $\omega$  from  $\nu$  to  $\mu$  becomes

$$\omega' = (\mu_1 - \gamma_1, \gamma_1, \gamma_2, \mu_2 - \gamma_2, \mu_3 - \gamma_3, \gamma_3, \gamma_4, \mu_4 - \gamma_4).$$

We then have equal cost in the two directions,  $\omega'c_{BA} = \omega c_{AB}$ .

For zero transport cost from  $\mathbf{A}$  to  $\mathbf{B}$ , the condition  $\mathbf{A}\omega\mathbf{B}$  is expressed by (11) and (12). On the other hand, for zero transport cost from  $\mathbf{B}$  to  $\mathbf{A}$ , the condition  $\mathbf{B}\omega'\mathbf{A}$  is expressed by

$$(13) \quad \alpha_{12} + \alpha_{14} = \alpha_{32} + \alpha_{34} = r \quad \text{and} \quad \alpha_{21} + \alpha_{23} = \alpha_{41} + \alpha_{43} = s$$

That is, the transport conditions  $\mathbf{A}\omega\mathbf{B}$  and  $\mathbf{B}\omega'\mathbf{A}$  place different restrictions on  $\mathbf{A}$ , which means that  $W(\mathbf{A}, \mathbf{B})$  and  $W(\mathbf{B}, \mathbf{A})$  are in general not simultaneously zero: for given  $(A, \mu)$  and  $\mathbf{B}$ , the values  $W(\mathbf{A}, \mathbf{B}) =$

0 and  $W(\mathbf{B}, \mathbf{A}) = 0$  are respectively reached on different sets of  $\alpha$ 's. In other words, there are  $\mathbf{A}$  and  $\mathbf{B}$  such that

$$(14) \quad W(\mathbf{A}, \mathbf{B}) = 0 \quad \text{and} \quad W(\mathbf{B}, \mathbf{A}) \neq 0,$$

as well as  $\mathbf{A}$  and  $\mathbf{B}$  such that

$$(15) \quad W(\mathbf{A}, \mathbf{B}) \neq 0 \quad \text{and} \quad W(\mathbf{B}, \mathbf{A}) = 0.$$

For example, in the case  $\alpha_{pq} > 0$  for all  $p$  and  $q$ , transform  $\alpha$  such that  $\alpha_{11} \mapsto \alpha_{11} + \varepsilon$ ,  $\alpha_{13} \mapsto \alpha_{13} - \varepsilon$ ,  $\mu_2\alpha_{21} \mapsto \mu_2\alpha_{21} - \mu_1\varepsilon$  and  $\mu_2\alpha_{23} \mapsto \mu_2\alpha_{23} + \mu_1\varepsilon$ , while all the other  $\alpha_{pq}$ 's are left unchanged. Then, for small enough  $|\varepsilon|$ , (6), (7) and (13) are preserved, but (12) not. So even if  $\mathbf{A}\omega\mathbf{B}$  and  $\mathbf{B}\omega'\mathbf{A}$  both hold initially, then after this transformation only  $\mathbf{B}\omega'\mathbf{A}$  continues to hold. In particular, in the case of the unique couplings  $\omega$  and  $\omega'$  (determined by  $\gamma_1 = \dots = \gamma_4 = 0$ ) which can respectively lead to  $W(\mathbf{A}, \mathbf{B}) = 0$  and  $W(\mathbf{B}, \mathbf{A}) = 0$ , only the latter still holds after the transformation.

The cost matrix

$$c_{AB} = |k_1 \otimes 1_2 - 1_4 \otimes l|^2 + |k_2 \otimes 1_2 - 1_4 \otimes l|^2$$

can similarly be studied, and as may be expected, leads to a weak form of the usual detailed balance condition  $\mu_1\alpha_{14} = \mu_4\alpha_{41}$  between the point (1, 1) and (2, 2) in  $\mathbf{A}$ .

## 5. QUANTUM DETAILED BALANCE AND KMS DUALS

In this section we discuss some points around quantum detailed balance and a related type of dual of u.p. maps, namely KMS-duals. The latter play a basic role in Sections 7 and 8, while the former provides background to how we connect detailed balance and Wasserstein metrics in those two sections. As in previous sections we only consider discrete time. To extend to continuous time, one merely has to replace  $\alpha$  by  $\alpha_t$  for all  $t \geq 0$ , throughout. Sections 7 and 8 will handle this more generally and systematically.

We are interested in defining detailed balance conditions and extensions thereof for a quantum system  $\mathbf{A}$ . As was seen in the previous section, for a classical Markov chain  $\mathbf{A}$  the dual system  $\mathbf{A}'$  is exactly the time-reversal of the dynamics in the classical sense. Detailed balance of a classical Markov chain  $\mathbf{A}$  is therefore given by

$$(16) \quad \mathbf{A}' = \mathbf{A}.$$

However, in the quantum or abstract noncommutative setting, this condition no longer makes sense, as  $\alpha' : A' \rightarrow A'$  as opposed to  $\alpha : A \rightarrow A$ , with  $A' \neq A$ . Therefore a direct mathematical translation of (16) to the quantum case does not appear possible. Consequently one has to explore other options to define quantum detailed balance. This has led to a range of possibilities being proposed and studied over the past five decades. This includes [5, 7, 8, 23, 34, 40, 43, 44, 54, 55, 56,

61], to mention only a few of the papers. Although our main concern is to develop a general approach which can ultimately extend such conditions into the non-equilibrium realm, we nevertheless hope that our approach may also shed some light on possible alternative quantum detailed balance conditions and their meaning. Indeed, there is still some uncertainty about the best way to approach quantum detailed balance, as has been pointed out in [63, 61]

There is in fact an alternative dual, the KMS-dual, of  $\alpha$ , denoted by  $\alpha^\sigma : A \rightarrow A$ , which does map from  $A$  to  $A$ , giving us the system  $\mathbf{A} = (A, \alpha^\sigma, \mu)$ . However, that does not necessarily mean that  $\mathbf{A}^\sigma = \mathbf{A}$  is a physically sensible definition of quantum detailed balance; also see Example 5.2. Nevertheless, the KMS dual does appear in what are known as standard quantum detailed balance conditions, one of which will be defined shortly.

**Definition 5.1.** Given a u.p. map  $E : A \rightarrow B$  satisfying  $\nu \circ E = \mu$  for some  $\mu \in \mathfrak{F}(A)$  and  $\nu \in \mathfrak{F}(B)$ , we define its *KMS-dual* (w.r.t.  $\mu$  and  $\nu$ ) as

$$E^\sigma := j_A \circ E' \circ j_B : B \rightarrow A.$$

Correspondingly  $E^\sigma$  is u.p. and  $\mu \circ E^\sigma = \nu$ , while  $(E^\sigma)^\sigma = E$  follows from  $(E')' = E$ . Under the given assumptions,  $E^\sigma$  is necessarily normal. If  $E$  is u.c.p., then so is  $E^\sigma$ . We note that KMS-duals have been discussed and used in [60, 58, 48, 27, 43, 41].

If  $A$  is abelian,  $j_A$  is the identity map, hence

$$\alpha^\sigma = \alpha',$$

which indicates that at least in some ways the KMS dual is a natural mathematical extension of time-reversal of the classical Markov chain in Subsection 4.1 to the general noncommutative framework.

The KMS-dual allows us to define a good example of a quantum detailed property, which we can use in subsequent sections to illustrate certain points about the general approach of this paper. This is done via a *reversing operation*  $\theta$  for  $(A, \mu)$ , which is a  $*$ -anti-homomorphism  $\theta : A \rightarrow A$  (i.e.,  $\theta$  is linear,  $\theta(a^*) = \theta(a)^*$ , and  $\theta(a_1 a_2) = \theta(a_2) \theta(a_1)$ ) such that  $\theta^2 = \text{id}_A$  and  $\mu \circ \theta = \mu$ . We then consider the *reverse* of  $\mathbf{A}$  (with respect to  $\theta$ ), namely

$$\mathbf{A}^\leftarrow := (A, \alpha^\leftarrow, \mu),$$

with

$$\alpha^\leftarrow := \theta \circ \alpha^\sigma \circ \theta$$

called the  $\theta$ -KMS dual of  $\alpha$  (see [18]). The latter is also denoted by  $\alpha^\theta$ , but the reversing operation will always be clear from context. It is easily checked that  $\alpha^{\leftarrow\leftarrow} \equiv (\alpha^\leftarrow)^\leftarrow = \alpha$  since  $\theta^\sigma = \theta$ ; see [41, Proposition 6.4]. Hence  $\mathbf{A}^{\leftarrow\leftarrow} = \mathbf{A}$ .

Now we define *standard quantum detailed balance with respect to the reversing operation*  $\theta$  of  $\mathbf{A}$ , abbreviated as  $\theta$ -sqdb, by requiring that

$$\mathbf{A}^{\leftarrow} = \mathbf{A}.$$

**Example 5.2.** Consider a system  $\mathbf{A} = (M_n, \alpha, \mu)$  on  $M_n$  with  $\alpha$  and  $\mu$  represented directly on  $M_n$  instead of on the standard form discussed in Example 2.1. Then

$$\alpha^\sigma(a) = \alpha'(a^\top)^\top,$$

with both these duals expressed in this representation, simply because  $j_{M_n \otimes 1_n}$  is given by transposition. Assuming that  $\mu$  is given by a diagonal density matrix, and taking the reversing operation  $\theta$  on  $M_n$  to be transposition (this is a standard choice), we consequently have  $\alpha^{\leftarrow} = \alpha'$ . In this case  $\theta$ -sqdb is therefore expressed by  $\alpha' = \alpha$ , i.e., by

$$\mathbf{A}' = \mathbf{A},$$

where  $\mathbf{A}' = (M_n, \alpha', \mu)$ , emphasizing the similarity of  $\theta$ -sqdb to the classical case (16). The condition  $\mathbf{A}^\sigma = \mathbf{A}$  instead says  $\theta \circ \alpha' \circ \theta = \alpha$ . Essentially  $j_A$  and  $\theta$  cancel in  $\theta$ -sqdb.

For more on  $\theta$ -sqdb, refer to [18, 43, 44]. Here we simply note that  $\theta$ -sqdb can be expressed in terms of transport plans (or balance) as set out in [41, Corollary 6.7]. The same is in fact true of usual detailed balance of a Markov chain, as was discussed for example in [67, Section II] and [40, Section 3], though from a conceptually different point of view and without connecting it to ideas from optimal transport.

## 6. A SIMPLE QUANTUM EXAMPLE

To get an impression of our framework for quantum systems, specifically in relation to detailed balance conditions, we take a brief look at a Wasserstein distance between a very simple spin 1/2 system and a 2-point classical system.

Let  $\mathbf{B}$  be as in Subsection 4.3. In this section the quantum system  $\mathbf{A} = (A, \alpha, \mu)$  will be defined directly on  $M_2$ , instead of in standard form (also see Example 5.2), with

$$A = M_2, \quad \alpha(a) = \lambda U_\eta^* a U_\eta + \tilde{\lambda} U_\varphi^* a U_\varphi \quad \text{and} \quad \mu(a) = \text{Tr}(\rho_\mu a)$$

for all  $a \in A$ , in terms of the unitary and density matrices

$$U_\eta = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\eta} \end{bmatrix} \quad \text{and} \quad \rho_\mu = \begin{bmatrix} \mu_1 & 0 \\ 0 & \mu_2 \end{bmatrix}$$

respectively, with  $\eta, \varphi \in \mathbb{R}$ ,  $0 \leq \lambda \leq 1$  and  $\tilde{\lambda} = 1 - \lambda$ . It is then elementary, though somewhat tedious, to deduce the results below.

With transposition in the given basis serving as a reversing operation  $\theta$ ,  $\mathbf{A}$  satisfies  $\theta$ -sqdb (Example 5.2 gives a definition sufficient for this example) for any values of  $\eta, \varphi$  and  $\lambda$ . However, depending on certain Wasserstein distances from  $\mathbf{A}$  to  $\mathbf{B}$ , the former can have an additional

property, which may also be interpreted as a form of detailed balance, as will be discussed below.

Taking the coordinates (as in Subsection 3.2) for  $\mathbf{A}$  as the Pauli spin matrices,

$$k_1 = \frac{1}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, k_2 = \frac{1}{2} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, k_3 = \frac{1}{2} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},$$

and again using (10) for  $\mathbf{B}$ , also setting  $l_3 = l$ , then via (3) and (5) for  $d = 3$ , the condition  $W(\mathbf{A}, \mathbf{B}) < 1$  implies that  $r + s > 0$  and

$$(17) \quad \lambda \sin \eta + \tilde{\lambda} \sin \varphi = 0.$$

In fact, if  $\mathbf{A}\omega\mathbf{B}$  for  $\omega \neq \mu \otimes \nu$ , and we assume  $r + s > 0$ , then (17) follows. However,  $W(\mathbf{A}, \mathbf{B}) < 1$  implies all of this, and this inequality can indeed be attained on certain sets of systems  $\mathbf{A}$  and  $\mathbf{B}$ .

To see the significance of (17), consider any density matrices  $X$  and  $Y$  for  $\mathbf{A}$ . Let

$$\alpha^*(X) = \lambda U_\eta X U_\eta^* + \tilde{\lambda} U_\varphi X U_\varphi^*$$

express the action of  $\alpha$  in terms of  $X$ . Set

$$V_{XY} = \text{Tr}(\alpha^*(X)Y) - \text{Tr}(XY).$$

One then finds that  $V_{XY} = V_{YX}$  if and only if (17) or  $\text{Im}(X_{21}Y_{12}) = 0$  holds, where the latter refers to entries of the matrices  $X$  and  $Y$ .

For pure states  $X$  and  $Y$ , this has a simple interpretation: If the physical system is currently in the state  $X$  (with  $\mu$  now viewed as a ‘‘reference’’ state, rather than necessarily being the state in which the system finds itself), then  $\text{Tr}(XY)$  is the probability for the system being found to be in state  $Y$  when measuring an observable with  $Y$  as an eigenstate at the current time. Correspondingly for  $\text{Tr}(\alpha^*(X)Y)$ , but one step into the future, when the system is in state  $\alpha^*(X)$ . Hence we can heuristically think of  $V_{XY}$  as a flow of probability from  $X$  to  $Y$  during one step of time evolution of the state  $X$ . The condition  $V_{XY} = V_{YX}$  tells us that this flow is the same in both directions, i.e., it can be viewed as a form of detailed balance, at least between pure states  $X$  and  $Y$  for which  $\text{Im}(X_{21}Y_{12}) \neq 0$ . The condition  $\text{Im}(X_{21}Y_{12}) = 0$ , on the other hand, describes a small set in the Cartesian product of the set of spin 1/2 pure states with itself, in the sense that the condition can cease to hold due to an arbitrarily small change in either of the states  $X$  or  $Y$ .

## 7. WASSERSTEIN DISTANCES

We now have the framework in place and our basic approach set out, motivated, and illustrated by simple examples. The next step is to systematically develop the quantitative tool, namely Wasserstein distance from one system to another, as well as related results, to provide the mathematical foundation for our approach. So far we only defined and



used Wasserstein distances in special situations and examples. Here we develop the more general theory that will in particular also cover those cases. This extends the definitions and some results on metric properties from [38, 39] (where all systems were on the same algebra).

The outlines of the arguments in this section are similar to those papers, but need to be adapted. The arguments in the next section, studying aspects of Wasserstein distances relevant to the properties and structure of systems, move further afield, however. We use the notation and conventions from Section 2, though the definition of a system will be extended and refined.

In Section 2 we only considered a simple case of the systems we are interested in. We now give a more abstract definition of systems, including the “coordinates” from Subsection 3.2, and allowing more general cases than just discrete time. We assume the minimum structure which still allows us to define Wasserstein distances from one system to another. In particular, we do not require semigroup properties for dynamics, which allows for non-Markovian systems. The definition is taken from [39, Section 3], though generalized to positive dynamics instead of just completely positive dynamics, for the reasons mentioned in Subsection 2.1, which become relevant in the next section.

**Definition 7.1.** A *system* is given by  $\mathbf{A} = (A, \alpha, \mu, k)$ , where  $\mu \in \mathfrak{F}(A)$  and  $k = (k_1, \dots, k_d)$  with  $k_1, \dots, k_d \in A$  for some  $d \in \{1, 2, 3, \dots\}$ , while  $\alpha$  consists of the following: Let  $\Upsilon$  be any set. To each  $v \in \Upsilon$  corresponds a set  $Z_v$  and *generalized dynamics*  $\alpha_v$  on  $A$ , which is given by a u.p. map

$$\alpha_{v,z} : A \rightarrow A$$

for every  $z \in Z_v$ , such that

$$\mu \circ \alpha_{v,z} = \mu$$

for all  $z \in Z_v$  and  $v \in \Upsilon$ . We then write

$$\alpha = (\alpha_v)_{v \in \Upsilon}.$$

We view  $Z_v$  as a set of “points in time” in an abstract sense. Each  $\alpha_v$  is viewed as dynamics, so  $\mathbf{A}$  is really a set of dynamical systems on  $A$ , one for each  $v$ , and all leaving the state  $\mu$  invariant. Lastly,  $k$  serves as “coordinates” for the system, in terms of which a quadratic cost of transport from one system to another will be defined. We also define  $\alpha'$  and  $\alpha^\sigma$  through

$$\alpha'_{v,z} = (\alpha_{v,z})' \quad \text{and} \quad \alpha^\sigma_{v,z} = (\alpha_{v,z})^\sigma.$$

In terms of Definition 5.1 we have the following type of dual of a system, which will play a key role in one of the types of Wasserstein distances to be defined shortly.

**Definition 7.2.** The *KMS-dual* of  $\mathbf{A}$  is defined to be  $\mathbf{A}^\sigma := (A, \alpha^\sigma, \mu, k)$ .

Note that  $\mathbf{A}^{\sigma\sigma} = \mathbf{A}$ . Extensions of the duals of  $\mathbf{A}$  in Subsection 2.1 and Section 5 will be defined in the next section to study corresponding symmetries of Wasserstein distances.

For the remainder of this section and the next, we fix  $\Upsilon$ , the  $Z_v$ 's, and  $d$ , i.e., they are the same for all systems our Wasserstein distances will be applied to. The following notational convention will be used:  $\mathbf{A}$  will denote  $(A, \alpha, \mu, k)$ , as in the definition above, and similarly we write

$$\mathbf{B} = (B, \beta, \nu, l) \quad \text{and} \quad \mathbf{C} = (C, \gamma, \xi, m).$$

Let

$$X$$

denote any set of such systems. Our Wasserstein distances will be defined on  $X$ .

Notationally it will be convenient to allow systems with one point  $\Upsilon$  and without coordinates (the case  $d = 0$ ) as well, written as  $(A, \alpha, \mu)$ , though they will not be viewed as members of  $X$ . This is needed to formulate certain conditions related to transport plans, involving modular dynamics, more conveniently in the definition below.

We are going to define Wasserstein distances from one system  $\mathbf{A}$  to another  $\mathbf{B}$ , as the square root of the infimum of the cost over an appropriate set of transport plans from  $\mathbf{A}$  to  $\mathbf{B}$ . One option is the full set  $T(\mathbf{A}, \mathbf{B})$  of transport plans as before, but there are further refinements that can be made to the set of transport plans, that can for example ensure symmetry of the resulting Wasserstein distance.

The sets of transport plans relevant to us are defined as follows, refining [39, Definition 3.5] with a corresponding change in notation and terminology.

**Definition 7.3.** We write

$$\mathbf{A}\omega\mathbf{B}$$

to express that  $\omega \in T(\mu, \nu)$  (see Subsection 2.2) and

$$(18) \quad \omega(\alpha_{v,z}(a) \otimes b') = \omega(a \otimes \beta'_{v,z}(b'))$$

for all  $a \in A$ ,  $b' \in B'$ ,  $z \in Z_v$  and  $v \in \Upsilon$ , in which case we call  $\omega$  a *transport plan* from  $\mathbf{A}$  to  $\mathbf{B}$ . The set of transport plans from  $\mathbf{A}$  to  $\mathbf{B}$  is written

$$T(\mathbf{A}, \mathbf{B}) := \{\omega \in T(\mu, \nu) : \mathbf{A}\omega\mathbf{B}\}.$$

The set of *modular* transport plans from  $\mathbf{A}$  to  $\mathbf{B}$  is

$$T_\sigma(\mathbf{A}, \mathbf{B}) := \{\omega \in T(\mathbf{A}, \mathbf{B}) : (A, \sigma^\mu, \mu)\omega(B, \sigma^\nu, \nu)\}.$$

where  $\sigma^\mu$  and  $\sigma^\nu$  denote the modular dynamics (from Tomita-Takesaki theory) associated to  $\mu$  and  $\nu$  respectively. The set of *KMS* transport plans from  $\mathbf{A}$  to  $\mathbf{B}$  is

$$T_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) := \{\omega \in T_\sigma(\mathbf{A}, \mathbf{B}) : \mathbf{A}^\sigma\omega\mathbf{B}^\sigma\}.$$

In connection to  $T_\sigma(\mathbf{A}, \mathbf{B})$  we point out that  $(\sigma_t^\nu)' = \sigma_t^{\nu'}$ . Note that the transport plans do not depend on the coordinates  $k$  and  $l$ . Furthermore, we always have  $\mu \odot \nu' \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ .

**Example 7.4.** Returning to our special case in Example 2.1, the modular dynamics (or modular group)  $\sigma^\mu$  is given by

$$\sigma_t^\mu(\pi(a)) = \pi(\rho_\mu^{it} a \rho_\mu^{-it})$$

for all  $a \in M_n$ . Along with the modular conjugation, the modular group is a natural component of the Tomita-Takesaki (or modular) theory of von Neumann algebras; see [19, 65] for expositions of the general theory.

Next we need to formulate the cost of a transport plan. In Subsection 2.2 we mentioned that a transport plan  $\omega \in T(\mu, \nu)$  from  $\mu$  to  $\nu$  can be represented as a channel (u.c.p. map)  $E_\omega : A \rightarrow B$ . To see this, we first define a state  $\delta_\nu$  on  $B \odot B'$  by requiring that

$$\delta_\nu(b \otimes b') = \langle \Lambda_\nu, b b' \Lambda_\nu \rangle$$

for all  $b \in B$  and  $b' \in B'$ .

**Definition 7.5.** For any  $\omega \in T(\mu, \nu)$ , the channel  $E_\omega$  is defined as the unique function from  $A$  to  $B$  such that

$$(19) \quad \omega(a \otimes b') = \delta_\nu(E_\omega(a) \otimes b').$$

This provides a correspondence between elements of  $T(\mu, \nu)$  and channels  $E : A \rightarrow B$  satisfying  $\nu \circ E = \mu$ . The map  $E_\omega$  in this condition necessarily exists and is indeed forced to be u.c.p. All this is demonstrated in [41, Section 3]. The state  $\delta_\nu$  generalizes the so-called diagonal state associated to a probability measure, but can also be viewed as an abstract version of the maximally entangled state of a quantum state with itself. In this way Definition 7.5 provides a generalization of the (finite dimensional) Choi-Jamiołkowski duality between channels and states as used in quantum physics [26, 53, 50], to a von Neumann algebra framework.

For our purposes,  $E_\omega$  has two uses. Firstly, we have  $\mathbf{A}\omega\mathbf{B}$  if and only if  $\omega \in T(\mu, \nu)$  and

$$(20) \quad E_\omega \circ \alpha_{v,z} = \beta_{v,z} \circ E_\omega$$

for all  $z \in Z_v$  and  $v \in \Upsilon$ , by [41, Theorem 4.1], which we also write simply as  $E_\omega \circ \alpha = \beta \circ E_\omega$ . This is often a convenient way to verify  $\mathbf{A}\omega\mathbf{B}$ .

Secondly,  $E_\omega$  allows us to define transport cost while avoiding the complications mentioned in Subsection 3.2, due to unbounded  $S_\nu$ :

**Definition 7.6.** The cost of a transport plan  $\omega \in T(\mathbf{A}, \mathbf{B})$  is defined as

$$(21) \quad I_{\mathbf{A}, \mathbf{B}}(\omega) = \sum_{i=1}^d [\mu(k_i^* k_i) + \nu(l_i^* l_i) - \nu(E_\omega(k_i)^* l_i) - \nu(l_i^* E_\omega(k_i))].$$

In general  $S_\nu b^* S_\nu$  is affiliated with  $B'$ , but it may be unbounded, hence not contained in  $B'$ . For cases where we do have  $S_\nu b^* S_\nu \in B'$ , the form of the cost above is in fact equivalent to the form used in (3). But unlike the latter, (21) only refers to bounded operators, thus avoiding complications even when some  $S_\nu l_i^* S_\nu$ 's are unbounded.

**Remark 7.7.** In terms of representation machinery built and used in [38, Section 2 and 3], but which will not be reviewed in any detail here, one can write

$$I_{\mathbf{A}, \mathbf{B}}(\omega) = \|\pi_\mu^\omega(k)\Omega - \pi_\nu^\omega(l)\Omega\|_{\oplus\omega}^2,$$

in terms of cyclic representations  $(H_\mu^\omega, \pi_\mu^\omega, \Omega)$  and  $(H_\nu^\omega, \pi_\nu^\omega, \Omega)$  of  $(A, \mu)$  and  $(B, \nu)$  inherited from a cyclic representation  $(H_\omega, \pi_\omega, \Omega)$  of  $(A \odot B', \omega)$ , and where  $\pi_\mu^\omega(k)\Omega \equiv (\pi_\mu^\omega(k_1)\Omega, \dots, \pi_\mu^\omega(k_d)\Omega) \in \bigoplus_{l=1}^n H_\omega$ , etc. This starts to give a more intuitive idea of why we expect to obtain distances from this cost. Indeed, the triangle inequality of our Wasserstein distances below follow from this form of  $I_{\mathbf{A}, \mathbf{B}}(\omega)$ . On the other hand, (21) is useful in relation to symmetry, as well as the consequences of zero Wasserstein distance in Section 8.

With this transport cost in hand, we can define our Wasserstein distances from one system to another. The cost  $I_{\mathbf{A}, \mathbf{B}}(\omega)$  does not depend directly on  $\alpha$  and  $\beta$ , but they play a central role in determining the allowed transport plans, namely  $T(\mathbf{A}, \mathbf{B})$ ,  $T_\sigma(\mathbf{A}, \mathbf{B})$  or  $T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ , and enter the definition of Wasserstein distance via this.

**Definition 7.8.** Given a set  $X$  of systems as above, we define the *Wasserstein distance*  $W$  on  $X$  by

$$W(\mathbf{A}, \mathbf{B}) := \inf_{\omega \in T(\mathbf{A}, \mathbf{B})} I_{\mathbf{A}, \mathbf{B}}(\omega)^{1/2},$$

the *modular Wasserstein distance*  $W_\sigma$  on  $X$  by

$$W_\sigma(\mathbf{A}, \mathbf{B}) := \inf_{\omega \in T_\sigma(\mathbf{A}, \mathbf{B})} I_{\mathbf{A}, \mathbf{B}}(\omega)^{1/2},$$

and the *KMS Wasserstein distance*  $W_{\sigma\sigma}$  on  $X$  by

$$W_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) := \inf_{\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})} I_{\mathbf{A}, \mathbf{B}}(\omega)^{1/2},$$

for all  $\mathbf{A}, \mathbf{B} \in X$ , in terms of Definitions 7.3 and 7.6.

Note that we thus obviously have

$$W(\mathbf{A}, \mathbf{B}) \leq W_\sigma(\mathbf{A}, \mathbf{B}) \leq W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$$

for all  $\mathbf{A}, \mathbf{B} \in X$ .

We proceed to prove the existence of optimal transport plans and the main metric properties of the functions  $W$ ,  $W_\sigma$  and  $W_{\sigma\sigma}$ . The proofs are similar to those appearing in [38] and [39, Section 3] for systems on the same von Neumann algebra. We simply show how to adapt them. Much of the framework of [38] was in fact already set up in terms of multiple von Neumann algebras, although the case of distance functions between states on different algebras was not treated there.

**Definition 7.9.** An *optimal* transport plan for  $W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  is any  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  such that  $I_{\mathbf{A}, \mathbf{B}}(\omega)^{1/2} = W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ . We say that optimal transport plans for  $W_{\sigma\sigma}$  *always exist* if they exist for  $W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  for all  $\mathbf{A}, \mathbf{B} \in X$ . Correspondingly for  $W$  and  $W_\sigma$ .

Recall that for any set  $Y$ , a real-valued function  $\rho$  on  $Y \times Y$  is called an *asymmetric pseudometric* if it satisfies the triangle inequality,  $\rho(x, y) \geq 0$  and  $\rho(x, x) = 0$  for all  $x, y \in Y$ . If in addition  $\rho(x, y) = \rho(y, x)$ , we call  $\rho$  a *pseudometric*. These properties of our Wasserstein distances will be proven below. The remaining standard property, namely that  $\rho(x, x) = 0$  implies  $x = x$ , will appear in a more refined form in the next section, and is essentially recovered in its usual form in the case of appropriate coordinates (the complication being that we allow systems on different algebras with different coordinate systems).

**Theorem 7.10.** *The functions  $W$  and  $W_\sigma$  are asymmetric pseudometrics, while  $W_{\sigma\sigma}$  is a pseudometric. In addition, optimal transport plans always exist for  $W$ ,  $W_\sigma$  and  $W_{\sigma\sigma}$ .*

*Proof.* We prove it for  $W_{\sigma\sigma}$ . The other cases are similar but simpler. By its definition,  $W_{\sigma\sigma}$  is real-valued and never negative, since by Kadison's inequality  $E_\omega(a^*a) \geq E_\omega(a)^*E_\omega(a)$  we have

$$\begin{aligned} (22) \quad & \mu(a^*a) + \nu(b^*b) - \nu(E_\omega(a)^*b) - \nu(b^*E_\omega(a)) \\ &= \nu(|b - E_\omega(a)|^2) + \nu(E_\omega(|a|^2) - |E_\omega(a)|^2) \\ &\geq \nu(|b - E_\omega(a)|^2) \\ &\geq 0 \end{aligned}$$

for all  $a \in A$  and  $b \in B$ . (Alternatively, one can use Remark 7.7, but (22) will come up again in the next section.) Note that for  $\omega = \delta_\mu$  we have  $E_\omega = \text{id}_A$ , from which  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{A})$  follows trivially by the test in (20). Consequently  $W_{\sigma\sigma}(\mathbf{A}, \mathbf{A}) = I_{\mathbf{A}, \mathbf{A}}(\delta_\mu) = 0$  from (21).

*The triangle inequality.* For  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  and  $\psi \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{C})$ , we define  $\varphi = \omega \circ \psi$  through

$$E_{\omega \circ \psi} = E_\psi \circ E_\omega.$$

Then  $\varphi \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{C})$ , since  $E_\varphi \circ \alpha_{v,z} = \gamma_{v,z} \circ E_\varphi$ , hence  $\mathbf{A}\varphi\mathbf{C}$ , and similarly  $\mathbf{A}^\sigma\varphi\mathbf{C}^\sigma$  and  $(A, \sigma^\mu, \mu)\varphi(B, \sigma^\xi, \xi)$ . As in the proof of [38, Proposition 4.3], but allowing multiple algebras as well as  $k$ ,  $l$  and  $m$

(rather than just  $k$ ), and using Remark 7.7, while skipping some details explained in [38], we have

$$\begin{aligned} I_{\mathbf{A},\mathbf{C}}(\varphi)^{1/2} &= \left\| \pi_{\mu}^{\varphi}(k)\Phi - \pi_{\xi}^{\varphi}(m)\Phi \right\|_{\oplus\varphi} \\ &\leq \left\| \pi_{\mu}^{\omega}(k)\Omega - \pi_{\nu}^{\omega}(l)\Omega \right\|_{\oplus\omega} + \left\| \pi_{\nu}^{\psi}(l)\Psi - \pi_{\xi}^{\psi}(m)\Psi \right\|_{\oplus\psi} \\ &= I_{\mathbf{A},\mathbf{B}}(\omega)^{1/2} + I_{\mathbf{B},\mathbf{C}}(\psi)^{1/2} \end{aligned}$$

by employing the triangle inequality in  $\bigoplus_{i=1}^d (H_{\omega} \otimes_{\nu} H_{\psi})$  as well as properties of the relative tensor product  $H_{\omega} \otimes_{\nu} H_{\psi}$  of the  $A$ - $B$ -bimodule  $H_{\omega}$  and  $B$ - $C$ -bimodule  $H_{\psi}$ . The role of  $H_{\omega} \otimes_{\nu} H_{\psi}$  (see [30, Appendix V.B], [45], [62] and [65, Section IX.3] for background) is to ensure that the “middle term” coming from the difference between  $\pi_{\nu}^{\omega}(l)\Omega$  and  $\pi_{\nu}^{\psi}(l)\Psi$  via imbedding into  $\bigoplus_{i=1}^d (H_{\omega} \otimes_{\nu} H_{\psi})$ , indeed disappears. Now take the infimum on the left over all  $\varphi \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{C})$ , which includes the compositions  $\omega \circ \psi$  for all  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  and  $\psi \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{C})$ , followed in turn by the infima over all  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  and  $\psi \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{C})$  on the right.

*Symmetry.* This is essentially verbatim as in the proof of [39, Theorem 3.9], but in terms of  $E_{\omega} : A \rightarrow B$ , instead of involving just one von Neumann algebra. However, note that the proof does not hold for  $W$  and  $W_{\sigma}$ , just for  $W_{\sigma\sigma}$ , as the KMS duals play a key role here.

*Optimal transport plans exist.* Without loss (see for example [36, Proposition 4.1]) we can view each element of  $T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  as a state on the maximal  $C^*$ -tensor product  $A \otimes_{\max} B'$ . Consequently  $T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  is weakly\* compact. From  $W_{\sigma\sigma}$ 's definition there is a sequence  $\omega_q \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  such that  $I_{\mathbf{A},\mathbf{B}}(\omega_q)^{1/2} \rightarrow W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ , and necessarily having a weak\* cluster point  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ . As a result,  $\omega$  is an optimal transport plan for  $W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ , by the following approximation:

Given  $\varepsilon > 0$ , there is a  $q_0$  such that

$$|I_{\mathbf{A},\mathbf{B}}(\omega_q) - W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})^2| < \varepsilon$$

for all  $q > q_0$ . Furthermore, there exist  $b'_1, \dots, b'_d \in B'$  such that

$$\|l_i \Lambda_{\nu} - b'_i \Lambda_{\nu}\| < \varepsilon$$

for  $i = 1, \dots, d$ . In addition there is a  $q > q_0$  such that

$$|\omega_q(k_i \otimes b'_i) - \omega(k_i \otimes b'_i)| < \varepsilon$$

for  $i = 1, \dots, d$ . Then as in the proof of [38, Lemma 6.2], using (21) and (19), we find

$$\begin{aligned} |I_{\mathbf{A},\mathbf{B}}(\omega) - I_{\mathbf{A},\mathbf{B}}(\omega_q)| &\leq 2 \sum_{i=1}^d |\nu(l_i^* E_{\omega_q}(k_i)) - \nu(l_i^* E_{\omega}(k_i))| \\ &= 2 \sum_{i=1}^d |\langle l_i \Lambda_{\nu}, (E_{\omega_q}(k_i) - E_{\omega}(k_i)) \Lambda_{\nu} \rangle| \\ &< 4\varepsilon \sum_{i=1}^d \|k_i\| + 2d\varepsilon. \end{aligned}$$

Thus

$$|I_{\mathbf{A},\mathbf{B}}(\omega) - W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})^2| < 4\varepsilon \sum_{i=1}^d \|k_i\| + 2d\varepsilon + \varepsilon$$

for all  $\varepsilon > 0$ . □

The remaining metric issue, namely under which conditions zero Wasserstein distance between  $\mathbf{A}$  and  $\mathbf{B}$  implies that they are in fact the same system (at least up to isomorphism), will be returned to in Corollary 8.14.

We note that optimal transport plans in general need not be unique.

**Example 7.11.** In (21), take  $A = B$ ,  $\mu = \nu$  and  $k_i = l_i$  for  $i = 1, \dots, d$ . Assume that the dynamics of  $\mathbf{A}$  is trivial (i.e., there is none, or each is taken as the identity map). Let  $F$  be any von Neumann subalgebra of  $A$  containing  $\{k_1, \dots, k_d\}$  such that  $\sigma_t^\mu(F) = F$ . Consider the unique conditional expectation  $E_F : A \rightarrow F$  such that  $\mu \circ E_F = \mu$ ; see [64] and [65, Theorem IX.4.2]. Then  $\omega_F$  defined from  $E_F$  through (19) trivially delivers  $I_{\mathbf{A},\mathbf{A}}(\omega_F) = 0$  simply because  $E_F(k_i) = k_i$ . This is true for any such  $F$ , hence in general multiple transport plans give the optimal cost 0. A simple instance is where  $\mu$  is tracial, in particular when  $A$  is abelian, in which case  $\sigma_t^\mu$  is trivial and the condition  $\sigma_t^\mu(F) = F$  is automatically satisfied.

What remains is to study relevant properties of these Wasserstein distances and take initial steps in showing how the general theory of these distances can be used to study the structure and properties of systems. This is what we turn to next.

## 8. PROPERTIES AND IMPLICATIONS OF WASSERSTEIN DISTANCES

Here we derive properties of Wasserstein distances relevant to the structure and characteristics of systems. These properties include symmetries related to dualities of systems. The symmetries along with the metric properties, in particular the triangle inequality, allow us to easily find simple bounds on how far a (quantum) system is from detailed

balance, in terms of its Wasserstein distance from other systems satisfying detailed balance (Subsection 8.1). The idea is that these other systems will typically be chosen as well understood or simpler, even classical, systems. This opens the door to analyzing a system via simpler systems, in line with the examples in Sections 4 and 6. In addition (Subsection 8.2) we also study implications of Wasserstein distances for the structure of systems, focussing in particular on the case of zero Wasserstein distance. The goal is to show that Wasserstein distance can give us information about common structure in two systems.

We continue with the notation from the previous section, again fixing  $\Upsilon$ , the  $Z_\nu$ 's, and  $d$  for all systems to be considered.

**8.1. Bounds on deviation from detailed balance.** The first step is to define two more duals of systems, in addition to the KMS-dual from Definition 7.2. The first of these extends the dual defined in Subsection 2.1:

**Definition 8.1.** The *dual* of  $\mathbf{A}$  is defined to be  $\mathbf{A}' := (A', \alpha', \mu', k')$  where  $k' = (k'_1, \dots, k'_d) := (j_A(k_1^*), \dots, j_A(k_d^*))$ .

It is easily seen that  $\mathbf{A}'' = \mathbf{A}$ . For systems  $\mathbf{A}$  and  $\mathbf{B}$ , and  $\omega \in T(\mu, \nu)$ , a useful fact is

$$(23) \quad \mathbf{A}\omega\mathbf{B} \Leftrightarrow \mathbf{B}'\omega'\mathbf{A}' \Leftrightarrow \mathbf{B}^\sigma\omega^\sigma\mathbf{A}^\sigma,$$

which was shown in [41, Corollary 4.6], where  $\omega'$  and  $\omega^\sigma$  are respectively defined via

$$\omega'(b' \otimes a) = \delta_{\mu'}(E'_\omega(b') \otimes a) = \delta_\nu(E_\omega(a) \otimes b') = \omega(a \otimes b')$$

for all  $a \in A$ ,  $b' \in B'$ , and

$$\omega^\sigma(b \otimes a') = \delta_\mu(E_\omega^\sigma(b) \otimes a'),$$

for all  $a' \in A'$ ,  $b \in B$ , in terms of the correspondence in Definition 7.5. I.e.,  $E_{\omega'} = E'_\omega$  and  $E_{\omega^\sigma} = E_\omega^\sigma$ .

The second of these duals, extending the reverse from Section 5, is defined in terms of a reversing operation as appearing in Section 5. In fact more generally we also need appropriate reversals for u.p. maps between von Neumann algebras, which we formalize as follows.

**Definition 8.2.** Given reversing operations  $\theta_\mu$  and  $\theta_\nu$  for  $(A, \mu)$  and  $(B, \nu)$  respectively, as well as a u.p. map  $E : A \rightarrow B$  satisfying  $\nu \circ E = \mu$ , we define its  $(\theta_\mu, \theta_\nu)$ -KMS dual  $E^{\leftarrow} : B \rightarrow A$  by

$$E^{\leftarrow} := \theta_\mu \circ E^\sigma \circ \theta_\nu.$$

For any  $\omega \in T(\mu, \nu)$  we can consequently define  $\omega^{\leftarrow} \in T(\nu, \mu)$  via

$$\omega^{\leftarrow}(b \otimes a') = \delta_\mu(E_\omega^{\leftarrow}(b) \otimes a')$$

for all  $a' \in A'$ ,  $b \in B$ , in terms of Definition 7.5, i.e.,  $E_{\omega^{\leftarrow}} = E_\omega^{\leftarrow}$ . (One could write  $E^{\theta_\mu, \theta_\nu}$  instead of  $E^{\leftarrow}$ , but  $\theta_\mu$  and  $\theta_\nu$  will always be clear from context.)



Note that  $E^\leftarrow = (\theta_\nu \circ E \circ \theta_\mu)^\sigma$ , since  $\theta_\mu^\sigma = \theta_\mu$  and  $\theta_\nu^\sigma = \theta_\nu$ , similar to Section 5, hence  $E^{\leftarrow\leftarrow} = E$ .

**Definition 8.3.** We call a system  $\mathbf{A}$  *reversible* if there is a distinguished  $\alpha_{v,z} = \theta_{\mathbf{A}}$  for some  $v \in \Upsilon$  with  $Z_v = \{z\}$  a 1-point set, where  $\theta_{\mathbf{A}}$  is a reversing operation for  $(A, \mu)$ , as defined in Section 5. The *reverse* of  $\mathbf{A}$  is then defined as the system

$$\mathbf{A}^\leftarrow = (A, \alpha^\leftarrow, \mu, k)$$

where  $\alpha_{v,z}^\leftarrow = (\alpha_{v,z})^\leftarrow$  for every  $z \in Z_v$  and  $v \in \Upsilon$ . A reversible system  $\mathbf{A}$  is said to satisfy  $\theta_{\mathbf{A}}$ -sqdb if  $\mathbf{A}^\leftarrow = \mathbf{A}$ , extending the definition from Section 5.

As in Section 5, one has  $\mathbf{A}^{\leftarrow\leftarrow} = \mathbf{A}$ . In this respect note that

$$\theta_{\mathbf{A}^\leftarrow}^\leftarrow = \theta_{\mathbf{A}},$$

i.e.,  $\mathbf{A}^\leftarrow$  has the same reversing operation as  $\mathbf{A}$ , since  $\theta_{\mathbf{A}^\leftarrow}^\sigma = \theta_{\mathbf{A}}$ . We aim to connect our Wasserstein distances to  $\theta_{\mathbf{A}}$ -sqdb.

We now have the following simple proposition in the vein of (23).

**Proposition 8.4.** *For reversible systems  $\mathbf{A}$  and  $\mathbf{B}$ , one has*

$$\mathbf{A}\omega\mathbf{B} \Leftrightarrow \mathbf{B}^\leftarrow\omega^\leftarrow\mathbf{A}^\leftarrow.$$

*Note in addition that if  $\omega \in T(\mathbf{A}, \mathbf{B})$  for reversible  $\mathbf{A}$  and  $\mathbf{B}$ , then  $\theta_{\mathbf{B}} \circ E_\omega \circ \theta_{\mathbf{A}} = E_\omega$ , hence  $E_\omega^\leftarrow = E_\omega^\sigma$  and  $\omega^\leftarrow = \omega^\sigma$ .*

*Proof.* Note that  $E_\omega \circ \alpha_{v,z} = \beta_{v,z} \circ E_\omega$  is equivalent to  $\alpha_{v,z}^\sigma \circ E_\omega^\sigma = E_\omega^\sigma \circ \beta_{v,z}^\sigma$ . Hence, for reversible systems,  $E_\omega \circ \alpha_{v,z} = \beta_{v,z} \circ E_\omega$  is also equivalent to  $\alpha_{v,z}^\leftarrow \circ E_\omega^\leftarrow = E_\omega^\leftarrow \circ \beta_{v,z}^\leftarrow$ , since  $\theta_{\mathbf{A}} \circ \theta_{\mathbf{A}} = \text{id}_A$  and  $\theta_{\mathbf{B}} \circ \theta_{\mathbf{B}} = \text{id}_B$ . The last statement in the proposition follows from  $T(\mathbf{A}, \mathbf{B})$ 's definition and the fact that the reversing operations are part of the systems' dynamics.  $\square$

In what follows we implicitly assume that we choose our set of systems  $X$  from Section 7 to contain all the duals that will be referred to. Then the Wasserstein distances  $W_\sigma$  and  $W_{\sigma\sigma}$  have the following symmetries with respect to the three types of duals discussed above.

**Theorem 8.5.** *For any  $\mathbf{A}$  and  $\mathbf{B}$  we have*

$$W_\sigma(\mathbf{A}, \mathbf{B}) = W_\sigma(\mathbf{B}', \mathbf{A}') = W_\sigma(\mathbf{B}^\sigma, \mathbf{A}^\sigma).$$

*For reversible systems  $\mathbf{A}$  and  $\mathbf{B}$  we in addition have*

$$W_\sigma(\mathbf{A}, \mathbf{B}) = W_\sigma(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow).$$

*The corresponding results also hold for  $W_{\sigma\sigma}$ , which can be written as  $W_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) = W_{\sigma\sigma}(\mathbf{A}', \mathbf{B}')$  etc., due to  $W_{\sigma\sigma}$ 's usual pseudometric symmetry (Theorem 7.10).*

*Proof.* For  $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$  (recall Definition 7.3)

$$\begin{aligned} I_{\mathbf{B}', \mathbf{A}'}(\omega') &= \sum_{i=1}^d [\nu'(l_i'^* l_i') + \mu'(k_i'^* k_i') - \mu'(E_{\omega'}(l_i')^* k_i') - \mu'(k_i'^* E_{\omega'}(l_i'))] \\ &= \sum_{i=1}^d [\nu(l_i^* l_i) + \mu(k_i^* k_i) - \mu(k_i^* E_\omega^\sigma(l_i)) - \mu(E_\omega^\sigma(l_i)^* k_i)] \\ &= I_{\mathbf{A}, \mathbf{B}}(\omega), \end{aligned}$$

using the definitions and properties of the various objects appearing, along with  $\mu(aE_\omega^\sigma(b)) = \nu(E_\omega(a)b)$ , which follows from  $E_\omega \circ \sigma_t^\mu = \sigma_t^\nu \circ E_\omega$  (see [38, Lemma 5.2] as well as the proof of [38, Lemma 5.3]). Similarly  $I_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}(\omega^\sigma) = I_{\mathbf{A}, \mathbf{B}}(\omega)$ . Because of (23) applied to the modular dynamics, along with  $(\sigma_t^\mu)' = \sigma_t^{\mu'}$  and  $(\sigma_t^\mu)^\sigma = \sigma_{-t}^\mu$ , to verify the modular transport plan properties, it follows that for  $\omega \in T(\mathbf{A}, \mathbf{B})$  we have  $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$  if and only if  $\omega' \in T_\sigma(\mathbf{B}', \mathbf{A}')$ , and if and only if  $\omega^\sigma \in T_\sigma(\mathbf{B}^\sigma, \mathbf{A}^\sigma)$ . Consequently, from the definition of  $W_\sigma$  we have  $W_\sigma(\mathbf{A}, \mathbf{B}) = W_\sigma(\mathbf{B}', \mathbf{A}') = W_\sigma(\mathbf{B}^\sigma, \mathbf{A}^\sigma)$ .

For reversible  $\mathbf{A}$  and  $\mathbf{B}$  and  $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$ , one has  $\mu(aE_\omega^\leftarrow(b)) = \mu(aE_\omega^\sigma(b)) = \nu(E_\omega(a)b)$  by Proposition 8.4. Similar to above, it follows that  $I_{\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow}(\omega^\leftarrow) = I_{\mathbf{A}, \mathbf{B}}(\omega)$ . Since  $\mu \circ \theta_{\mathbf{A}} = \mu$ , we have  $\sigma_t^\mu \circ \theta_{\mathbf{A}} = \theta_{\mathbf{A}} \circ \sigma_t^\mu$  (similar to the proof of [41, Proposition 6.4] for example), hence  $(\sigma_t^\mu)^\leftarrow = \sigma_{-t}^\mu$ , which along with Proposition 8.4 tells us that for  $\omega \in T(\mathbf{A}, \mathbf{B})$  we have  $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$  if and only if  $\omega^\leftarrow \in T_\sigma(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow)$ . Thus  $W_\sigma(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow) = W_\sigma(\mathbf{A}, \mathbf{B})$ .

The case of  $W_{\sigma\sigma}$  is very similar. One has to verify that  $(\mathbf{A}')^\sigma = (\mathbf{A}^\sigma)'$  and  $(\mathbf{A}^\leftarrow)^\sigma = (\mathbf{A}^\sigma)^\leftarrow$ , which are straightforward from the definitions and general properties of these constructions, including  $(j_\nu \circ E \circ j_\mu)' = j_\mu \circ E' \circ j_\nu$  (see [41, Proposition 2.8]). This allows us to check that for  $\omega \in T(\mathbf{A}, \mathbf{B})$  and reversible  $\mathbf{A}$  and  $\mathbf{B}$ , one has  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$  if and only if  $\omega^\leftarrow \in T_{\sigma\sigma}(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow)$ . Consequently,  $W_{\sigma\sigma}(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow) = W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ , but by Theorem 7.10,  $W_{\sigma\sigma}(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow) = W_{\sigma\sigma}(\mathbf{A}^\leftarrow, \mathbf{B}^\leftarrow)$ . Similarly for the other two dualities.  $\square$

This result along with the basic metric properties in Theorem 7.10, lead to simple consequences for quantifying and bounding the deviation of a system from satisfying a detailed balance condition, in terms of the Wasserstein distance of the system from another system which does satisfy some detailed balance condition.

**Corollary 8.6.** *Consider reversible systems  $\mathbf{A}$  and  $\mathbf{B}$ . If  $\mathbf{B}$  satisfies  $\theta_{\mathbf{B}}$ -sqdb, then*

$$W_\sigma(\mathbf{A}, \mathbf{A}^\leftarrow) \leq 2W_\sigma(\mathbf{A}, \mathbf{B}) \quad \text{and} \quad W_\sigma(\mathbf{A}^\leftarrow, \mathbf{A}) \leq 2W_\sigma(\mathbf{B}, \mathbf{A})$$

and

$$W_{\sigma\sigma}(\mathbf{A}, \mathbf{A}^\leftarrow) \leq 2W_{\sigma\sigma}(\mathbf{A}, \mathbf{B}).$$

*Proof.* By the triangle inequality (from Theorem 7.10)

$$W_\sigma(\mathbf{A}, \mathbf{A}^\leftarrow) \leq W_\sigma(\mathbf{A}, \mathbf{B}) + W_\sigma(\mathbf{B}, \mathbf{A}^\leftarrow) = 2W_\sigma(\mathbf{A}, \mathbf{B}).$$

Similarly for the other cases.  $\square$

Keep in mind that  $\mathbf{A}^\leftarrow = \mathbf{A}$  would tell us that  $\mathbf{A}$  satisfies  $\theta_{\mathbf{A}}$ -sqdb. This condition indeed follows from  $W_\sigma(\mathbf{A}, \mathbf{A}^\leftarrow) = 0$  if  $k$  generates  $A$  and  $\{k_1^*, \dots, k_d^*\} = \{k_1, \dots, k_d\}$ , as can be seen from [39, Theorems 3.9 and 3.10] and [38, Section 6] as well as the arguments used there (those papers do not explicitly cover  $W_\sigma$  as defined in this paper). Similarly for the other cases in the corollary above. For  $W_\sigma$  and  $W_{\sigma\sigma}$  we in fact discuss this from a more general point of view in Subsection 8.2 (Theorem 8.11 and Corollary 8.14).

Since we do not have corresponding symmetries for  $W$  (from the proof of Theorem 8.5 it is clear that the modular dynamics and KMS duals played a key role in obtaining those symmetries, and  $W$  simply does not have the required structure built in) we only have the triangle inequality

$$W(\mathbf{A}, \mathbf{A}^\leftarrow) \leq W(\mathbf{A}, \mathbf{B}) + W(\mathbf{B}, \mathbf{A}^\leftarrow)$$

and similarly for  $W(\mathbf{A}^\leftarrow, \mathbf{A})$ . However, the central point remains the same, namely to be able to bound the deviation of  $\mathbf{A}$  from detailed balance in terms of its Wasserstein distance from another system.

**Example 8.7.** Applying the corollary when  $\mathbf{B}$  is classical, i.e.,  $B$  is abelian, we take  $\mathbf{B}$ 's reversing operation to be the identity map, in which case  $\mathbf{B}^\leftarrow = \mathbf{B}$ , and  $\theta_{\mathbf{B}}$ -sqdb simply says that  $\mathbf{B}' = \mathbf{B}$  (refer to Section 5), which generalizes detailed balance of a Markov chain. Thus we have the deviation  $W_\sigma(\mathbf{A}, \mathbf{A}^\leftarrow)$  of  $\mathbf{A}$  from  $\theta_{\mathbf{A}}$ -sqdb bounded in terms of its distance  $W_\sigma(\mathbf{A}, \mathbf{B})$  from a system  $\mathbf{B}$  satisfying usual classical detailed balance. Similarly for  $W_\sigma(\mathbf{A}^\leftarrow, \mathbf{A})$ .

When both  $\mathbf{A}$  and  $\mathbf{B}$  are classical, the triviality of the modular dynamics gives  $W_\sigma = W$ . Hence the inequalities for  $W_\sigma$  can be stated as

$$W(\mathbf{A}, \mathbf{A}') \leq 2W(\mathbf{A}, \mathbf{B}) \quad \text{and} \quad W(\mathbf{A}', \mathbf{A}) \leq 2W(\mathbf{B}, \mathbf{A}).$$

As illustrated in Subsection 4.3,  $W$  is not symmetric in general, even for classical systems. To ensure the usual metric symmetry,  $W_{\sigma\sigma}$  still has to be used.

**Conclusion.** The various inequalities above illustrate that considering a set of systems at most some specified Wasserstein distance away from a given system  $\mathbf{B}$  satisfying a detailed balance property, sensibly relates to the deviation (as measured by Wasserstein distance) of systems in that set from detailed balance. In addition, we can choose  $\mathbf{B}$  to be simple or well understood, say some appropriately chosen classical system. In this way we can obtain what we expect to be sets of non-equilibrium systems  $\mathbf{A}$  having structure close enough to detailed balance to make them amenable to further analysis.

**8.2. Zero Wasserstein distance and common structure.** To shed light on this issue regarding the structure of a system  $\mathbf{A}$ , we turn to the implications of zero Wasserstein distance in relation to common structure in two systems. Our basic result in this regard is stated as Theorem 8.11 below. This in fact boils down to a generalization of the “faithfulness” of an (asymmetric) metric  $\rho$ , namely the property that  $\rho(x, y) = 0$  implies  $x = y$ , which was not discussed in the previous section. We leave the case of non-zero Wasserstein distance, which appears to much more involved, for future work. Again modular properties and KMS duals play a key role, hence our strongest results will be for  $W_\sigma$  and  $W_{\sigma\sigma}$ .

This is intimately related to the coordinates of a system, in particular the algebra generated by them, hence we introduce the following terminology and notation to be used in the remainder of this section.

**Definition 8.8.** The *coordinate algebra*  $M$  of a system  $\mathbf{A}$  is the von Neumann subalgebra of  $A$  generated by  $\{k_1, \dots, k_d\}$ .

This notation  $M$  will be used as a convention below. Similarly,  $N$  will denote the coordinate algebra of  $\mathbf{B}$ .

Given any  $\mathbf{A}$ , the condition  $\{k_1^*, \dots, k_d^*\} = \{k_1, \dots, k_d\}$  will now become relevant. (Note that this does not mean that  $k_1^* = k_1$ , etc.) In [38, 39] this condition was needed as part of the proof of faithfulness of an asymmetric metric. This will now be obtained in a generalized form for  $W_\sigma$  and  $W_{\sigma\sigma}$ . For later convenience, we give this condition a name:

**Definition 8.9.** A system  $\mathbf{A}$  is called *hermitian* if  $\{k_1^*, \dots, k_d^*\} = \{k_1, \dots, k_d\}$ .

We need the following lemma extending a basic technical point from [38, Lemma 6.3].

**Lemma 8.10.** *Consider systems  $\mathbf{A}$  and  $\mathbf{B}$ , with  $\mathbf{A}$  hermitian. Assume that there is an  $\omega \in T(\mathbf{A}, \mathbf{B})$  such that  $I_{\mathbf{A}, \mathbf{B}}(\omega) = 0$ . Then the restriction of  $E_\omega$  to  $M$  is a normal unital  $*$ -homomorphism*

$$E_\omega|_M : M \rightarrow N$$

and  $E_\omega(k_i) = l_i$  for  $i = 1, \dots, d$ .

*Proof.* As in (22),

$$\nu(|l_i - E_\omega(k_i)|^2) + \nu(E_\omega(|k_i|^2) - |E_\omega(k_i)|^2) = 0,$$

due to  $I_{\mathbf{A}, \mathbf{B}}(\omega) = 0$ . Thus  $E_\omega(k_i) = l_i$  and  $E_\omega(|k_i|^2) = |E_\omega(k_i)|^2$ , since  $\nu$  is faithful and  $E_\omega(|k_i|^2) \geq |E_\omega(k_i)|^2$ . Let  $M_0$  be the unital  $*$ -algebra generated by  $\{1_A, k_1, \dots, k_d\}$ . Applying [25, Theorem 3.1] and using the fact that  $\mathbf{A}$  is hermitian, we find that  $E_\omega|_{M_0} : M_0 \rightarrow N$  is a unital  $*$ -homomorphism. As  $E_\omega$  is normal (i.e.,  $\sigma$ -weakly continuous) and  $M_0$  is  $\sigma$ -weakly dense in  $M$ , the lemma follows, simply because the maps  $a_1 \mapsto a_1 a_2$  and  $a_2 \mapsto a_1 a_2$  are  $\sigma$ -weakly continuous.  $\square$

Note that this lemma is applicable when  $W(\mathbf{A}, \mathbf{B}) = 0$ , due to the existence of optimal transport plan in Theorem 7.10, which indeed led to  $\mathbf{A} = \mathbf{B}$  for the case of  $A = B$  and  $k = l$  in [39, Theorem 3.10]. However, to make any appreciable further progress in our current more general context, we need the additional structure of modular and KMS transport plans in the definitions of  $W_\sigma$  and  $W_{\sigma\sigma}$ .

To formulate our results below more succinctly, we are going to use the notation

$$\alpha|_M$$

to refer to the restrictions  $(\alpha|_M)_{v,z} := \alpha_{v,z}|_M$  and

$$E_\omega \circ \alpha$$

to refer to  $(E_\omega \circ \alpha)_{v,z} := E_\omega \circ \alpha_{v,z}$ , etc., for all  $z \in Z_v$  and  $v \in \Upsilon$ , in line with Definition 7.1. I.e., we are going to suppress  $v$  and  $z$  in our notation.

Also recall that a  $*$ -isomorphism from one von Neumann algebra to another is a linear map that is one to one (injective), onto (surjective) and preserves all algebraic structure.

**Theorem 8.11.** *Let  $\mathbf{A}$  and  $\mathbf{B}$  be hermitian systems such that  $W_\sigma(\mathbf{A}, \mathbf{B}) = 0$ . Then there is a  $*$ -isomorphism  $\iota_{\mathbf{A},\mathbf{B}} : M \rightarrow N$  between the coordinate algebras of  $\mathbf{A}$  and  $\mathbf{B}$ , uniquely determined by  $\iota_{\mathbf{A},\mathbf{B}}(k_i) = l_i$  for  $i = 1, \dots, d$ , such that*

$$(24) \quad E_\omega \circ \alpha|_M = \beta \circ \iota_{\mathbf{A},\mathbf{B}}$$

for any optimal transport plan  $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$ .

*Proof.* By Theorem 7.10 and Lemma 8.10 we have a normal unital  $*$ -homomorphism  $\iota_{\mathbf{A},\mathbf{B}} := E_\omega|_M : M \rightarrow N$ , necessarily uniquely determined by  $\iota_{\mathbf{A},\mathbf{B}}(k_i) = l_i$  for  $i = 1, \dots, d$ . As in Theorem 8.5's proof we have  $I_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}(\omega^\sigma) = 0$ . We therefore also have a normal unital  $*$ -homomorphism  $\iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} := E_\omega^\sigma|_M : N \rightarrow M$ , uniquely determined by  $\iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}(l_i) = k_i$  for  $i = 1, \dots, d$ . From this it is easily seen that  $\iota_{\mathbf{A},\mathbf{B}}$  and  $\iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}$  are each other's inverses:  $\iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} \circ \iota_{\mathbf{A},\mathbf{B}}(k_i) = k_i$  meaning that  $\iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} \circ \iota_{\mathbf{A},\mathbf{B}}|_{M_0} = \text{id}_{M_0}$  with  $M_0$  as in the lemma's proof, hence  $\iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} \circ \iota_{\mathbf{A},\mathbf{B}} = \text{id}_M$  by  $\sigma$ -weak continuity; similarly  $\iota_{\mathbf{A},\mathbf{B}} \circ \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} = \text{id}_N$ . Hence  $\iota_{\mathbf{A},\mathbf{B}}$  is indeed a  $*$ -isomorphism from  $M$  onto  $N$ .

Now  $E_\omega \circ \alpha|_M = \beta \circ \iota_{\mathbf{A},\mathbf{B}}$  follows directly from  $E_\omega \circ \alpha = \beta \circ E_\omega$ , which is part of  $T_\sigma(\mathbf{A}, \mathbf{B})$ 's definition; see (20) and Definition 7.3.  $\square$

In particular (24) tells us (by applying  $\iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}$  from the right) that

$$(25) \quad \beta|_N = E_\omega \circ \alpha|_M \circ \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma},$$

showing that  $\beta|_N$  is determined by  $\alpha|_M$ , while  $\alpha|_M$  is at least constrained by  $\beta|_N$ . This clearly illustrates our main point about common structure in the dynamics of the two systems when  $W_\sigma(\mathbf{A}, \mathbf{B}) = 0$ .

Building on this result, and in preparation for the corollaries below, we state the following:

**Definition 8.12.** Two systems  $\mathbf{A}$  and  $\mathbf{B}$  are called *isomorphic* if there is a  $*$ -isomorphism  $\iota : A \rightarrow B$  such that  $\iota \circ \alpha = \beta \circ \iota$ ,  $\nu \circ \iota = \mu$  and  $\iota(k_i) = l_i$  for  $i = 1, \dots, d$ .

For all intents and purposes isomorphic systems are the same, but possibly represented differently. Below we show how isomorphic systems can be identified inside  $\mathbf{A}$  and  $\mathbf{B}$  in Theorem 8.11 when additional assumptions are made. In particular, in Theorem 8.11 we did not assume that  $\alpha(M) \subset M$ , i.e., that  $\alpha(M)$  is contained in  $M$ , or that  $\beta(N) \subset N$ , hence we could not necessarily restrict the systems  $\mathbf{A}$  or  $\mathbf{B}$  to systems on  $M$  and  $N$  respectively.

**Corollary 8.13.** *Assuming that  $\alpha(M) \subset M$ , in addition to Theorem 8.11's assumptions, it follows that  $\beta(N) \subset N$  and*

$$\iota_{\mathbf{A},\mathbf{B}} \circ \alpha|_M = \beta \circ \iota_{\mathbf{A},\mathbf{B}}.$$

*Consequently we can restrict all the structures in  $\mathbf{A}$  and  $\mathbf{B}$  to  $M$  and  $N$  respectively to obtain isomorphic systems  $\mathbf{M}$  and  $\mathbf{N}$  respectively.*

*Proof.* This follows directly from Theorem 8.11 and  $\iota_{\mathbf{A},\mathbf{B}} := E_\omega|_M$  in its proof. Keep in mind that  $\nu \circ \iota_{\mathbf{A},\mathbf{B}} = \nu \circ E_\omega|_M = \mu|_M$ ; see Definition 7.5.  $\square$

This is a very clear cut case of common structure in  $\mathbf{A}$  and  $\mathbf{B}$ . It suggests that when we aim to analyze a system  $\mathbf{B}$  by comparison to simple or well understood systems, one strategy would be to choose each of the latter as a system  $\mathbf{A}$  with  $A$  generated by  $\mathbf{A}$ 's coordinates  $k_1, \dots, k_d$ . For  $W_\sigma(\mathbf{A}, \mathbf{B}) = 0$ , this corollary then implies that

$$\beta|_N = \iota_{\mathbf{A},\mathbf{B}} \circ \alpha \circ \iota_{\mathbf{A},\mathbf{B}}^{-1},$$

giving a precise expression of how  $\mathbf{A}$  is contained in  $\mathbf{B}$ , and how  $\mathbf{A}$ 's properties and behaviour are consequently reflected in that of  $\mathbf{B}$ . Theorem 8.11 can be viewed as weaker version of this situation.

To show explicitly how Theorem 8.11 relates to the faithfulness of an asymmetric metric, we state the following special case of this corollary:

**Corollary 8.14.** *Consider two hermitian systems  $\mathbf{A}$  and  $\mathbf{B}$ , where  $A$  is generated by  $k_1, \dots, k_d$  and  $B$  by  $l_1, \dots, l_d$ . If  $W_\sigma(\mathbf{A}, \mathbf{B}) = 0$ , it then follows that  $\mathbf{A}$  and  $\mathbf{B}$  are isomorphic.*

Note that the relationship between  $\alpha|_M$  and  $\beta|_N$  in Theorem 8.11 and Corollary 8.13 is not symmetric, as may be expected from the lack of symmetry of the asymmetric pseudometric  $W_\sigma$ .

**Example 8.15.** In the example treated in Subsection 4.3, where  $N = B$ , one can show that  $W_\sigma(\mathbf{A}, \mathbf{B}) = 0$  is not sufficient to ensure that  $\mathbf{B}$  is isomorphic to a system on  $M$  obtained by restriction of  $\mathbf{A}$ . Indeed,  $W_\sigma(\mathbf{A}, \mathbf{B}) = 0$  does not imply that  $\alpha(M) \subset M$ , despite  $\beta(N) \subset N$  being true. This is closely related to (14) and (15); keep in mind

that  $W = W_\sigma$  for classical systems, as the modular dynamics for such systems are trivial.

To attain a symmetric relationship, we of course need to resort to the (symmetric) pseudometric  $W_{\sigma\sigma}$ . One can indeed expect that the requirement  $W_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) = 0$  may place stronger restrictions than  $W_\sigma(\mathbf{A}, \mathbf{B}) = 0$  on  $\alpha$ , given  $\beta$ , simply because by definition we always have  $W_\sigma(\mathbf{A}, \mathbf{B}) \leq W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ .

**Corollary 8.16.** *Let  $\mathbf{A}$  and  $\mathbf{B}$  be hermitian systems such that  $W_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) = 0$ . Then*

$$E_\omega \circ \alpha|_M = \beta \circ \iota_{\mathbf{A}, \mathbf{B}} \quad \text{and} \quad E_\omega^\sigma \circ \beta|_N = \alpha \circ \iota_{\mathbf{B}, \mathbf{A}}$$

for any optimal transport plan  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ , in which case  $\omega^\sigma \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$  is also optimal.

*Proof.* Here  $W_\sigma(\mathbf{A}, \mathbf{B}) = 0$  and  $W_\sigma(\mathbf{B}, \mathbf{A}) = 0$ . The former follows from the definitions of  $W_\sigma$  and  $W_{\sigma\sigma}$ , which ensure that  $W_\sigma(\mathbf{A}, \mathbf{B}) \leq W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ . The latter follows from the symmetry of  $W_{\sigma\sigma}$  given by Theorem 7.10. By  $T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ 's definition, we have  $\omega^\sigma \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$  for any  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ . Hence for an optimal  $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ , the cost  $I_{\mathbf{B}, \mathbf{A}}(\omega^\sigma)$  is defined and as in Theorem 8.5's proof we have  $I_{\mathbf{B}, \mathbf{A}}(\omega^\sigma) = 0$ , so  $\omega^\sigma$  is indeed optimal. Now we can simply apply Theorem 8.11 to both directions.  $\square$

We then have a corresponding symmetric version of Corollary 8.13 as well, where we could assume either  $\alpha(M) \subset M$  or  $\beta(N) \subset N$ .

More generally, for any optimal transport plan, including for the case of  $W$ , the condition  $E_\omega \circ \alpha = \beta \circ E_\omega$  implies a relation between  $\mathbf{A}$  and  $\mathbf{B}$  which can be viewed as a weaker condition than an isomorphism between systems. This is the case even when the systems are not hermitian or the Wasserstein distance being used is not zero. Theorem 8.11 and its corollaries simply state strong forms of such a relation.

The general case can possibly be fruitfully viewed from the perspective of normal u.c.p. maps as morphisms, or, in keeping with the bimodule approach, from that of Connes' correspondences as morphisms. This will not be pursued here, but see [30, Appendix V.B] and [41, Section 5] for background on this matter, as well as [11] in relation to dynamical systems with automorphic (i.e., unitary) dynamics.

What is needed in addition to our development above, is a fitting notion of the "size" of  $E_\omega(A)$  in  $B$ , or of  $E_\psi(B)$  in  $A$ , in particular for optimal transport plans (for any of our Wasserstein distances)  $\omega$  from  $\mathbf{A}$  to  $\mathbf{B}$  or  $\psi$  from  $\mathbf{B}$  to  $\mathbf{A}$ . This is relevant, simply because

$$\beta(E_\omega(a)) = E_\omega(\alpha(a))$$

for all  $a \in A$ , hence  $\alpha$  and the transport plan  $\omega$  determines the behaviour of  $\beta$  on  $E_\omega(A)$ . The role of different optimal transport plans, when not unique, may also be of interest.

## 9. OUTLOOK

This paper developed the conceptual and technical foundations of a novel framework for expressing and studying deviation from detailed balance via optimal transport, in both the quantum and classical cases. In the process it tied together the ideas built up in the papers [41, 38, 39], leading to an optimal transport perspective on [41]. Corollary 8.6 together with its discussion is a fairly representative illustration of our aims. More broadly the goal is to study (quantum) dynamical systems via the optimal transport ideas and tools developed in this paper.

Much remains to be explored. In particular, to systematically apply the theory to analyze systems, including in the context of non-equilibrium statistical mechanics, as mentioned in the introduction. We expect that it should be of broader use, though, for example in non-commutative as well as classical ergodic theory to quantify and study how far a systems is from satisfying a particular ergodic property.

The theory itself could also be developed further, some lines of investigation having been discussed at the end of Section 8. In addition, it would be worth investigating the case where the coordinates  $k$  of a system  $\mathbf{A}$  are not necessarily bounded. In this case they will not be elements of  $A$ , but a natural assumption would be that they are affiliated to  $A$ .

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