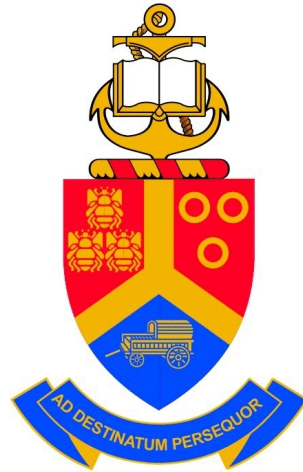


Extending quantum detailed balance through optimal transport



by

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degree*

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Declaration

I, Samuel Skosana, declare that the thesis, which I hereby submit for the degree Philosophiae Doctor at the University of Pretoria, is my own work and has not previously been submitted by me for a degree at this or any other tertiary institution.

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Degree: Philosophiae Doctor

Summary

We develop a general framework for studying classes of quantum dynamical systems that are close to and structurally similar to other systems satisfying specified properties, in particular quantum detailed balance conditions. This is done in terms of optimal transport plans and Wasserstein distances between systems on possibly different observable algebras. Basic metric properties of Wasserstein distances are proven. As a possible application of our framework to non-equilibrium statistical mechanics, bounds on deviations from detailed balance are derived.

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Science offers the boldest metaphysics of the age. It is a thoroughly human construct, driven by the faith that if we dream, press to discover, explain, and dream again, thereby plunging repeatedly into new terrain, the world will somehow come clearer and we will grasp the true strangeness of the universe. And the strangeness will all prove to be connected, and make sense.

–Edward O. Wilson, 1998.

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Index of Symbols and Conventions

General symbols.

- \emptyset : The empty set. \mathbb{N} : Natural numbers, $\{1, 2, 3, \dots\}$.
 \mathbb{R} : Field of real numbers. \mathbb{C} : Field of complex numbers.

Conventions.

- $\mathfrak{H}, \mathfrak{K}$: Typical (complex) Hilbert spaces.
 $\langle \cdot, \cdot \rangle$: An inner product on a Hilbert space; linear in the second argument and conjugate linear in the first argument.
 $\overline{\mathfrak{H}}$: The conjugate Hilbert space of \mathfrak{H} .
 $\mathfrak{H} \otimes \mathfrak{K}$: The tensor product of Hilbert spaces \mathfrak{H} and \mathfrak{K} .
 x, y, z : Typical elements of a Hilbert space.
 \bar{x} : The element $x \in \mathfrak{H}$ viewed as an element of the conjugate Hilbert space $\overline{\mathfrak{H}}$.
 $x \otimes y$: The elementary tensor of x and y .
 α, β : Typical complex numbers.
 $\bar{\alpha}$: The conjugate of a complex number α .
 $\mathcal{B}(\mathfrak{H}, \mathfrak{K})$: The space of bounded linear operators $\mathfrak{H} \rightarrow \mathfrak{K}$ for Hilbert spaces \mathfrak{H} and \mathfrak{K} .
 A, B, C : Typical (σ -finite) von Neumann algebras.
 A' : The commutant of the algebra A .
 A_+ : The set of positive elements of the algebra A .
 M, N : The subsets (or subspaces) of von Neumann algebras A and B , respectively.
 μ, ν, ξ : The faithful normal states on von Neumann algebras A, B and C , respectively.
 (A, μ) : A von Neumann algebra and faithful normal state pair.
 $1, 1_A$: The unit element of the algebra A .
 id_A : The identity operator on the algebra A .
 a, b, c : Typical bounded linear operators on Hilbert spaces, and elements of von Neumann algebras.
 a^* : The adjoint of an operator a .
 $\|a\|$: The operator norm of a .
 $a|_{\mathcal{S}}$: The restriction of operator a onto the set \mathcal{S} .
 $a \otimes b$: The algebraic elementary tensor product of the elements a and b of the algebras A and B , respectively.
 Λ, Ω, Ψ : Typical cyclic (and/or separating) vectors for von Neumann algebras A, B , and C , respectively.
 π, π' : A $*$ -homomorphism (respectively, $*$ -antihomomorphism) from a von Neumann algebra A to the space of all bounded linear operators on some Hilbert space \mathfrak{H} .
 (\mathfrak{H}, π) : A representation of an algebra A on Hilbert space \mathfrak{H} .
 $(\mathfrak{H}, \pi, \Lambda)$: A cyclic representation of algebra A on Hilbert space \mathfrak{H} .
 $\{A, \mathfrak{H}\}$: Spatially represented von Neumann algebra.

Symbols defined in the text.

$\mathbf{A}, \mathbf{B}, \mathbf{C}$	40.	ι_ω, ι_ψ	69.	$W, W_\sigma, W_{\sigma\sigma}$	64.
$\mathbf{A}', \mathbf{A}^\sigma, \mathbf{A}^{\leftarrow}$	41.	$\iota_{\mathbf{A}, \mathbf{B}}$	84.	V_{XY}	96.
$\mathbf{A}\omega\mathbf{B}$	45.	J_A	16.	X, Y	17.
Ax, \overline{Ax}	4.	j_A	16.	$x \otimes y$	11.
$A \odot B, A \otimes B$	11.	K	35.	$x \otimes_\nu y$	31.
B°	19.	$L^2(A)$	15.	Z_ν	40.
$B(\cdot, \cdot), B'(\cdot, \cdot)$	29.	L_ν, R_ν	26.		
\mathfrak{A}	41.	Λ_μ	7.		
$a \odot b, a \otimes b$	11.	λ	95.		
$a \otimes_s b$	17.	M, N	43.		
$a \otimes_\nu b$	31.	$M_n, M_n(\mathbb{C})$	9.		
α, β, γ	41.	N_μ, n_μ	3.		
α^*	96.	μ, ν, ξ	41.		
$\alpha_\nu, \alpha_{\nu, z}$	40.	μ'	8.		
$\mathcal{B}({}_A\mathfrak{H}, {}_A\mathfrak{K})$	21.	$\mu \odot \nu'$	12.		
$\mathcal{B}(\mathfrak{H}_B, \mathfrak{K}_B)$	22.	$\Omega \otimes_\nu \Psi$	69.		
$\mathcal{B}({}_A\mathfrak{H}_B)$	22.	ω_E	48.		
C_x, C_y	26.	ω, ψ, φ	14.		
Δ_μ	7.	$\omega', \omega^\sigma, \omega^{\leftarrow}$	48.		
c	44.	P_ν	14.		
c_{AB}	92.	$\mathcal{P}, \widehat{\mathcal{P}}$	15.		
d	67.	\mathcal{P}_A	16.		
Δ_μ^{it}	8.	π, π_t	4.		
$\Delta'_\mu, \Delta_\mu^{-1}$	10.	$\pi_{\mathfrak{H}}, \pi'_{\mathfrak{K}}$	19.		
δ_μ	11.	$\pi_\mu^\omega, \pi_\nu^\omega$	13.		
$\mathfrak{D}(\mathfrak{H}, \nu), \mathfrak{D}'(\mathfrak{K}, \nu)$	26.	ϖ_A	11.		
E	34.	r	22.		
E'	34.	ρ_μ	9.		
E^σ	35.	$S_{0, \mu}, S_\mu$	8.		
E^{\leftarrow}	35.	$\sigma_t, \sigma_t^\Omega, \sigma_t^\mu$	8.		
E_ω	47.	$\sigma'_t, \sigma_t^{\mu'}$	10.		
η_μ	5.	Tr	9.		
$F_{0, \mu}, F_\mu$	7.	$T(\mu, \nu)$	11.		
$\mathfrak{F}(A)$	3.	$T(\mathbf{A}, \mathbf{B})$	46.		
f	94.	$T_\sigma(\mathbf{A}, \mathbf{B})$	46.		
\mathfrak{H}_A	15.	$T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$	46.		
\mathfrak{H}_μ	5.	τ_A	36.		
$\mathfrak{H}_\mu^\omega, \mathfrak{H}_\nu^\omega$	13.	θ_μ	35.		
$\mathfrak{H} \otimes_\nu \mathfrak{K}$	31.	$\theta_{\mathbf{A}}$	41.		
${}_A\mathfrak{H}, \mathfrak{H}_B, {}_A\mathfrak{H}_B$	22.	U_η	95.		
$I_{\mathbf{A}, \mathbf{B}}$	62.	u	5.		
ι	22, 43.	u_ν	13.		
$\iota\mathfrak{H}_\nu$	47.	W_2	44.		

Introduction

Every beginning is in time, and every limit of extension in space.
–Immanuel Kant, 1781.

The main motivation for this thesis is to develop a natural framework for studying quantum dynamical systems, in which one can obtain extensions or generalized versions of properties of a system relative to another system satisfying some specified property of interest. In particular, we study extensions (including weaker forms) of quantum detailed balance (QDB) 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. In other words, we establish a novel approach to deviation from detailed balance, even in the classical case. Our approach is via transport plans. We also develop a point of view that motivates the bimodule (or correspondences in the sense of Connes) approach to non-commutative optimal transport, as developed in [41, 42] and [43], and how it fits perfectly with dynamical systems possessing steady states, and thus provides a framework for their analysis. This thesis is mainly based on the work done in [43].

The essence of our framework is to extend detailed balance conditions by considering balance between two systems, in the sense of [45], making use of couplings of the states of the two systems. Moreover, these couplings can also be viewed as a form of transport between systems. By using optimal transport, through Wasserstein distances between the two systems, we can develop a quantitative version of the theory in [45], effectively quantifying the similarity or difference between systems. In particular, if one of the systems is relatively simple or well-understood, and it satisfies certain detailed balance conditions, this framework can be used to extend those conditions to the other, possibly more complex system, thus generalizing detailed balance. In essence, some properties of one system are carried over to the other in a very structured and quantifiable way. Notably, this approach works even if the two systems have different observable algebras, as long as there is a natural physical relationship between certain observables. This relationship is built into the Wasserstein distance, which uses these observables as coordinates in the respective systems.

We adopt a transport plan approach to quadratic Wasserstein distances between systems, building on [41, 42]. However, we need to adapt this approach to accommodate systems with 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 needed to obtain certain bounds on deviation from detailed balance.

Although our main goal is to extend quantum detailed balance properties, it appears that our approach is new even in the classical case, 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, e.g., ergodic properties.

Our approach will be formulated in terms of von Neumann algebras, which provide a clear and powerful framework for studying systems. This enables us to draw on the insights and tools of Tomita-Takesaki theory, along with the related theory of bimodules, which are essential for developing a general theory. Furthermore, this von Neumann algebra setting is conceptually clear, for example in terms of comparison to the classical case, making it an ideal choice. We use unital completely positive (u.c.p.) maps to describe the dynamics of the systems, although we also allow for unital positive (u.p.) maps.

There are alternative approaches to quantum Wasserstein distances, at least between states (rather than systems) on the same algebra. Some key papers on this include [14, 23, 27, 31, 35, 60, 89], among many others. While some of these use a dynamical (see [12]) rather than transport plan approach, the framework in [41, 42] appears most appropriate to fit with [45], due to its bimodule setup and level of generality. 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.

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, 22, 46, 47, 48, 82]. Our approach offers an alternative and complementary perspective. However, we will not attempt to connect our approach to those mentioned above or to entropy production, leaving this for future work. Nevertheless, it is worth noting that [10, 34, 88] have linked entropy production to optimal transport and Wasserstein distance by following very different routes than ours.

The mathematical background necessary for the thesis is covered in Chapter 1. In particular, we discuss canonical representations of von Neumann algebras on certain Hilbert spaces, in which case the former are said to be in standard form. A natural bimodule structure on the Hilbert space is identified through the tools of Tomita-Takesaki theory. The relative tensor product of bimodules ultimately allows us to obtain the triangle inequality of Wasserstein distances.

In Chapter 2 we introduce a noncommutative version of optimal transport between systems on possibly different von Neumann algebras as adopted and used in this thesis. The basic feature of our framework, namely extending dynamical properties through transport, is discussed with detailed balance as a particular instance.

In Chapter 3 the basic metric properties of Wasserstein distances are demonstrated. Due to direction of transport, these distances are typically asymmetric pseudometrics, since the two directions relate to different (though dual) aspects of the dynamics. In particular, zero distance between two systems does not mean that they are the same. However, our bimodule setup for Wasserstein metrics indeed provide symmetric and asymmetric Wasserstein distances, depending on the restrictions we place on the transport plans. Chapter 4 investigates further properties of Wasserstein distances, including certain symmetries, which along with the metric properties allow us to find bounds on deviation from detailed balance. We also explore how zero Wasserstein distance between two systems relates to common structure in the systems.

In Chapter 5 we treat simple finite dimensional examples to clarify our approach and to illustrate how extended or refined detailed balance conditions are obtained, in the special cases where the systems are given on either an $n \times n$ matrix algebra or a classical Markov chain on finite sets.

CHAPTER 1

The Tomita-Takesaki theory and bimodules

*When a solid foundation is laid, if the mason is able
and his materials good, a strong house can be built.*
– Haile Selassie I, 1963.

A key property we want a distance function to have is the triangle inequality. This is certainly one of the most distinctive properties of a distance function. But it turns out to be difficult to obtain from the transport plan approach to Wasserstein distances in the noncommutative case. However, by Tomita-Takesaki (or modular) theory, the resulting bimodules and their relative tensor products, provide a way to obtain the triangle inequality in our von Neumann algebra framework using a transport plan approach.

In this chapter we review the construction of the *relative tensor product* of a pair consisting of a left module and a right module over a common von Neumann algebra. We view a Hilbert space equipped with the usual action of a von Neumann algebra as a *left module* over the von Neumann algebra. Similarly, we take a *right module* over a von Neumann as a Hilbert space with a right action, i.e. an anti-representation, of the von Neumann algebra on that Hilbert space. Naturally, we view a *bimodule* over a pair of von Neumann algebras as a Hilbert space equipped with a left action of one algebra and a right action of another such that the two actions commute.

Unlike the ordinary (i.e. spatial) tensor product of Hilbert spaces, the relative tensor product depends on the choice of a faithful normal state on the common von Neumann algebra, hence the use of the description *relative*. In approximate terms, the basic idea behind the construction of the relative tensor product is as follows: given a faithful normal state ν on a von Neumann algebra B , and Hilbert spaces \mathfrak{H} and \mathfrak{K} with a representation and an anti-representation of B respectively, then the goal is to produce a new Hilbert space, say $\mathfrak{H} \otimes_{\nu} \mathfrak{K}$, by factoring out the actions of B on \mathfrak{H} and \mathfrak{K} . The precise construction is quite involved.

The purpose of this chapter is twofold, firstly to fix the notation we adopt and secondly to introduce the necessary mathematical background required in this thesis. In Section 1.1 we discuss the representation theory of von Neumann algebras on Hilbert spaces. This is a useful and a common way of thinking of von Neumann algebras, i.e.

presented spatially as $\{A, \mathfrak{H}\}$. Such representations always exist and are essentially unique (up to unitary equivalence), and will be exploited in the construction of the relative tensor product. A general overview of the Tomita-Takesaki theory is given in Section 1.2, in which the very precise and intimate connection between an algebra and its commutant is discussed along with a one-parameter group of automorphisms. A von Neumann algebra can be identified as a subspace of $\mathcal{B}(\mathfrak{H})$ in various ways. In Section 1.3 we discuss a canonical representation of von Neumann algebras on a Hilbert space known as a *standard form*. In Section 1.4 we introduce the notion of *modules* over one or two von Neumann algebras as well as discuss their morphisms. Section 1.5 presents the theory of *bimodules* and correspondences. The theory of correspondences was originally developed by Connes, but never published in full, although it is discussed briefly in his book [33, Appendix V.B]. In short, a *correspondence* from one von Neumann algebra, A , to another, B , is an A - B -bimodule (where the direction *from* A to B , is the convention we adopt in this thesis). The relative tensor product can be viewed as the composition of such correspondences.

We adopt the following notational conventions. Unless explicitly stated otherwise, any Hilbert space or algebra will be over the field of complex numbers. An inner product of a (pre-) Hilbert space will always be taken to be linear in the second argument and conjugate linear in the first argument, as is conventional in physics. Throughout the text, A , B , and C denote von Neumann algebras, which are assumed to be σ -finite (or countably decomposable); that is, all collections of mutually orthogonal projections have at most a countable cardinality. We denote identity operators on Hilbert spaces by 1. In particular, the unit 1_A of a von Neumann algebra A will usually be denoted by 1 when no confusion may arise.

1.1. States and the Gelfand-Naimark-Segal construction

The Gelfand-Naimark-Segal (GNS-) construction is a fundamental correspondence between *cyclic $*$ -representations* of a C^* -algebra and positive linear functionals on the algebra. It offers a way of manufacturing *representations* of algebras. In this section we give a summary of the main definitions and results that will be useful to us. For a more thorough treatment, we refer the reader to [15, §1.8 and §2.3], [20, §2.3], [62, §4.5] and [69, §3.4].

DEFINITION 1.1.1. Let A be a unital $*$ -algebra on a Hilbert space \mathfrak{H} , and μ a linear functional on A .

- (1) μ is *positive*, denoted by $\mu \geq 0$, if $\mu(a^*a) \geq 0$, $\forall a \in A$.
- (2) μ is a *state* if it is normalized and positive, i.e. if it satisfies $\mu(1_A) = 1$ and $\mu \geq 0$.
- (3) A state μ is said to be:

faithful if $\mu(a^*a) > 0, \forall a \neq 0$.

tracial if $\mu(ab) = \mu(ba), \forall a, b \in A$.

- (4) If A is a von Neumann algebra on a Hilbert space \mathfrak{H} , a state μ is said to be a *vector state* if there is a vector $x \in \mathfrak{H}$ such that $\mu(a) = \langle x, ax \rangle, \forall a \in A$.

Note that if $\mu \geq 0$, then we have $\|\mu\| = \mu(1), \mu(a^*) = \overline{\mu(a)}, \forall a \in A$, and the Cauchy-Schwarz inequality

$$(1.1.1) \quad |\mu(a^*b)|^2 \leq \mu(a^*a)\mu(b^*b), \forall a, b \in A.$$

Denote the set of all positive elements of a C^* -algebra A by A_+ , i.e.

$$A_+ := \{a^*a : a \in A\}.$$

DEFINITION 1.1.2. Let A be a von Neumann algebra on a Hilbert space \mathfrak{H} .

- (1) A linear functional μ is *normal* if it is σ -weakly continuous.
- (2) A linear functional μ on A is a *normal state* if it is normal, positive and normalized. If, in addition, μ is faithful, it is said to be a *faithful normal state*. Denote the set of all faithful normal states on A by $\mathfrak{F}(A)$.

For characterizations of normality of states, see [19, Theorem III.2.1.4]. The normal states are exactly those given by density matrices (see [20, Theorem 2.4.21]). Moreover, vector states are normal.

A linear subspace I of an algebra A is called a *left* (respectively, *right*) *ideal* in A if

$$a \in A \text{ and } b \in I \implies ab \in I \text{ (respectively, } ba \in I).$$

We call I an *ideal* in A if it is simultaneously a left and right ideal, i.e. $AI, IA \subseteq I$. For any algebra A , it is easily verified that 0 and A are both ideals in A ; they are called *trivial ideals* for A .

Note that for any C^* -algebra A we have

$$(1.1.2) \quad (ab)^*ab \leq \|a\|^2 b^*b,$$

for all $a, b \in A$ (see [19, Proposition II.3.1.9]).

PROPOSITION 1.1.3. For a linear functional μ on a C^* -algebra A , set

$$n_\mu := \{a \in A : \mu(a^*a) < +\infty\}$$

and

$$N_\mu := \{a \in A : \mu(a^*a) = 0\}.$$

Then n_μ and N_μ are both left ideals of A .

PROOF. Let $a \in A$, then

$$(1.1.3) \quad \mu((ab)^*ab) = \mu(b^*a^*ab) \leq \|a\|^2 \mu(b^*b), \forall b \in A,$$

by the inequality (1.1.2). Thus, if $b \in n_\mu$ it then follows from (1.1.3) that $ab \in n_\mu$, so that n_μ is a left ideal of A . Again, by (1.1.3) it follows that $ab \in N_\mu$ whenever $b \in N_\mu$. Thus, N_μ is a left ideal of A . \square

Note that a state on a C^* -algebra is bounded by [20, Proposition 2.3.11]. Thus, if μ is a state on A , then $n_\mu = A$.

DEFINITION 1.1.4. Let A and B be $*$ -algebras. The map $\pi : A \rightarrow B$ is said to be a $*$ -homomorphism if it satisfies

- (1) $\pi(\alpha a + \beta b) = \alpha\pi(a) + \beta\pi(b)$
- (2) $\pi(ab) = \pi(a)\pi(b)$
- (3) $\pi(a^*) = \pi(a)^*$

$\forall a, b \in A, \alpha, \beta \in \mathbb{C}$. If, in addition, π is bijective, it is called a $*$ -isomorphism. A $*$ -automorphism of A is a $*$ -isomorphism $\pi : A \rightarrow A$. The set $\{\pi_t : t \in \mathbb{R}\}$ is a *one-parameter $*$ -automorphism group* if π_t is a $*$ -automorphism for every $t \in \mathbb{R}$ and has the group property that $\pi_{t+s} = \pi_t \circ \pi_s \forall t, s \in \mathbb{R}$.

DEFINITION 1.1.5. A $*$ -homomorphism $\pi : A \rightarrow B$ between von Neumann algebras is said to be *normal* if π is continuous for the σ -weak topologies on A and B .

DEFINITION 1.1.6. Let A be a C^* -algebra on a Hilbert space \mathfrak{H} , then a vector $x \in \mathfrak{H}$ is said to be:

- (1) *cyclic* for A if $\overline{Ax} = \mathfrak{H}$, i.e the closure of the set $Ax := \{ax : a \in A\}$ is dense in \mathfrak{H} .
- (2) *separating* for A if $ax = bx, a, b \in A$ if and only if $a = b$.

DEFINITION 1.1.7. Let A be a C^* -algebra.

- (1) A *representation* of A is a pair (\mathfrak{H}, π) where \mathfrak{H} is a (complex) Hilbert space, and $\pi : A \rightarrow \mathcal{B}(\mathfrak{H})$ is a $*$ -homomorphism, where $\mathcal{B}(\mathfrak{H})$ denotes the set of bounded linear operators on \mathfrak{H} . We say that (\mathfrak{H}, π) is a *faithful representation*, if in addition, π is injective.
- (2) A *cyclic representation* of A is defined as the triple $(\mathfrak{H}, \pi, \Lambda)$, where (\mathfrak{H}, π) is a representation of A , and Λ is a vector in \mathfrak{H} which is cyclic for $\pi(A)$, i.e. $\pi(A)\Lambda = \{\pi(a)\Lambda : a \in A\}$ is dense in \mathfrak{H} .
- (3) Two representations (\mathfrak{H}_1, π_1) and (\mathfrak{H}_2, π_2) of A are *unitarily equivalent* if there exists a unitary operator u from \mathfrak{H}_1 onto \mathfrak{H}_2 such that

$$u\pi_1(a)u^* = \pi_2(a), \forall a \in A.$$

Note that if (\mathfrak{H}, π) is a representation of a C^* -algebra A and if $\Lambda \in \mathfrak{H}$ is a unit vector, then the map

$$\mu(a) := \langle \Lambda, \pi(a)\Lambda \rangle \quad (a \in A)$$

clearly defines a vector state (and thus normal) on $\pi(A)$.

LEMMA 1.1.8 (Unitarily equivalent representations). *Let $(\mathfrak{H}_1, \pi_1, \Lambda_1)$ and $(\mathfrak{H}_2, \pi_2, \Lambda_2)$ be two cyclic representations of (A, μ) . Then π_1 and π_2 are unitarily equivalent representations of A , i.e. there is a unitary map $u : \mathfrak{H}_1 \rightarrow \mathfrak{H}_2$ such that*

$$u\pi_1(a)u^* = \pi_2(a), \quad \forall a \in A.$$

PROOF. For all $a \in A$, we have

$$\begin{aligned} \|\pi_1(a)\Lambda_1\|^2 &= \langle \pi_1(a)\Lambda_1, \pi_1(a)\Lambda_1 \rangle \\ &= \langle \Lambda_1, \pi_1(a^*a)\Lambda_1 \rangle \\ &= \mu(a^*a) \\ &= \langle \Lambda_2, \pi_2(a^*a)\Lambda_2 \rangle \\ &= \|\pi_2(a)\Lambda_2\|^2. \end{aligned}$$

Similarly (with the role of a replaced by $a - b$ in the above calculation), if $\pi_1(a)\Lambda_1 = \pi_1(b)\Lambda_1$, it follows that $\pi_2(a)\Lambda_2 = \pi_2(b)\Lambda_2$, for $a, b \in A$. Consequently, the map

$$u_0\pi_1(a)\Lambda_1 = \pi_2(a)\Lambda_2 \quad (a \in A)$$

defines a norm-preserving linear map from $\pi_1(A)\Lambda_1$ to $\pi_2(A)\Lambda_2$. Since $\overline{\pi_1(A)\Lambda_1} = \mathfrak{H}_1$ and $\overline{\pi_2(A)\Lambda_2} = \mathfrak{H}_2$, it follows that u_0 extends uniquely by boundedness to an isomorphism u from \mathfrak{H}_1 to \mathfrak{H}_2 , and

$$u\Lambda_1 = u_0\pi_1(1)\Lambda_1 = \pi_2(1)\Lambda_2 = \Lambda_2.$$

Then, for all $a, b \in A$,

$$\begin{aligned} u\pi_1(a)\pi_1(b)\Lambda_1 &= u\pi_1(ab)\Lambda_1 \\ &= \pi_2(ab)\Lambda_2 \\ &= \pi_2(a)\pi_2(b)\Lambda_2 \\ &= \pi_2(a)u\pi_1(b)\Lambda_1, \end{aligned}$$

and $u\pi_1(a) = \pi_2(a)u$, since $\overline{\pi_1(A)\Lambda_1} = \mathfrak{H}_1$. Thus $u\pi_1(a)u^* = \pi_2(a)$, for all $a \in A$. \square

The existence of a cyclic representation for (A, μ) is guaranteed by the following:

THEOREM 1.1.9 (The GNS-construction). *Let $\mu : A \rightarrow \mathbb{C}$ be a state on the C^* -algebra A . Then there exists a unique (up to unitary equivalence) cyclic representation $(\mathfrak{H}_\mu, \pi_\mu, \Lambda_\mu)$ of (A, μ) such that*

$$(1.1.4) \quad \mu(a) = \langle \Lambda_\mu, \pi_\mu(a)\Lambda_\mu \rangle, \quad \forall a \in A.$$

PROOF. Construction of the Hilbert space \mathfrak{H}_μ . Let

$$N_\mu := \{a \in A : \mu(a^*a) = 0\}.$$

The set N_μ is called the left kernel of μ . Then, by Proposition 1.1.3, N_μ is a left ideal of A . Furthermore, N_μ is closed since μ is bounded. Let

$$\eta_\mu : A \rightarrow A/N_\mu$$

be the quotient map from A onto A/N_μ given by $\eta_\mu(a) := a + N_\mu$. Then we can define

$$(1.1.5) \quad \langle \eta_\mu(a), \eta_\mu(b) \rangle := \mu(a^*b), \quad \forall a, b \in A.$$

It is straightforward to verify that $\langle \cdot, \cdot \rangle$ is an inner product on A/N_μ . Denote the completion of A/N_μ with respect to the norm induced by this inner product by \mathfrak{H}_μ .

Construction of the representation π_μ : For any $a \in A$, define $\pi_\mu(a)$ as the left multiplication by a on A/N_μ , i.e.

$$(1.1.6) \quad \pi_\mu(a)\eta_\mu(b) := ab + N_\mu = \eta_\mu(ab).$$

Then $\pi_\mu(a)$ is a linear map on A/N_μ , and

$$\|\pi_\mu(a)\eta_\mu(b)\|^2 = \mu(b^*a^*ab) \leq \|a\|^2\mu(b^*b) = \|a\|^2\|\eta_\mu(b)\|^2, \quad \forall b \in A,$$

by (1.1.2). Then $\pi_\mu(a)$ is bounded and has a unique extension to a bounded linear map on \mathfrak{H}_μ . Denote this extension also by $\pi_\mu(a)$. It is then easily verified that the map $\pi_\mu : A \rightarrow \mathcal{B}(\mathfrak{H}_\mu)$ is a $*$ -homomorphism.

Identifying the unit cyclic vector Λ_μ : Let $\Lambda_\mu := \eta_\mu(1) = 1_A + N_\mu$. Clearly, $\Lambda_\mu \in \mathfrak{H}_\mu$, and

$$\pi_\mu(a)\Lambda_\mu = \pi_\mu(a)(1_A + N_\mu) = a + N_\mu \quad (a \in A).$$

Thus $\pi_\mu(A)\Lambda_\mu$ is a dense subset of \mathfrak{H}_μ , and Λ_μ is cyclic for $\pi_\mu(A)$. Moreover,

$$\begin{aligned} \langle \Lambda_\mu, \pi_\mu(a)\Lambda_\mu \rangle &= \langle \eta_\mu(1_A), \pi_\mu(a)\eta_\mu(1_A) \rangle = \langle \eta_\mu(1_A), \eta_\mu(a) \rangle = \mu(a1^*) \\ &= \mu(a) \end{aligned}$$

for all $a \in A$. □

The foregoing result states that, for a state on a C^* -algebra, the corresponding GNS-construction is essentially uniquely determined because of the cyclic property. It is easily seen that μ is faithful if and only if π_μ is faithful and Λ_μ is separating for $\pi_\mu(A)$, since $\mu(a^*a) = \|\pi_\mu(a)\Lambda_\mu\|^2$.

THEOREM 1.1.10. *Consider any state μ on a von Neumann algebra A , and let $(\mathfrak{H}_\mu, \pi_\mu, \Lambda_\mu)$ be the GNS-representation for (A, μ) . Then μ is normal if and only if $\pi_\mu : A \rightarrow \mathcal{B}(\mathfrak{H}_\mu)$ is normal. Moreover, in this case $\pi_\mu(A)$ is a von Neumann algebra on \mathfrak{H}_μ .*

For proof, see [19, Theorem III.2.2.3] or [20, Theorem 2.4.24].

In this section we established that every C^* -algebra has a concrete representation, this is the essence of the Gelfand-Naimark theorem (see [62, Theorem 4.5.6] or [69, Theorem 3.4.1]). Thus, every C^* -algebra can be realized as a C^* -subalgebra of $\mathcal{B}(\mathfrak{H})$ for some Hilbert space \mathfrak{H} .

1.2. Tomita-Takesaki theory

In this section we give a general overview of Tomita-Takesaki theory (or modular theory) and state, without proof, some of its main results. Details and proofs of statements may be found, for example, in [20, Sect. 2.5], [63, Sect. 9.2], or [81, Chap. VIII]. See [77] for a treatment of the theory on the von Neumann algebra $\mathcal{B}(\mathfrak{H})$ of bounded linear operators on a separable Hilbert space \mathfrak{H} .

The Tomita-Takesaki theory is one of the most important and useful developments in operator algebras for its many applications to mathematical physics. The theory gives a very precise and intimate connection between an algebra and its commutant, along with a one-parameter group of automorphisms [19, Section III.4]. Of particular importance is its use, in the mathematical description of thermodynamic equilibrium states using the *Kubo-Martin-Schwinger (KMS) boundary condition* in theoretical physics, which was developed by Haag, Hugenholtz, and Winnink [57] at the same time as the theory itself by Tomita [84], later expanded upon by Takesaki [79].

Consider the pair (A, μ) where A is a von Neumann algebra and $\mu \in \mathfrak{F}(A)$. We assume that the pair is in standard form, meaning that A is a von Neumann algebra on a Hilbert space \mathfrak{H}_μ with a cyclic and separating vector $\Lambda_\mu \in \mathfrak{H}_\mu$ for A (and for its commutant A') such that

$$(1.2.1) \quad \mu(a) = \langle \Lambda_\mu, a\Lambda_\mu \rangle, \quad \forall a \in A.$$

In other words, we omit to mention the normal representation π_μ and identify A and A' with $\pi_\mu(A)$ and $\pi_\mu(A')$, respectively. The vector Λ_μ is then cyclic and separating for both A and A' .

The conjugate-linear map $S_{0,\mu} : A\Lambda_\mu \subseteq \mathfrak{H}_\mu \rightarrow \mathfrak{H}_\mu$ defined by

$$S_{0,\mu}a\Lambda_\mu := a^*\Lambda_\mu, \quad \forall a \in A$$

extends to a closed conjugate linear map S_μ , called the *Tomita operator* for (A, μ) . Let J_μ the unique anti-unitary operator and Δ_μ be the unique positive, self-adjoint operator in the polar decomposition of S_μ , i.e.

$$S_\mu = J_\mu \Delta_\mu^{1/2}.$$

The adjoint S_μ^* of the Tomita operator is the closure the of conjugate linear map $F_{0,\mu} : A'\Lambda_\mu \subseteq \mathfrak{H}_\mu \rightarrow \mathfrak{H}_\mu$ defined by

$$F_{0,\mu}a'\Lambda_\mu := (a')^*\Lambda_\mu, \quad \forall a' \in A',$$

with the polar decomposition given by $S_\mu^* = J_\mu \Delta_\mu^{-1/2}$.

Note that if, in addition, the state μ is *tracial* then we have

$$\begin{aligned}
\|S_{0,\mu}a\Lambda_\mu\|^2 &= \|a^*\Lambda_\mu\|^2 \\
&= \langle a^*\Lambda_\mu, a^*\Lambda_\mu \rangle \\
&= \langle \Lambda_\mu, aa^*\Lambda_\mu \rangle \\
&= \mu(aa^*) \\
&= \mu(a^*a) \\
&= \|a\Lambda_\mu\|^2.
\end{aligned}$$

Thus $S_{0,\mu}$, in this case, is an isometry and $S_\mu = J_\mu$ and $\Delta_\mu = id_A$.

The *modular conjugation* (or *modular involution*) associated with the pair (A, μ) is the conjugate linear map $J_\mu : \mathfrak{H}_\mu \rightarrow \mathfrak{H}_\mu$ satisfying $J_\mu^2 = 1$ and

$$\langle J_\mu x, J_\mu y \rangle = \langle x, y \rangle \quad \forall x, y \in \mathfrak{H}_\mu.$$

It follows that $J_\mu^* = J_\mu$. The modular conjugation J_μ gives a $*$ -anti-isomorphism between A and its commutant A' defined by

$$(1.2.2) \quad j_\mu := J_\mu(\cdot)^* J_\mu : \mathcal{B}(\mathfrak{H}_\mu) \rightarrow \mathcal{B}(\mathfrak{H}_\mu)$$

i.e., $j_\mu(a) := J_\mu a^* J_\mu$ for every bounded linear $a : \mathfrak{H}_\mu \rightarrow \mathfrak{H}_\mu$. That is, j_μ is linear, bijective and $j_\mu(a^*) = j_\mu(a)^*$, but $j_\mu(ab) = j_\mu(b)j_\mu(a)$ for all $a, b \in \mathcal{B}(\mathfrak{H}_\mu)$. From this we can define

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

on the commutant A' of A for every $\mu \in \mathfrak{F}(A)$, i.e., $\mu'(a') = \mu(j_\mu(a'))$ for all $a' \in A'$. Since every $\mu \in \mathfrak{F}(A)$ is given by a (unique) cyclic and separating vector $\Lambda_\mu \in \mathfrak{H}_\mu$ for A , through (1.2.1), we can represent μ' by

$$\mu'(a') = \langle \Lambda_\mu, a'\Lambda_\mu \rangle, \quad \forall a' \in A'.$$

The *modular operator* $\Delta_\mu : \mathfrak{H}_\mu \rightarrow \mathfrak{H}_\mu$ is the invertible operator $\Delta_\mu = S_\mu^* S_\mu$ satisfying $J_\mu \Delta_\mu J_\mu = \Delta_\mu^{-1}$, as well as

$$S_\mu = J_\mu \Delta_\mu^{1/2} = \Delta_\mu^{-1/2} J_\mu$$

and

$$S_\mu^* = J_\mu \Delta_\mu^{-1/2} = \Delta_\mu^{1/2} J_\mu.$$

From the functional calculus of Δ_μ we construct an operator

$$\Delta_\mu^{it} = \exp(it(\ln \Delta_\mu)), \quad \forall t \in \mathbb{R},$$

such that Δ_μ^{it} is unitary for all $t \in \mathbb{R}$ and the set $\{\Delta_\mu^{it} : t \in \mathbb{R}\}$ forms a strongly continuous unitary group, called the *modular group*. Furthermore, $\Delta_\mu^{it} J_\mu = J_\mu \Delta_\mu^{it}$ and $J_\mu \Lambda_\mu = \Delta_\mu^{it} \Lambda_\mu = \Lambda_\mu$ for all $t \in \mathbb{R}$.

The unitaries $\{\Delta_\mu^{it} : t \in \mathbb{R}\}$ induce a one-parameter automorphism group $\sigma^\mu := \{\sigma_t^\mu : t \in \mathbb{R}\}$ of A by

$$(1.2.3) \quad \sigma_t^\mu(a) = \Delta_\mu^{it} a \Delta_\mu^{-it}, \quad \forall a \in A, t \in \mathbb{R}.$$

This is the so-called *modular automorphism group* of A (relative to μ).

THEOREM 1.2.1 (Tomita-Takesaki). *Let μ be a faithful normal state on a von Neumann algebra A . Then:*

- (1) $\sigma_t^\mu(A) = A, \quad t \in \mathbb{R},$
- (2) $J_\mu A J_\mu = A'.$

Furthermore, from the one-to-one correspondence between faithful normal states on A and the cyclic and separating vectors Λ_μ , the state μ is invariant under the automorphism group σ^μ , i.e.

$$(1.2.4) \quad \mu(\sigma_t^\mu(a)) = \mu(a), \quad \forall a \in A, t \in \mathbb{R}.$$

We will consider finite dimensional examples in this thesis, and according to Tomita-Takesaki theory we have the following:

EXAMPLE 1.2.2. Let \mathbb{C}^n be an n -dimensional Hilbert space with an orthonormal basis $\{e_j : j = 1, \dots, n\} \subseteq \mathbb{C}^n$. Consider the von Neumann algebra $M_n := M_n(\mathbb{C}) \cong \mathcal{B}(\mathbb{C}^n)$ of $n \times n$ complex valued matrices, with the operations given by the usual matrix multiplication and conjugate-transpose. First note that any faithful state (necessarily normal in finite dimensions) on M_n is given by

$$\mu(a) := \text{Tr}(\rho_\mu a), \quad \forall a \in M_n,$$

where $\rho_\mu \in M_n$ is some density matrix whose eigenvalues are strictly positive, i.e. $\rho_\mu \geq 0$ and $\text{Tr} \rho_\mu = 1$ such that $\rho_\mu e_j = p_j e_j$ with $0 < p_j \leq 1$, for all $j = 1, \dots, n$. Let $\mathfrak{H}_A := \mathbb{C}^n \otimes \mathbb{C}^n = M_n$ be a Hilbert space with the inner product given by

$$\langle x, y \rangle := \text{Tr}(x^* y).$$

We represent M_n on \mathfrak{H}_A as

$$A := M_n \otimes 1_n$$

with 1_n the $n \times n$ identity matrix. Denote this representation by π . Then

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

where $\pi(a) := a \otimes 1_n$, for all $a \in M_n$, and

$$\Lambda_\mu := \rho_\mu^{1/2} = \sum_{i=1}^n \sqrt{p_i} e_i \otimes e_i \in \mathfrak{H}_A.$$

The commutant of A is

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

with elements given by $\pi'(b) := 1_n \otimes b$, for all $b \in M_n$, where π' is the representation of M_n on \mathfrak{H}_A .

The Tomita-Takesaki theory yields a conjugate linear map

$$S_\mu \pi(a) \Lambda_\mu := \pi(a^*) \Lambda_\mu, \quad \forall a \in M_n,$$

whose adjoint S_μ^* is given by

$$S_\mu^* \pi(a) \Lambda_\mu = \pi(\rho_\mu a^* \rho_\mu^{-1}) \Lambda_\mu, \quad \forall a \in M_n.$$

Indeed, we have

$$\begin{aligned}
\langle \pi(b)\Lambda_\mu, S_\mu^* \pi(a)\Lambda_\mu \rangle &= \langle \pi(a)\Lambda_\mu, S_\mu \pi(b)\Lambda_\mu \rangle \\
&= \langle \Lambda_\mu, \pi(a^*b^*)\Lambda_\mu \rangle \\
&= \mu(a^*b^*) \\
&= \text{Tr}(\rho_\mu a^*b^*) \\
&= \text{Tr}[\rho_\mu b^* (\rho_\mu a^* \rho_\mu^{-1})] \\
&= \mu(b^* (\rho_\mu a^* \rho_\mu^{-1})) \\
&= \langle \pi(b)\Lambda_\mu, \pi(\rho_\mu a^* \rho_\mu^{-1})\Lambda_\mu \rangle
\end{aligned}$$

for all $a, b \in M_n$. Thus $S_\mu^* \pi(a) = \pi(\rho_\mu a^* \rho_\mu^{-1})$, for all $a, b \in M_n$. Similarly, J_A is given by

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

(which is indeed independent of the faithful state μ) and one has

$$(1.2.5) \quad j_A(\pi(a)) = \pi'(a^\top) \quad \text{and} \quad j_A(\pi'(a)) = \pi(a^\top)$$

for $a \in M_n$, where a^\top is the transpose of $a \in M_n$. Note that this means that

$$\mu'(\pi'(a)) = \mu(\pi(a^\top)) = \text{Tr}(\rho_\mu a^\top) = \text{Tr}(\rho_\mu^\top a), \quad \forall a \in M_n.$$

Furthermore, for all $a \in M_n$, we have

$$\begin{aligned}
\Delta_\mu \pi(a) &= (S_\mu^* J_A) (S_\mu^* J_A) \pi(a) \\
&= S_\mu^* J_A S_\mu^* \pi'((a^*)^\top) \\
&= S_\mu^* J_A \pi'(\rho_\mu a^\top \rho_\mu^{-1}) \\
&= S_\mu^* \pi((\rho_\mu a^\top \rho_\mu^{-1})^*) \\
&= \pi(a),
\end{aligned}$$

thus Δ_μ is simply given by the identity map in the finite dimensional case, and can be expressed as $\Delta_\mu = \rho_\mu \otimes \rho_\mu^{-1}$. It then follows from the functional calculus of the modular operator that

$$\Delta_\mu^{it} \pi(a) \Delta_\mu^{-it} = [\rho_\mu^{it} a \rho_\mu^{-it}] \otimes 1_n,$$

and the modular dynamics (or modular group) σ^μ is given by

$$(1.2.6) \quad \sigma_t^\mu(\pi(a)) = \pi(\rho_\mu^{it} a \rho_\mu^{-it})$$

for all $a \in M_n$, and $t \in \mathbb{R}$. Similarly, for the modular dynamics on the commutant of A , we have

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

since $\Delta'_\mu = \Delta_\mu^{-1}$ and $(\Delta_\mu^{it})^* = \Delta_\mu^{-it}$, for all $a \in M_n$, and $t \in \mathbb{R}$.

We conclude this section with a description of how when given a composite space, the constituent spaces inherit its cyclic representation and modular structure. Consider two von Neumann algebras A and B , and denote by $A \odot B$ their algebraic tensor product, this is the space linearly spanned by finitely many linear combinations of *elementary tensors* $a \otimes b$ ($a \in A, b \in B$). The space $A \odot B$ has a natural structure as a $*$ -algebra with multiplication

$$(a_1 \otimes b_1)(a_2 \otimes b_2) = a_1 a_2 \otimes b_1 b_2$$

and involution $(a \otimes b)^* = a^* \otimes b^*$. Similarly $A \odot B'$, where B' is the commutant of B , has a natural $*$ -algebraic structure.

DEFINITION 1.2.3. Let A and B be von Neumann algebras with $\mu \in \mathfrak{F}(A)$ and $\nu \in \mathfrak{F}(B)$. A *coupling* of (A, μ) and (B, ν) is a state ω on the algebraic tensor product $A \odot B'$ such that

$$(1.2.7) \quad \omega(a \otimes 1) = \mu(a) \quad \text{and} \quad \omega(1 \otimes b') = \nu'(b')$$

for all $a \in A, b' \in B'$. We also call such an ω of a *coupling* of μ and ν . Denote the set of all couplings of μ and ν by $T(\mu, \nu)$.

REMARKS 1.2.4. In Section 2.3, we will introduce refined versions of the set of couplings and motivate why couplings can be viewed as transport plans in our approach to Wasserstein distances.

Note that ω is bounded with respect to the maximal C^* -norm on $A \odot B'$ and therefore has a unique extension to a state on $A \odot B'$, which we may call ω_m . Therefore the GNS-construction Theorem 1.1.9 applies to ω_m , which means that we have a cyclic representation for $(A \odot B', \omega)$ as well, despite $A \odot B'$ not being a C^* -algebra in general, with $\pi_\omega := \pi_{\omega_m}|_{A \odot B'}$ and $\pi_\omega(A \odot B')\Omega$ dense in \mathfrak{H}_ω , where $\Omega := \Lambda_\omega$ (see for example [39, Theorem 4.1]).

We now define two simple, yet important, examples of couplings that always exist:

PROPOSITION 1.2.5. Consider two von Neumann algebras A and B with $\mu \in \mathfrak{F}(A)$ and $\nu \in \mathfrak{F}(B)$. Let $(\mathfrak{H}_\mu, id_A, \Lambda_\mu)$ and $(\mathfrak{H}_\nu, id_B, \Lambda_\nu)$ be the cyclic representations of (A, μ) and (B, ν) , respectively.

- (1) Let $\varpi_A : A \odot A' \rightarrow \mathcal{B}(\mathfrak{H}_\mu)$ be the unital $*$ -homomorphism obtained by extending the bilinear map

$$A \times A' \rightarrow \mathcal{B}(\mathfrak{H}_\mu) : (a, a') \mapsto aa',$$

by the universal property of tensor products. Then the diagonal coupling of μ with itself, is defined by

$$(1.2.8) \quad \delta_\mu(d) := \langle \Lambda_\mu, \varpi_A(d)\Lambda_\mu \rangle \quad \forall d \in A \odot A',$$

i.e. $\delta_\mu(a \otimes a') = \langle \Lambda_\mu, aa'\Lambda_\mu \rangle$ for all $a \in A$ and $a' \in A'$.

(2) Let $\mu \odot \nu'$ be the linear functional on $A \odot B'$ defined by

$$(1.2.9) \quad \mu \odot \nu'(a \otimes b') := \mu(a)\nu'(b') \quad \forall a \in A, b' \in B'.$$

Then $\mu \odot \nu'$ is a coupling of μ and ν , called the product (or trivial) coupling.

PROOF. (1) The functional δ_μ is clearly linear. Since ϖ_A is a unital $*$ -homomorphism on $A \odot A'$, it follows that

$$\delta_\mu(1 \otimes 1) = \langle \Lambda_\mu, 1 \cdot 1\Lambda_\mu \rangle = \|\Lambda_\mu\|^2 = 1,$$

and for any $d = \sum_{j=1}^n a_j \otimes a'_j \in A \odot A'$

$$\begin{aligned} \delta_\mu(d^*d) &= \langle \Lambda_\mu, \varpi_A(d)^* \varpi_A(d) \Lambda_\mu \rangle \\ &= \langle \varpi_A(d) \Lambda_\mu, \varpi_A(d) \Lambda_\mu \rangle \\ &= \|\varpi_A(d) \Lambda_\mu\|^2 \\ &\geq 0. \end{aligned}$$

Thus δ_μ defines a state on $A \odot A'$. It is a coupling of μ and ν since

$$\delta_\mu(a \otimes 1) = \langle \Lambda_\mu, \varpi_A(a \otimes 1) \Lambda_\mu \rangle = \langle \Lambda_\mu, a\Lambda_\mu \rangle = \mu(a),$$

and

$$\delta_\mu(1 \otimes a') = \langle \Lambda_\mu, \varpi_A(1 \otimes a') \Lambda_\mu \rangle = \langle \Lambda_\mu, a'\Lambda_\mu \rangle = \mu'(a')$$

for all $a \in A, a' \in A'$.

(2) The functional $\mu \odot \nu' : A \odot B' \rightarrow \mathbb{C}$ is well-defined by the universal property of tensor products, since the map

$$A \times B' \rightarrow \mathbb{C} : (a, b') \mapsto \mu(a)\nu'(b')$$

is bilinear. Furthermore $\mu \odot \nu'$ is linear, and

$$\mu \odot \nu'(1 \otimes 1) = \mu(1)\nu'(1) = 1.$$

To see that $\mu \odot \nu'$ is positive, consider the inner product space representation of (1.2.9):

$$\begin{aligned} \mu \odot \nu'(a \otimes b') &= \mu(a)\nu'(b') \\ &= \langle \Lambda_\mu, a\Lambda_\mu \rangle \langle \Lambda_\nu, b'\Lambda_\nu \rangle \\ &= \langle \Lambda_\mu \otimes \Lambda_\nu, (a \otimes b')\Lambda_\mu \otimes \Lambda_\nu \rangle \end{aligned}$$

$\forall a \otimes b' \in A \odot B'$. Then extending by linearity, it follows that

$$\mu \odot \nu'(d) = \langle \Lambda_\mu \otimes \Lambda_\nu, d(\Lambda_\mu \otimes \Lambda_\nu) \rangle, \quad \forall d \in A \odot B'.$$

Thus,

$$\begin{aligned} \mu \odot \nu'(d^*d) &= \langle \Lambda_\mu \otimes \Lambda_\nu, d^*d(\Lambda_\mu \otimes \Lambda_\nu) \rangle \\ &= \langle d(\Lambda_\mu \otimes \Lambda_\nu), d(\Lambda_\mu \otimes \Lambda_\nu) \rangle \\ &= \|d(\Lambda_\mu \otimes \Lambda_\nu)\|^2 \\ &\geq 0 \end{aligned}$$

for all $d \in A \odot B'$. Hence $\mu \odot \nu'$ defines a state on $A \odot B'$. Furthermore, $\mu \odot \nu'$ is a coupling of μ and ν , since by definition

$$\mu \odot \nu'(a \otimes 1) = \mu(a)\nu'(1) = \mu(a),$$

and

$$\mu \odot \nu'(1 \otimes a) = \mu(1)\nu'(b') = \nu'(b')$$

for all $a \in A, b' \in B'$. \square

Let ω be a coupling of μ and ν . To clarify certain points made in subsequent chapters, we consider multiple (but necessarily unitarily equivalent) cyclic representations corresponding to a state on a von Neumann algebra (see Lemma 1.1.8). This requires us to have the appropriate notations. We assume without loss of generality that (B, ν) is in its cyclic representation, denoted $(\mathfrak{H}_\nu, id_B, \Lambda_\nu)$, which means that $(\mathfrak{H}_\nu, id_{B'}, \Lambda_\nu)$ is a cyclic representation of (B', ν') . Similarly, we assume that (A, μ) is in the cyclic representation $(\mathfrak{H}_\mu, id_A, \Lambda_\mu)$.

Let $(\mathfrak{H}_\omega, \pi_\omega, \Omega)$ be a cyclic representation of $(A \odot B', \omega)$, i.e. $\Omega \in \mathfrak{H}_\omega$ is cyclic for $\pi_\omega(A \odot B')$ and

$$\omega = \langle \Omega, \pi_\omega(\cdot)\Omega \rangle_\omega,$$

where for emphasis we write the inner product of \mathfrak{H}_ω as $\langle \cdot, \cdot \rangle_\omega$. This induces a second cyclic representation $(\mathfrak{H}_\mu^\omega, \pi_\mu^\omega, \Omega_\mu)$ of (A, μ) by setting

$$(1.2.10) \quad \mathfrak{H}_\mu^\omega := \overline{\pi_\omega(A \odot 1)\Omega}, \quad \pi_\mu^\omega(a) := \pi_\omega(a \otimes 1)|_{\mathfrak{H}_\mu^\omega} \quad \text{and} \quad \Omega_\mu := \Omega,$$

for all $a \in A$, since

$$\langle \Omega_\mu, \pi_\mu^\omega(a)\Omega_\mu \rangle = \langle \Omega, \pi_\omega(a \otimes 1)\Omega \rangle_\omega = \omega(a \otimes 1) = \mu(a).$$

Similarly,

$$(1.2.11) \quad \mathfrak{H}_\nu^\omega := \overline{\pi_\omega(1 \odot B')\Omega}, \quad \pi_{\nu'}^\omega(b') := \pi_\omega(1 \otimes b')|_{\mathfrak{H}_\nu^\omega} \quad \text{and} \quad \Omega_\nu := \Omega,$$

for all $b' \in B'$, gives a second representation $(\mathfrak{H}_\nu^\omega, \pi_{\nu'}^\omega, \Omega_\nu)$ of (B', ν') . In particular, \mathfrak{H}_μ^ω and \mathfrak{H}_ν^ω are (closed) subspaces of \mathfrak{H}_ω .

By the unitary equivalence of the cyclic representations $(\mathfrak{H}_\nu, id_{B'}, \Lambda_\nu)$ and $(\mathfrak{H}_\nu^\omega, \pi_{\nu'}^\omega, \Omega_\nu)$ of (B', ν') , there exists a unitary operator

$$(1.2.12) \quad u_\nu : \mathfrak{H}_\nu \rightarrow \mathfrak{H}_\nu^\omega$$

defined by

$$u_\nu b' \Lambda_\nu := \pi_{\nu'}^\omega(b')\Omega_\nu, \quad \forall b' \in B'.$$

More generally, since \mathfrak{H}_ν and \mathfrak{H}_ν^ω are essentially the “same” through u_ν , any operator $t \in \mathcal{B}(\mathfrak{H}_\nu)$ can alternatively be viewed as an operator $utu^* \in \mathcal{B}(\mathfrak{H}_\nu^\omega)$. Then

$$(1.2.13) \quad \pi_{\nu'}^\omega(b') = u_\nu b' u_\nu^*, \quad \forall b' \in B'.$$

By setting

$$(1.2.14) \quad \pi_\nu^\omega(b) := u_\nu b u_\nu^*, \quad \forall b \in B,$$

we obtain a second cyclic representation $(\mathfrak{H}_\nu^\omega, \pi_\nu^\omega, \Omega_\nu)$ of (B, ν) with the property

$$\pi_\nu^\omega(B)' = \pi_{\nu'}^\omega(B').$$

Let $P_\nu \in \mathcal{B}(\mathfrak{H}_\omega)$ be the projection of \mathfrak{H}_ω onto \mathfrak{H}_ν^ω , i.e., $P_\nu = P_\nu^* = P_\nu^2$ and

$$(1.2.15) \quad P_\nu \pi_\nu^\omega(b) \Omega = \pi_\nu^\omega(b) \Omega, \quad \forall b \in B.$$

Then, for any $a \in A$, we have that

$$(1.2.16) \quad \pi_\omega(a \otimes 1) \in \mathcal{B}(\mathfrak{H}_\omega),$$

$$(1.2.17) \quad P_\nu \pi_\omega(a \otimes 1) P_\nu^* \in \mathcal{B}(\mathfrak{H}_\nu^\omega), \quad \text{and}$$

$$(1.2.18) \quad u_\nu^* P_\nu \pi_\omega(a \otimes 1) P_\nu^* u_\nu \in \mathcal{B}(\mathfrak{H}_\nu),$$

by [45, Proposition 3.1]. That is, we can directly compare the elements of A to those of B (and B') as operators on the same Hilbert space.

The foregoing discussion also holds for the couplings $\psi \in T(\nu, \xi)$ and $\varphi \in T(\mu, \xi)$, using appropriate notation for the corresponding induced representations and modular structures. Analogously, denoting the cyclic representations of $(B \odot C', \psi)$ and $(A \odot C', \varphi)$ by $(\mathfrak{H}_\psi, \pi_\psi, \Psi)$ and $(\mathfrak{H}_\varphi, \pi_\varphi, \Phi)$ respectively, we have

$$\psi = \langle \Psi, \pi_\psi(\cdot) \Psi \rangle_\psi \quad \text{and} \quad \varphi = \langle \Phi, \pi_\varphi(\cdot) \Phi \rangle_\varphi,$$

where $\pi_\psi : B \odot C' \rightarrow \mathcal{B}(\mathfrak{H}_\psi)$ and $\pi_\varphi : A \odot C' \rightarrow \mathcal{B}(\mathfrak{H}_\varphi)$ are *-homomorphisms. In particular, it follows by restricting the former cyclic representation that

$$(1.2.19) \quad \mathfrak{H}_\nu^\psi := \overline{\pi_\psi(B \odot 1) \Psi}, \quad \pi_\nu^\psi(b) := \pi_\psi(b \otimes 1)|_{\mathfrak{H}_\nu^\psi} \quad \text{and} \quad \Psi_\nu := \Psi,$$

gives a third cyclic representation $(\mathfrak{H}_\nu^\psi, \pi_\nu^\psi, \Psi_\nu)$ of (B, ν) , and that

$$(1.2.20) \quad \mathfrak{H}_\xi^\psi := \overline{\pi_\psi(1 \odot C') \Psi}, \quad \pi_{\xi'}^\psi(c') := \pi_\psi(1 \otimes c')|_{\mathfrak{H}_\xi^\psi} \quad \text{and} \quad \Psi_\xi := \Psi,$$

gives a cyclic representation $(\mathfrak{H}_\xi^\psi, \pi_{\xi'}^\psi, \Psi_\xi)$ of (C', ξ') . The unitary equivalence of the representations $(\mathfrak{H}_\nu, id_B, \Lambda_\nu)$ and $(\mathfrak{H}_\nu^\psi, \pi_\nu^\psi, \Psi_\nu)$ for (B, ν) , is established through the unitary operator $v_\nu : \mathfrak{H}_\nu \rightarrow \mathfrak{H}_\nu^\psi$ defined by

$$v_\nu b \Lambda_\nu := \pi_\nu^\psi(b) \Psi_\nu, \quad \forall b \in B,$$

which satisfies

$$(1.2.21) \quad \pi_\nu^\psi(b) = v_\nu b v_\nu^*, \quad \forall b \in B',$$

from which it in turn follows that $\pi_\nu^\psi(B)' = \pi_{\nu'}^\psi(B')$, where we have set

$$(1.2.22) \quad \pi_{\nu'}^\psi(b) := v_\nu b v_\nu^*, \quad \forall b \in B.$$

Denoting the modular conjugation for B associated to Λ_ν by J_ν , while the modular conjugation for B associated to Ω_ν is denoted by J_ν^ω , one finds

$$J_\nu^\omega u_\nu = u_\nu J_\nu$$

from which it follows that

$$\pi_\nu^\omega = j_\nu^\omega \circ \pi_{\nu'}^\omega \circ j_\nu$$

where $j_\nu^\omega := J_\nu^\omega(\cdot)^* J_\nu^\omega$ and $j_\nu := J_\nu(\cdot)^* J_\nu$ on $\mathcal{B}(\mathfrak{H}_\nu^\omega)$ and $\mathcal{B}(\mathfrak{H}_\nu)$ respectively.

1.3. Standard forms of von Neumann algebras

It is commonplace to think of von Neumann algebras presented spatially, i.e. we consider the pair $\{A, \mathfrak{H}\}$ [49]. Even if the von Neumann algebra A is given as acting on a Hilbert space \mathfrak{H} , we will see that it has other privileged representations. As we saw in Section 1.1, the GNS-construction associated to any von Neumann algebra A with a faithful normal state μ yields a faithful normal representation, and remarkably such representations are unitarily equivalent.

In this section we show that (A, μ) has a canonical representation on a certain Hilbert space, called *standard*. This is a particular instance of the GNS-construction, and it will play a major role in the study of all normal representations of the von Neumann algebra A , as will seen in Section 1.5.

The theory of standard forms of von Neumann algebras was developed independently by Araki [9] and Connes [32] in the case of σ -finite von Neumann algebras, and by Haagerup [58] in the general case. See [50], [59, Appendix A.3] and [78, Chap. 10] for more details on the standard forms. The reader is referred to [20, Section 2.5.4] for a very good treatment.

DEFINITION 1.3.1. Let A be a von Neumann algebra and $\mu \in \mathfrak{F}(A)$. We call the GNS-representation $\pi_\mu : A \rightarrow \mathcal{B}(\mathfrak{H}_\mu)$ the *standard representation* of (A, μ) and write

$$L^2(A) := \mathfrak{H}_\mu$$

for the GNS Hilbert space.

The standard representation is faithful and normal. The former follows from the faithfulness of μ while the latter follows from Proposition 1.1.10. In this case we identify A with its image $\pi_\mu(A) \subset \mathcal{B}(L^2(A))$, and A is said to be in *standard representation on $L^2(A)$* . Denote the image of $1 \in A$ in $L^2(A)$ by Λ_μ , which we use to differentiate between the operator $a \in A$ and the vector $a\Lambda_\mu \in L^2(A)$. Note that the vector Λ_μ is both cyclic and separating for A . To simplify the notation, we will sometimes identify $a \in A$ with $\pi_\mu(a)$ and write ax in place of $\pi_\mu(a)x$.

DEFINITION 1.3.2. Let \mathfrak{H} be a Hilbert space.

(1) A subset $\mathcal{P} \subseteq \mathfrak{H}$ is called a *cone in \mathfrak{H}* if

$$tx \in \mathcal{P}, \quad \forall t \geq 0, x \in \mathcal{P}.$$

(2) The *dual of a cone* \mathcal{P} is the closed cone

$$\widehat{\mathcal{P}} := \{x \in \mathfrak{H} : \langle y, x \rangle \geq 0, \forall y \in \mathcal{P}\}.$$

(3) A cone \mathcal{P} is *self-dual* if $\widehat{\mathcal{P}} = \mathcal{P}$.

A self-dual cone is closed.

DEFINITION 1.3.3. A von Neumann algebra $A \subseteq \mathcal{B}(\mathfrak{H})$ is said to be in *standard form* if A has a representation on a Hilbert space \mathfrak{H} with an anti-unitary involution J on \mathfrak{H} (called the *conjugation*) and a self-dual cone $\mathcal{P} \subseteq \mathfrak{H}$ such that:

- (1) $JAJ = A'$.
- (2) $Jx = x, \forall x \in \mathcal{P}$.
- (3) $aJa\mathcal{P} \subset \mathcal{P}, \forall a \in A$.
- (4) $JaJ = a^*, \forall a \in A \cap A'$.

We denote by $(A, \mathfrak{H}, J, \mathcal{P})$ a von Neumann algebra in standard form.

This is the abstract (or axiomatic) definition. The aim of this section is to demonstrate the existence of a standard form for any σ -finite von Neumann algebra.

A standard form is unique in the sense that any two $*$ -isomorphic forms are spatially isomorphic:

PROPOSITION 1.3.4 (Uniqueness of standard forms). *If $(A, \mathfrak{H}, J, \mathcal{P})$ and $(\tilde{A}, \tilde{\mathfrak{H}}, \tilde{J}, \tilde{\mathcal{P}})$ are two standard forms, and $\Phi : A \rightarrow \tilde{A}$ is a $*$ -isomorphism, then there is a unique unitary $u : \mathfrak{H} \rightarrow \tilde{\mathfrak{H}}$ such that*

- (1) $\Phi(a) = uau^*, \forall a \in A$,
- (2) $\tilde{J} = uJu^*$, and
- (3) $\tilde{\mathcal{P}} = u(\mathcal{P})$.

For proof see [58] or [78, Corollary 10.15].

DEFINITION 1.3.5. The *natural positive cone* \mathcal{P}_A in \mathfrak{H} associated with (A, Λ_μ) is defined by

$$\mathcal{P}_A := \overline{\{aJ_\mu a\Lambda : a \in A\}},$$

where J_μ is the modular conjugation corresponding to (A, μ) for $\mu \in \mathfrak{F}(A)$.

REMARKS 1.3.6. The natural positive cone is self-dual (by [20, Proposition 2.5.28]), and thus a closed subset. By the universality of the natural positive cone \mathcal{P}_A associated to A , the cyclic Hilbert space and modular conjugation associated to all $\mu \in \mathfrak{F}(A)$ are the same and will be denoted

$$\mathfrak{H}_A \text{ and } J_A$$

respectively (see [20, Proposition 2.5.30]). The modular conjugation J_A gives a $*$ -anti-isomorphism between A and its commutant A' defined by

$$(1.3.1) \quad j_A := J_A(\cdot)^* J_A : \mathcal{B}(\mathfrak{H}_A) \rightarrow \mathcal{B}(\mathfrak{H}_A)$$

i.e., $j_A(a) = J_A a^* J_A$ for every $a \in \mathfrak{B}(\mathfrak{H}_A)$.

Note that A is a σ -finite von Neumann algebra if and only if it has a faithful normal state (see Theorem [20, 2.5.6]). The GNS-construction then yields a standard representation for A , i.e., A has a faithful normal representation on the Hilbert space $\mathfrak{H}_A = L^2(A)$ (by Theorem 1.1.10). From Tomita-Takesaki theory we have the anti-unitary involution given by the modular conjugation and the self-dual cone given by the natural positive cone, i.e. $J = J_A$ and $\mathcal{P} = \mathcal{P}_A$, such that A is in standard form $(A, \mathfrak{H}_A, J_A, \mathcal{P}_A)$ (see [59, Appendix A.3]). We summarize this in the following result:

PROPOSITION 1.3.7. *Every σ -finite von Neumann algebra has a standard form which is unique up to spatial isomorphisms.*

We note that faithful normal states are uniquely determined by the elements of the natural positive cone (see Theorem [20, 2.5.31]). That is, for each $x \in \mathcal{P}_A$ the vector state $\mu_x : A \rightarrow \mathbb{C}$ defined by

$$\mu_x(a) := \langle x, ax \rangle$$

is such that $\mu_x \in \mathfrak{F}(A)$. Conversely, for all $\mu \in \mathfrak{F}(A)$, there is a unique $x \in \mathcal{P}_A$ such that $\mu = \mu_x$.

EXAMPLE 1.3.8. This example briefly recounts a standard form for the von Neumann algebra M_n of $n \times n$ complex-valued matrices. As in Example 1.2.2, 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. (When ρ_μ 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 Λ_μ as in Example 1.2.2, but our standard form is more convenient below for the general case.) However, in the general theory we do not use this representation directly. We rather use a standard form, one formulation of which is as follows. Write

$$\mathfrak{H}_A := \mathbb{C}^n \otimes_s \mathbb{C}^n = M_n,$$

where elementary tensors in \mathfrak{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 \mathfrak{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 \mathfrak{H}_A as

$$A := M_n \otimes_s 1_n$$

and its commutant is

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

with 1_n the $n \times n$ identity matrix. In this representation we use the notation $\pi(a) := a \otimes_s 1_n$ and $\pi'(b) := 1_n \otimes_s b$ for $a, b \in M_n$. 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 π' . Furthermore, the representations π and π' of M_n on \mathfrak{H}_A are normal, 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

$$\Lambda_\mu := \rho_\mu^{1/2} \in \mathfrak{H}_A.$$

The modular conjugation J_A on \mathfrak{H}_A is given by

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

(which is independent of the faithful state μ) and one has

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

for $a \in M_n$. It then follows that

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

for all $a \in M_n$.

The natural positive cone is defined (see [20, 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 \mathfrak{H}_A . Thus, M_n is in standard form $(A, \mathfrak{H}_A, J_A, \mathcal{P}_A)$.

Here we use the notation \otimes_s to represent the tensor product $M_n \otimes M_n$ on $\mathfrak{H}_A = M_n$ 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 $\mathfrak{H}_A = \mathbb{C}^n \otimes \mathbb{C}^n$ 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 3.4.2. (Also see [44, Section 2].)

Keeping these points in mind, one can 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 Λ_μ becomes less convenient for our purposes.

1.4. Module and bimodule morphisms

In this section we discuss the notion of modules over one or two von Neumann algebras, which is mainly concerned with the study of normal representations. This notion allows the introduction of the *relative tensor product* of a pair of a left module and a right module over a common von Neumann algebra. We also discuss morphisms between modules and bimodules. The reader is referred to [33, Appendix V.B], [16], [72] for further background on bimodules; see also [49], [81, Section IX.3].

DEFINITION 1.4.1. Let A and B be von Neumann algebras.

- (1) A *left A -module* is a Hilbert space \mathfrak{K} equipped with a *left A -action*, i.e. a normal unital $*$ -homomorphism $\pi_{\mathfrak{K}} : A \rightarrow \mathcal{B}(\mathfrak{K})$, or equivalently, if \mathfrak{K} has a normal representation of A . We write ${}_A\mathfrak{K}$ to emphasize that \mathfrak{K} has a left A -module structure.
- (2) A *right B -module* is a Hilbert space \mathfrak{H} equipped with a *right B -action*, i.e. a normal unital $*$ -anti-homomorphism $\pi'_{\mathfrak{H}} : B \rightarrow \mathcal{B}(\mathfrak{H})$ (that is, $\pi'_{\mathfrak{H}}$ is linear, $\pi'_{\mathfrak{H}}(b^*) = \pi'_{\mathfrak{H}}(b)^*$, but $\pi'_{\mathfrak{H}}(ab) = \pi'(b)_{\mathfrak{H}}\pi'_{\mathfrak{H}}(a)$, $a, b \in B$). Equivalently, if \mathfrak{H} has a normal anti-representation of B . We write \mathfrak{H}_B to emphasize that \mathfrak{H} has a right B -module structure.
- (3) An *A - B -bimodule* is a Hilbert space \mathfrak{H} equipped with a left A -action and a right B -action such that $\pi(A)$ and $\pi'(B)$ commute, i.e.

$$(1.4.1) \quad \pi(a)\pi'(b)x = \pi'(b)\pi(a)x, \quad \forall a \in A, b \in B, x \in \mathfrak{H}.$$

In other words, an A - B bimodule is a Hilbert space \mathfrak{H} equipped with normal representation and anti-representation π and π' of A and B on \mathfrak{H} , respectively, which commute. We write ${}_A\mathfrak{H}_B$ to emphasize that \mathfrak{H} has a left A -module and a right B -module structure. We call an A - A bimodule simply an *A -bimodule*.

Note that, if \mathfrak{H} is an A - B bimodule, then we have that $\pi(A) \subseteq \pi'(B)'$ and $\pi'(B) \subseteq \pi(A)'$ in $\mathcal{B}(\mathfrak{H})$. Furthermore, a right B -module \mathfrak{H} means canonically a $\mathcal{B}(\mathfrak{H}_B)$ - B bimodule.

REMARKS 1.4.2 (Opposite von Neumann algebra). In literature, the notion of modules is often equivalently defined in terms of opposite algebras (see, for example [49, 81, 83]). Given a von Neumann algebra B , the *opposite von Neumann algebra* B° is the von Neumann algebra obtained by reversing the product operation on B , i.e. as a linear space equipped with a $*$ -operation we take B° to be B , we denote by b° the element in B° corresponding to $b \in B$, and then define the product on B° by

$$a^\circ b^\circ = (ba)^\circ, \quad \forall a, b \in B.$$

It can be shown that the map $B \rightarrow B^\circ : b \mapsto b^\circ$ is an anti-automorphism. From which it then follows that left (respectively, right) B -modules

correspond bijectively with right (respectively, left) B° -modules. In particular, an A - B bimodule is a B° - A° bimodule.

An A - B bimodule introduces a link between the von Neumann algebras A and B . It is also referred to as a *correspondence* between A and B (see [33, 72]).

An important example of a B -bimodule is the GNS Hilbert space associated to a faithful normal state on a von Neumann algebra:

PROPOSITION 1.4.3 (Standard bimodule). *Let B be a von Neumann algebra with $\nu \in \mathfrak{F}(B)$. Then the GNS Hilbert space $L^2(B)$ is a B -bimodule with the structure given by:*

$$(1.4.2) \quad \pi_\nu : B \rightarrow \mathcal{B}(L^2(B)) \text{ and } \pi'_\nu := j_B \circ \pi_\nu,$$

where π_ν is the standard representation of B on $L^2(B)$ associated to ν (see Definition 1.3.1) and $j_B = J_B(\cdot)^*J_B$, with J_B the canonical modular conjugation associated to all $\nu \in \mathfrak{F}(B)$. The Hilbert space $L^2(B)$ is called the standard B -bimodule.

PROOF. The map π_ν is a unital $*$ -homomorphism, by the GNS-construction (Theorem 1.1.9). Furthermore, it is normal by Proposition 1.1.10. Thus, $L^2(B)$ is a left B -module. On the other hand, the map $\pi'_\nu : B \rightarrow \mathcal{B}(L^2(B))$ is linear because J_B and the conjugation operation are both conjugate-linear. Furthermore, we have $\pi'_\nu(1) = J_B 1^* J_B = J_B^2 = 1$,

$$\pi'_\nu(b^*) = J_B \pi_\nu(b) J_B = (J_B \pi_\nu(b)^* J_B)^* = \pi'_\nu(b)^*,$$

and

$$\pi'_\nu(ab) = J_B \pi_\nu(b^* a^*) J_B = J_B \pi_\nu(b)^* J_B J_B \pi_\nu(a)^* J_B = \pi'_\nu(b) \pi'_\nu(a),$$

for all $a, b \in B$. So π'_ν is a unital $*$ -anti-homomorphism. Since j_B and π_ν are both normal, it follows that π'_ν is also normal. Thus, $L^2(B)$ is a right B -module.

Finally, $\pi'(b) \in B'$, for all $b \in B$, by Theorem 1.2.1. Thus, for every $a, b \in B$, we have that $\pi(a)$ commutes with $\pi'(b)$. Then the space $L^2(B)$ is a B -bimodule. \square

The standard bimodule can be used to construct other bimodules and it also plays a central role in the construction of the relative tensor product.

REMARKS 1.4.4 (Colloquial notation). We now adopt the notation in which we suppress the representations of the left and right modules, and we set $ax := \pi(a)x$ and $xb := \pi'(b)x$, then the condition (1.4.1) can be expressed as associativity:

$$(1.4.3) \quad a(xb) = (ax)b, \quad \forall a \in A, b \in B, x \in \mathfrak{H}.$$

By Proposition 1.1.3, the set $N_\nu := \{b \in B : \nu(b^*b) = 0\}$ is a left ideal of B , from which it then follows that the quotient space n_ν/N_ν is a left B -module. We define a map $\eta'_\nu : B \rightarrow L^2(B)$ by

$$(1.4.4) \quad \eta'_\nu(b) := J_B \eta_\nu(b^*), \quad \forall b \in B,$$

where $\eta_\nu : B \rightarrow L^2(B)$ is the quotient map. The anti-representation π'_ν of B on $L^2(B)$ satisfies

$$(1.4.5) \quad \pi'_\nu(a) \eta'_\nu(b) = J_B \pi_\nu(a^*) \eta_\nu(b^*) = J_B \eta_\nu((ba)^*) = \eta'_\nu(ba),$$

and

$$(1.4.6) \quad \langle \eta'_\nu(a), \eta'_\nu(b) \rangle = \langle J_B \eta_\nu(a^*), J_B \eta_\nu(b^*) \rangle = \langle \eta_\nu(b^*), \eta_\nu(a^*) \rangle = \nu(ba^*),$$

for all $a, b \in B$. Note that $\eta_\nu(1) = \eta'_\nu(1) = \Lambda_\nu$.

LEMMA 1.4.5. *Let ν be a positive linear functional on a von Neumann algebra B . Then*

$$\eta_\nu(ab) = a\eta_\nu(b) \quad \text{and} \quad \eta'_\nu(ba) = \eta'_\nu(b)a$$

for all $a, b \in B$. In particular,

$$\eta_\nu(b) = b\Lambda_\nu \quad \text{and} \quad \eta'_\nu(b) = \Lambda_\nu b,$$

for all $b \in B$.

PROOF. Let $a, b \in B$. Then

$$\eta_\nu(ab) = \pi_\nu(a) \eta_\nu(b) = a\eta_\nu(b),$$

and

$$\begin{aligned} \eta'_\nu(ba) &= J_B \eta_\nu(a^*b^*) \\ &= J_B \pi_\nu(a^*) \eta_\nu(b^*) \\ &= J_B \pi_\nu(a^*) J_B J_B \eta_\nu(b^*) \\ &= J_B \eta_\nu(b^*) a \\ &= \eta'_\nu(b) a, \end{aligned}$$

by Equations (1.4.3) and (1.4.5). The last part follows as special cases of the above. \square

DEFINITION 1.4.6 (Module, bimodule morphisms). Let A and B be von Neumann algebras.

- (1) A *morphism of left A -modules* \mathfrak{K}_1 and \mathfrak{K}_2 is an operator $t \in \mathcal{B}(\mathfrak{K}_1, \mathfrak{K}_2)$ such that

$$t(ax) = at(x), \quad \forall a \in A, x \in \mathfrak{K}_1.$$

Denote the set of left A -module morphisms by $\mathcal{B}(A(\mathfrak{K}_1), A(\mathfrak{K}_2))$, and for $\mathcal{B}(A\mathfrak{K}, A\mathfrak{K})$ we simply write $\mathcal{B}(A\mathfrak{K})$.

- (2) A *morphism of right B -modules* \mathfrak{H}_1 and \mathfrak{H}_2 is an operator $t \in \mathcal{B}(\mathfrak{H}_1, \mathfrak{H}_2)$ such that

$$t(yb) = t(y)b, \quad \forall b \in B, y \in \mathfrak{H}_1.$$

Denote the set of right B -module morphisms by $\mathcal{B}((\mathfrak{H}_1)_B, (\mathfrak{H}_2)_B)$, and for $\mathcal{B}(\mathfrak{H}_B, \mathfrak{H}_B)$, we simply write $\mathcal{B}(\mathfrak{H}_B)$.

- (3) A *morphism of A - B bimodules* \mathfrak{H} and \mathfrak{K} is an operator $t \in \mathcal{B}(\mathfrak{H}, \mathfrak{K})$ such that

$$t(axb) = at(x)b, \quad \forall a \in A, b \in B, x \in \mathfrak{H}.$$

Denote the set of A - B bimodule morphisms by $\mathcal{B}({}_A\mathfrak{H}_B, {}_A\mathfrak{K}_B)$, and for $\mathcal{B}({}_A\mathfrak{H}_B, {}_A\mathfrak{H}_B)$ we simply write $\mathcal{B}({}_A\mathfrak{H}_B)$.

The *Banach dual* $\overline{\mathfrak{H}}$ of a Hilbert space \mathfrak{H} is the set of all continuous linear functionals $f : \mathfrak{H} \rightarrow \mathbb{C}$ equipped with the operator norm:

$$\|f\| = \sup_{\|x\| \leq 1} |f(x)|.$$

By the Riesz Representation Theorem (see [65, Theorem 3.8-1]), for every continuous linear functional f on a Hilbert space \mathfrak{H} , there exists a unique vector $y \in \mathfrak{H}$ such that

$$f(x) = \langle x, y \rangle \quad \forall x \in \mathfrak{H},$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product on the Hilbert space. This implies that every continuous linear functional on \mathfrak{H} can be represented as an inner product with a vector from \mathfrak{H} . Consequently, the Banach dual of a Hilbert space \mathfrak{H} is isometrically isomorphic to \mathfrak{H} itself:

$$\overline{\mathfrak{H}} \cong \mathfrak{H}.$$

DEFINITION 1.4.7. If \mathfrak{H} is an A - B bimodule, then its Banach space dual $\overline{\mathfrak{H}} := \{\bar{x} : x \in \mathfrak{H}\}$, where $\bar{x} : \mathfrak{H} \rightarrow \mathbb{C} : y \mapsto \langle x, y \rangle$, is a B - A bimodule by the action

$$b\bar{x}a := \overline{a^*xb^*}, \quad \forall a \in A, b \in B, x \in \mathfrak{H},$$

where \bar{x} denotes the vector in $\overline{\mathfrak{H}}$ corresponding to $x \in \mathfrak{H}$. We call this B - A bimodule $\overline{\mathfrak{H}}$ the *conjugate* bimodule or the bimodule *dual* to the original bimodule \mathfrak{H} .

If there is a bimodule morphism between a bimodule \mathfrak{H} and its dual $\overline{\mathfrak{H}}$, we say that the bimodule \mathfrak{H} is *self-dual*.

PROPOSITION 1.4.8 (Self duality of the standard bimodule). *For a von Neumann algebra B with $\nu \in \mathfrak{F}(B)$, the standard bimodule $L^2(B)$ is self-dual under the correspondence: $x^* \leftrightarrow \bar{x}$, $\forall x \in L^2(B)$.*

PROOF. Denote the representation and the anti-representation of B on $L^2(B)$ by π and π' , respectively. Consider the Banach space dual $\overline{L^2(B)}$ of $L^2(B)$ and a map

$$r : L^2(B) \rightarrow \overline{L^2(B)} : x \mapsto \bar{x}.$$

Clearly, r is bijective. Since $\langle \alpha x, y \rangle = \bar{\alpha} \langle x, y \rangle$, for all $x, y \in L^2(B)$ and $\alpha \in \mathbb{C}$, then r is a conjugate-linear map. Define an inner product on $\overline{L^2(B)}$ by

$$\langle r(x), r(y) \rangle = \langle \bar{x}, \bar{y} \rangle = \langle y, x \rangle, \forall x, y \in L^2(B).$$

Thus r is isometric.

Define a map $\iota := r \circ J_B : L^2(B) \rightarrow \overline{L^2(B)}$, i.e., $\iota(x) = \overline{J_B x}$, where J_B is the modular conjugation associated to (B, ν) . Then ι is unitary since r and J_B are respectively conjugate linear and anti-unitary, and is bijective since r is bijective and J_B is isometric.

Define the map $\bar{\pi} : B \rightarrow \mathcal{B}(\overline{L^2(B)})$ by $\bar{\pi}(b)\bar{x} := \overline{\pi(b^*)x} = r(\pi(b^*)x)$.

Then $\bar{\pi}$ is an anti-representation of B on $\overline{L^2(B)}$, since

$$\begin{aligned} \bar{\pi}(\alpha a + b)\bar{x} &= r(\pi(\bar{\alpha}a^* + b^*)x) \\ &= r(\bar{\alpha}\pi(a^*)x + \pi(b^*)x) \\ &= \alpha r(\pi(a^*)x) + r(\pi(b^*)x) \\ &= \alpha \bar{\pi}(a)\bar{x} + \bar{\pi}(b)\bar{x} \\ &= [\alpha \bar{\pi}(a) + \bar{\pi}(b)]\bar{x}, \end{aligned}$$

$$\begin{aligned} \langle \bar{x}, \bar{\pi}(a^*)\bar{y} \rangle &= \langle \bar{x}, \overline{\pi(a)y} \rangle \\ &= \langle \pi(a)y, x \rangle \\ &= \langle y, \pi(a^*)x \rangle \\ &= \langle \overline{\pi(a^*)x}, \bar{y} \rangle \\ &= \langle \bar{\pi}(a)\bar{x}, \bar{y} \rangle \\ &= \langle \bar{x}, \bar{\pi}(a)^*\bar{y} \rangle, \end{aligned}$$

and

$$\begin{aligned} \bar{\pi}(ab)\bar{x} &= \overline{\pi(b^*a^*)x} \\ &= \overline{\pi(b^*)\pi(a^*)x} \\ &= \bar{\pi}(b) \left(\overline{\pi(a^*)x} \right) \\ &= \bar{\pi}(b)\bar{\pi}(a)\bar{x}, \end{aligned}$$

for all $a, b \in B, x \in L^2(B)$. Similarly, the map $\bar{\pi}' : B \rightarrow \mathcal{B}(\overline{L^2(B)})$ given by $\bar{\pi}'(b)\bar{x} := \overline{\pi'(b^*)x} = r(\pi'(b^*)x)$ defines a representation of B on $\overline{L^2(B)}$.

The mutual commutativity of $\bar{\pi}(B)$ and $\bar{\pi}'(B)$ follows from that of $\pi(B)$ and $\pi'(B)$:

$$b\bar{x}a := \bar{\pi}(a)\bar{\pi}'(b)\bar{x} = \overline{\pi(a^*)\pi'(b^*)x} = \overline{\pi'(b^*)\pi(a^*)x} = \overline{a^*xb^*},$$

for all $a, b \in B, x \in L^2(B)$. Thus, $\overline{L^2(B)}$ is a B -bimodule. Furthermore, since $L^2(B)$ is itself a B -bimodule, we have

$$\begin{aligned}
a\iota(x)b &= a(\overline{J_B x})b \\
&= \overline{b^* J_B x a^*} \\
&= \overline{b^* (J_B a J_B) J_B x} \\
&= \overline{b^* J_B a x} \\
&= \overline{J_B (J_B b^* J_B) a x} \\
&= \overline{J_B a (J_B b^* J_B) x} \\
&= \overline{J_B (a x b)} \\
&= \iota(a x b)
\end{aligned}$$

for all $a, b \in B, x \in L^2(B)$. Thus, ι is a bimodule morphism. Consequently, $L^2(B)$ is self-dual. \square

PROPOSITION 1.4.9. *Let A and B be von Neumann algebras in standard form. Then*

- (1) $\mathcal{B}(L^2(A)_A) = A$.
- (2) $\mathcal{B}({}_B L^2(B)) = B'$.

PROOF. (1) Let $a \in A$, then for all $b \in A$ and $x \in L^2(A)$,

$$\begin{aligned}
a(xb) &= a j_A(b)x \\
&= j_A(b)ax \text{ (since } j_A(A) = A', \text{ by Theorem 1.2.1)} \\
&= (ax)b.
\end{aligned}$$

Thus $a \in \mathcal{B}(L^2(A)_A)$. Conversely, suppose that $a \in \mathcal{B}(L^2(A)_A)$, then for all $b \in A$ and $x \in L^2(A)$,

$$\begin{aligned}
a(xb) &= (ax)b \\
\implies a j_A(b)x &= j_A(b)ax.
\end{aligned}$$

Thus $a j_A(b) = j_A(b)a$ for all $b \in A$. It then follows that $a \in j_A(A)' = A$. Hence $\mathcal{B}(L^2(A)_A) = A$.

- (2) Let $a \in B'$, then $a(bx) = b(ax)$ for all $b \in B$ and $x \in L^2(B)$. Thus, $a \in \mathcal{B}({}_B L^2(B))$. Conversely, if $a \in \mathcal{B}({}_B L^2(B))$ then $a(bx) = b(ax)$ for all $b \in B$ and $x \in L^2(B)$. Thus,

$$ab = ba, \quad \forall b \in B,$$

and $a \in B'$. Together, we have $\mathcal{B}({}_B L^2(B)) = B'$. \square

PROPOSITION 1.4.10. *Let A and B be von Neumann algebras, and let $\mathfrak{K}_1, \mathfrak{K}_2$ be left A -modules and $\mathfrak{H}_1, \mathfrak{H}_2$ be right B -modules.*

- (1) *If $a \in \mathcal{B}({}_A(\mathfrak{K}_1), {}_A(\mathfrak{K}_2))$, then $a^* \in \mathcal{B}({}_A(\mathfrak{K}_2), {}_A(\mathfrak{K}_1))$ and $a^*a \in \mathcal{B}({}_A(\mathfrak{K}_1)) = A'$.*

(2) If $b \in \mathcal{B}((\mathfrak{H}_1)_B, (\mathfrak{H}_2)_B)$, then $b^* \in \mathcal{B}((\mathfrak{H}_2)_B, (\mathfrak{H}_1)_B)$ and $b^*b \in \mathcal{B}((\mathfrak{H}_1)_B) = B$.

PROOF. By the definition of the adjoint of an operator, if $a \in \mathcal{B}(\mathfrak{K}_1, \mathfrak{K}_2)$ and $b \in \mathcal{B}(\mathfrak{H}_1, \mathfrak{H}_2)$, then $a^* \in \mathcal{B}(\mathfrak{K}_2, \mathfrak{K}_1)$, $b^* \in \mathcal{B}(\mathfrak{H}_2, \mathfrak{H}_1)$ and $a^*a \in \mathcal{B}(\mathfrak{K}_1)$, $b^*b \in \mathcal{B}(\mathfrak{H}_1)$.

(1) If $a \in \mathcal{B}(A(\mathfrak{K}_1), A(\mathfrak{K}_2))$, then

$$\begin{aligned} \langle a^*(bx), y \rangle_{\mathfrak{K}_1} &= \langle bx, ay \rangle_{\mathfrak{K}_2} \\ &= \langle x, b^*(ay) \rangle_{\mathfrak{K}_2} \\ &= \langle x, a(b^*y) \rangle_{\mathfrak{K}_2} \\ &= \langle a^*x, b^*y \rangle_{\mathfrak{K}_1} \\ &= \langle b(a^*x), y \rangle_{\mathfrak{K}_1}, \end{aligned}$$

for all $b \in A$, $x \in \mathfrak{K}_2$, and $y \in \mathfrak{K}_1$. Thus,

$$(1.4.7) \quad a^*(xb) = (a^*x)b, \forall b \in A, x \in \mathfrak{K}_2,$$

and $a^* \in \mathcal{B}(A(\mathfrak{K}_2), A(\mathfrak{K}_1))$. By (1.4.7), we have

$$a^*a(bx) = a^*[b(ax)] = b[a^*(ax)] = b(a^*ax)$$

for all $b \in A$ and $x \in \mathfrak{K}_1$. Thus, $a^*a \in \mathcal{B}(A(\mathfrak{K}_1)) = A'$, by Proposition 1.4.9(2).

(2) Denote the anti-representations of B on \mathfrak{H}_1 and \mathfrak{H}_2 by π'_1 and π'_2 , respectively. If $b \in \mathcal{B}((\mathfrak{H}_1)_B, (\mathfrak{H}_2)_B)$,

$$\begin{aligned} \langle b^*(xa), y \rangle_{\mathfrak{H}_1} &= \langle ax, by \rangle_{\mathfrak{H}_2} \\ &= \langle \pi'_2(a)x, by \rangle_{\mathfrak{H}_2} \\ &= \langle x, \pi'_2(a^*)by \rangle_{\mathfrak{H}_2} \\ &= \langle x, (by)a^* \rangle_{\mathfrak{H}_2} \\ &= \langle x, b(ya^*) \rangle_{\mathfrak{H}_2} \\ &= \langle b^*x, ya^* \rangle_{\mathfrak{H}_1} \\ &= \langle b^*x, \pi'_1(b^*)y \rangle_{\mathfrak{H}_1} \\ &= \langle \pi'_1(a)b^*x, y \rangle_{\mathfrak{H}_1} \\ &= \langle (b^*x)a, y \rangle_{\mathfrak{H}_1}, \end{aligned}$$

for all $a \in B$, $x \in \mathfrak{H}_2$, and $y \in \mathfrak{H}_1$. Thus,

$$(1.4.8) \quad b^*(xa) = (b^*x)a, \forall b \in B, x \in \mathfrak{H}_2,$$

and $b^* \in \mathcal{B}((\mathfrak{H}_2)_B, (\mathfrak{H}_1)_B)$. By (1.4.8), we have

$$b^*b(xa) = b^*[(bx)a] = [b^*(bx)]a = (b^*bx)a$$

for all $a \in B$ and $x \in \mathfrak{H}_1$. Thus, $a^*a \in \mathcal{B}((\mathfrak{H}_1)_B) = B$, by Proposition (1.4.9)(1). □

1.5. The relative tensor product of bimodules

In this section we discuss the construction of the relative tensor product for a pair consisting of a right B -module \mathfrak{H} and a left B -module \mathfrak{K} , which will depend on the choice of a faithful normal state ν on B . In essence, relative tensor products are algebraic objects. However, there are subtle differences between the operator algebraic approach and a purely algebraic one. In the context of operator algebras, the requirement that the output of the construction be a Hilbert space equipped with a certain mathematical structure causes analytical obstructions [75]. For example, the relative tensor product of an arbitrary pair of vectors does not make sense unless we are in the very special case of atomic von Neumann algebras [81]. As a consequence, in general, a purely algebraic approach to their theory is insufficient. Fortunately, von Neumann algebras have a sufficiently simple representation theory to allow a reformulation of relative tensor products in algebraic terms [75].

The relative tensor product for Hilbert spaces over commutative von Neumann algebras was defined by Sauvageot [74]. Connes generalized the construction to the noncommutative case [33, Appendix V.B]. The reader is referred to [49], [75], [81, Section IX.3] and [83] for further background.

DEFINITION 1.5.1. Let B be a von Neumann algebra, $\nu \in \mathfrak{F}(B)$, \mathfrak{H} be a right B -module and \mathfrak{K} be a left B -module. Denote the representation and anti-representation of B on \mathfrak{K} and \mathfrak{H} by $\pi_{\mathfrak{K}}$ and $\pi'_{\mathfrak{H}}$, respectively.

(1) Define a subset of \mathfrak{H} by

$$\mathfrak{D}(\mathfrak{H}, \nu) := \{x \in \mathfrak{H} : \|xb\| \leq C_x \|\eta'_\nu(b)\|, b \in B \text{ for some } C_x \geq 0\}.$$

For each $x \in \mathfrak{D}(\mathfrak{H}, \nu)$, we define a map $L_\nu(x) : \eta'_\nu(B) \rightarrow \mathfrak{H}$ by

$$(1.5.1) \quad L_\nu(x)\eta'_\nu(b) := xb = \pi'_{\mathfrak{H}}(b)x, \quad \forall b \in B.$$

The elements of $\mathfrak{D}(\mathfrak{H}, \nu)$ are called *left B -bounded vectors*.

(2) Define a subset of \mathfrak{K} by

$$\mathfrak{D}'(\mathfrak{K}, \nu) := \{y \in \mathfrak{K} : \|by\| \leq C_y \|\eta_\nu(b)\|, b \in B \text{ for some } C_y \geq 0\}.$$

For each $y \in \mathfrak{D}'(\mathfrak{K}, \nu)$, we define a map $R_\nu(y) : \eta_\nu(B) \rightarrow \mathfrak{K}$ by

$$(1.5.2) \quad R_\nu(y)\eta_\nu(b) := by = \pi_{\mathfrak{K}}(b)y, \quad \forall b \in B.$$

The elements of $\mathfrak{D}'(\mathfrak{K}, \nu)$ are called *right B -bounded vectors*.

Note that B -bounded vectors depend on the choice of the faithful normal state ν on B . For the cyclic vector Λ_ν associated with (B, ν) , if $x \in \mathfrak{D}(\mathfrak{H}, \nu)$, then

$$L_\nu(x)\Lambda_\nu = L_\nu(x)\eta'_\nu(1) = x1 = \pi'_{\mathfrak{H}}(1)x = x.$$

Similarly, $R_\nu(y)\Lambda_\nu = \pi_{\mathfrak{K}}(1)y = y$, for all $y \in \mathfrak{D}'(\mathfrak{K}, \nu)$.

PROPOSITION 1.5.2. *The sets $\mathfrak{D}(\mathfrak{H}, \nu)$ and $\mathfrak{D}'(\mathfrak{K}, \nu)$ are dense subspaces of \mathfrak{H} and \mathfrak{K} , respectively.*

We do not give a proof but we refer the reader to [49, Lemma 2.3], or [81, Lemma IX.3.3].

We now collect a few facts about $\mathfrak{D}(\mathfrak{H}, \nu)$ (respectively, $\mathfrak{D}'(\mathfrak{K}, \nu)$) and L_ν (respectively, R_ν):

PROPOSITION 1.5.3. *Let B be a von Neumann algebra, $\nu \in \mathfrak{F}(B)$, \mathfrak{H} be a right B -module and \mathfrak{K} be a left B -module.*

- (1) $\forall x \in \mathfrak{D}(\mathfrak{H}, \nu)$, $L_\nu(x) \in \mathcal{B}(L^2(B)_B, \mathfrak{H}_B)$.
- (2) $\forall y \in \mathfrak{D}'(\mathfrak{K}, \nu)$, $R_\nu(y) \in \mathcal{B}({}_B L^2(B), {}_B \mathfrak{K})$.

PROOF. (1) Let $x \in \mathfrak{D}(\mathfrak{H}, \nu)$, then for all $a, b \in B$ and $\alpha \in \mathbb{C}$,

$$\begin{aligned} L_\nu(x) [\alpha \eta'_\nu(a) + \eta'_\nu(b)] &= L_\nu(x) \eta'_\nu(\alpha a + b) \\ &= x(\alpha a + b) \\ &= \alpha(xa) + xb \\ &= \alpha L_\nu(x) \eta'_\nu(a) + L_\nu(x) \eta'_\nu(b), \end{aligned}$$

and

$$\|L_\nu(x) \eta'_\nu(b)\| = \|xb\| \leq C_x \|\eta'_\nu(b)\| \text{ for some } C_x \geq 0.$$

The latter follows from the definition of $\mathfrak{D}(\mathfrak{H}, \nu)$. Thus $L_\nu(x)$ is a bounded linear operator on $\eta'_\nu(B)$. Since $\overline{\eta'_\nu(B)\Lambda_\nu} = L^2(B)$ it then follows that $L_\nu(x)$ has a bounded linear extension, which we also denote by $L_\nu(x)$, on $L^2(B)$, i.e. $L_\nu(x) \in \mathcal{B}(L^2(B), \mathfrak{H})$. Furthermore,

$$[L_\nu(x) \eta'_\nu(a)] b = (xa)b = x(ab) = L_\nu(x) \eta'_\nu(ab) = L_\nu(x) [\eta'_\nu(a)b],$$

for all $a, b \in B$, by Lemma 1.4.5. Thus, $L_\nu(x) \in \mathcal{B}(L^2(B)_B, \mathfrak{H}_B)$.

- (2) That $R_\nu(y) \in \mathcal{B}(L^2(B), \mathfrak{K})$, for $y \in \mathfrak{D}'(\mathfrak{K}, \nu)$, follows similarly to the proof in the first part of this proposition. Furthermore,

$$\begin{aligned} a [R_\nu(y) \eta_\nu(b)] &= a(by) \\ &= (ab)y \\ &= R_\nu(y) \eta_\nu(ab) \\ &= R_\nu(y) [a \eta_\nu(b)] \end{aligned}$$

for all $a, b \in B$, by Lemma 1.4.5. Thus, $R_\nu(y) \in \mathcal{B}({}_B L^2(B), {}_B \mathfrak{K})$. \square

Note that $x \in \mathfrak{D}(\mathfrak{H}, \nu)$ if the map $b\Lambda_\nu \mapsto xb$ extends to a bounded operator $L_\nu(x) : L^2(B) \rightarrow \mathfrak{H}$. Similarly, $y \in \mathfrak{D}'(\mathfrak{K}, \nu)$ if the map $b\Lambda_\nu \mapsto by$ extends to a bounded operator $R_\nu(y) : L^2(B) \rightarrow \mathfrak{K}$. The subspaces $\mathfrak{D}(\mathfrak{H}, \nu)$ and $\mathfrak{D}'(\mathfrak{K}, \nu)$ are defined to ensure that the operators $L_\nu(x)$ and $R_\nu(y)$ are indeed bounded.

PROPOSITION 1.5.4. *Let B be a von Neumann algebra, $\nu \in \mathfrak{F}(B)$, \mathfrak{H} a right B -module and \mathfrak{K} a left B -module.*

(1) *For all $x_1, x_2 \in \mathfrak{D}(\mathfrak{H}, \nu)$,*

$$\langle x_1, x_2 \rangle = \nu(L_\nu(x_1)^* L_\nu(x_2))$$

and

$$\eta_\nu(L_\nu(x_1)^* L_\nu(x_2)) = L_\nu(x_1)^* x_2.$$

(2) *For all $y_1, y_2 \in \mathfrak{D}'(\mathfrak{K}, \nu)$,*

$$\langle y_1, y_2 \rangle = \nu(j_B(R_\nu(y_1)^* R_\nu(y_2)))$$

and

$$\eta'_\nu(j_B(R_\nu(y_1)^* R_\nu(y_2))) = R_\nu(y_1)^* y_2.$$

PROOF. (1) If $x_1, x_2 \in \mathfrak{D}(\mathfrak{H}, \nu)$ then $L_\nu(x_1), L_\nu(x_2) \in \mathcal{B}(L^2(B)_B, \mathfrak{H}_B)$ by Proposition 1.5.3; and thus $L_\nu(x_1)^* \in \mathcal{B}(\mathfrak{H}_B, L^2(B)_B)$ by Proposition 1.4.10. It follows by Proposition 1.4.9 that $L_\nu(x_1)^* L_\nu(x_2) \in \mathcal{B}(L^2(B)_B) = B$. By Lemma 1.4.5, we have

$$\begin{aligned} \nu(L_\nu(x_1)^* L_\nu(x_2)) &= \langle \Lambda_\nu, L_\nu(x_1)^* L_\nu(x_2) \Lambda_\nu \rangle \\ &= \langle L_\nu(x_1) \eta'_\nu(1), L_\nu(x_2) \eta'_\nu(1) \rangle \\ &= \langle x_1, x_2 \rangle, \end{aligned}$$

and by Lemma 1.4.5

$$\begin{aligned} \eta_\nu(L_\nu(x_1)^* L_\nu(x_2)) &= L_\nu(x_1)^* L_\nu(x_2) \Lambda_\nu \\ &= L_\nu(x_1)^* L_\nu(x_2) \eta'_\nu(1) \\ &= L_\nu(x_1)^* x_2, \end{aligned}$$

for all $x_1, x_2 \in \mathfrak{D}(\mathfrak{H}, \nu)$.

(2) If $y_1, y_2 \in \mathfrak{D}'(\mathfrak{K}, \nu)$ then $R_\nu(y_1)^* R_\nu(y_2) \in \mathcal{B}({}_B L^2(B)) = B'$, by Propositions 1.4.9 and 1.4.10. By Lemma 1.4.5, we have

$$\begin{aligned} \nu(j_B(R_\nu(y_1)^* R_\nu(y_2))) &= \nu'(R_\nu(y_1)^* R_\nu(y_2)) \\ &= \langle \Lambda_\nu, R_\nu(y_1)^* R_\nu(y_2) \Lambda_\nu \rangle \\ &= \langle R_\nu(y_1) \eta_\nu(1), R_\nu(y_2) \Lambda_\nu \rangle \\ &= \langle y_1, y_2 \rangle, \end{aligned}$$

and by Lemma 1.4.5, using $\eta_\nu(1) = \Lambda_\nu$ and $J_B \Lambda_\nu = \Lambda_\nu$

$$\begin{aligned} \eta'_\nu(j_B(R_\nu(y_1)^* R_\nu(y_2))) &= J_B j_B(R_\nu(y_1)^* R_\nu(y_2))^* \eta_\nu(1) \\ &= J_B [J_B R_\nu(y_1)^* R_\nu(y_2) J_B] \eta_\nu(1) \\ &= R_\nu(y_1)^* R_\nu(y_2) \eta_\nu(1) \\ &= R_\nu(y_1)^* y_2, \end{aligned}$$

for all $y_1, y_2 \in \mathfrak{D}'(\mathfrak{K}, \nu)$.

□

Recall that to every sesquilinear form on a complex linear space there corresponds a Hilbert space through a standard construction: we first factor out the null space of the form, and then complete the resulting quotient space with respect to the norm corresponding to the form (see the proof of Theorem 1.1.9).

LEMMA 1.5.5. *Let B be a von Neumann algebra, $\nu \in \mathfrak{F}(B)$, \mathfrak{H} a right B -module and \mathfrak{K} a left B -module. Denote the anti-representation and representation of B on \mathfrak{H} and \mathfrak{K} by $\pi'_{\mathfrak{H}}$ and $\pi_{\mathfrak{K}}$, respectively.*

(1) *The sesquilinear form $B : \mathfrak{D}(\mathfrak{H}, \nu) \odot \mathfrak{K} \rightarrow \mathbb{C}$ given by*

$$(1.5.3) \quad B(x_1 \otimes y_1, x_2 \otimes y_2) := \langle y_1, \pi_{\mathfrak{K}}(L_{\nu}(x_1)^* L_{\nu}(x_2)) y_2 \rangle_{\mathfrak{K}}$$

is positive semi-definite, and so defines a semi-inner product on $\mathfrak{D}(\mathfrak{H}, \nu) \odot \mathfrak{K}$. Denote the Hilbert space associated to the form B via a quotient by $\mathfrak{H} \otimes_{\nu} \mathfrak{K}$.

(2) *The sesquilinear form $B' : \mathfrak{H} \odot \mathfrak{D}'(\mathfrak{K}, \nu) \rightarrow \mathbb{C}$ given by*

$$(1.5.4) \quad B'(x_1 \otimes y_1, x_2 \otimes y_2) := \langle x_1, \pi'_{\mathfrak{H}}(j_B(R_{\nu}(y_1)^* R_{\nu}(y_2))) x_2 \rangle_{\mathfrak{H}}$$

is positive semi-definite, and so defines a semi-inner product on $\mathfrak{H} \odot \mathfrak{D}'(\mathfrak{K}, \nu)$. Denote the Hilbert space associated to the form B' via a quotient by $\mathfrak{H} \otimes'_{\nu} \mathfrak{K}$.

(3) *The restrictions of the sesquilinear forms defined in parts (1) and (2) to $\mathfrak{D}(\mathfrak{H}, \nu) \odot \mathfrak{D}'(\mathfrak{K}, \nu)$ coincide. Moreover, the Hilbert spaces associated to these forms are isomorphic.*

PROOF. In order to simplify the notation, we set

$$\begin{aligned} V &:= \mathfrak{H} \odot \mathfrak{K}, \\ X &:= \mathfrak{D}(\mathfrak{H}, \nu) \odot \mathfrak{K}, \\ Y &:= \mathfrak{H} \odot \mathfrak{D}'(\mathfrak{K}, \nu), \quad \text{and} \\ Z &:= \mathfrak{D}(\mathfrak{H}, \nu) \odot \mathfrak{D}'(\mathfrak{K}, \nu). \end{aligned}$$

Let $N := \{z \in X : B(z, z) = 0\}$ and $N' := \{z \in Y : B'(z, z) = 0\}$.

(1) Let $z := x \otimes y \in \mathfrak{D}(\mathfrak{H}, \nu) \odot \mathfrak{K}$, then

$$\begin{aligned} B(z, z) &= \langle y, \pi_{\mathfrak{K}}(L_{\nu}(x)^* L_{\nu}(x)) y \rangle_{\mathfrak{K}} \\ &= \langle y, L_{\nu}(x)^* L_{\nu}(x) y \rangle_{\mathfrak{K}} \\ &= \langle L_{\nu}(x) y, L_{\nu}(x) y \rangle_{\mathfrak{H}} \\ &= \|L_{\nu}(x) y\|_{\mathfrak{H}}^2 \\ &\geq 0. \end{aligned}$$

Thus, the sesquilinear form B is non-negative.

Let $\eta : V \rightarrow V/N$ be the quotient map, then the form B induces an inner product on the quotient space V/N given by

$$\langle \eta(z_1), \eta(z_2) \rangle := B(z_1, z_2), \quad \forall z_1, z_2 \in X.$$

Denote the Hilbert space completion of V/N with respect to the norm corresponding to the inner product $\langle \cdot, \cdot \rangle$ by $\mathfrak{H} \otimes_{\nu} \mathfrak{K}$, i.e.

$$\mathfrak{H} \otimes_{\nu} \mathfrak{K} := \overline{\eta(X)} = \overline{\eta(\mathfrak{D}(\mathfrak{H}, \nu) \odot \mathfrak{K})}.$$

(2) Let $z := x \otimes y \in \mathfrak{H} \odot \mathfrak{D}'(\mathfrak{K}, \nu)$, then

$$\begin{aligned} B'(z, z) &= \langle x, \pi'_{\mathfrak{H}}(j_B(R_{\nu}(y)^* R_{\nu}(y))) x \rangle_{\mathfrak{H}} \\ &= \langle x, x j_B(R_{\nu}(y)^* R_{\nu}(y)) \rangle_{\mathfrak{H}} \\ &= \langle x, R_{\nu}(y)^* R_{\nu}(y) x \rangle_{\mathfrak{H}} \\ &= \langle R_{\nu}(y) x, R_{\nu}(y) x \rangle_{\mathfrak{K}} \\ &= \|R_{\nu}(y) x\|_{\mathfrak{K}}^2 \\ &\geq 0. \end{aligned}$$

Thus, the sesquilinear form B' is non-negative.

Let $\eta' : V \rightarrow V/N'$ be the quotient map, then the form B' induces an inner product on the quotient space V/N' given by

$$\langle \eta'(z_1), \eta'(z_2) \rangle' := B'(z_1, z_2), \quad \forall z_1, z_2 \in Y.$$

Denote the Hilbert space completion of V/N' with respect to the norm corresponding to the inner product $\langle \cdot, \cdot \rangle'$ by $\mathfrak{H} \otimes'_{\nu} \mathfrak{K}$, i.e.

$$\mathfrak{H} \otimes'_{\nu} \mathfrak{K} := \overline{\eta'(Y)} = \overline{\eta'(\mathfrak{H} \odot \mathfrak{D}'(\mathfrak{K}, \nu))}.$$

(3) For all $x_1, x_2 \in \mathfrak{D}(\mathfrak{H}, \nu)$ and $y_1, y_2 \in \mathfrak{D}'(\mathfrak{K}, \nu)$, we have

$$\begin{aligned} B(x_1 \otimes y_1, x_2 \otimes y_2) &= \langle y_1, \pi_{\mathfrak{K}}(L_{\nu}(x_1)^* L_{\nu}(x_2)) y_2 \rangle_{\mathfrak{K}} \\ &= \langle y_1, R_{\nu}(y_2) \eta_{\nu}(L_{\nu}(x_1)^* L_{\nu}(x_2)) \rangle_{\mathfrak{K}} \\ &= \langle R_{\nu}(y_2)^* y_1, L_{\nu}(x_1)^* x_2 \rangle_{\mathfrak{H}} \\ &= \langle \eta'_{\nu}(j_B(R_{\nu}(y_2)^* R_{\nu}(y_1))), L_{\nu}(x_1)^* x_2 \rangle_{\mathfrak{H}} \\ &= \langle L_{\nu}(x_1) \eta'_{\nu}(j_B(R_{\nu}(y_2)^* R_{\nu}(y_1))), x_2 \rangle_{\mathfrak{H}} \\ &= \langle \pi'_{\mathfrak{H}}(j_B(R_{\nu}(y_2)^* R_{\nu}(y_1))) x_1, x_2 \rangle_{\mathfrak{H}} \\ &= \langle x_1, \pi'_{\mathfrak{H}}(j_B(R_{\nu}(y_2)^* R_{\nu}(y_1)))^* x_2 \rangle_{\mathfrak{H}} \\ &= \langle x_1, \pi'_{\mathfrak{H}}(j_B(R_{\nu}(y_1)^* R_{\nu}(y_2))) x_2 \rangle_{\mathfrak{H}} \\ &= B'(x_1 \otimes y_1, x_2 \otimes y_2). \end{aligned}$$

Then $Z \cap N = Z \cap N'$, since

$$\begin{aligned} z \in Z \cap N &\iff z \in Z \text{ and } B(z, z) = 0 \\ &\iff z \in Z \text{ and } B'(z, z) = 0 \\ &\iff z \in Z \cap N'. \end{aligned}$$

For all $z \in Z$, we have

$$\begin{aligned} \|\eta(z)\|^2 &= \langle \eta(z), \eta(z) \rangle \\ &= B(z, z) \\ &= B'(z, z) \\ &= \langle \eta'(z), \eta'(z) \rangle \\ &= \|\eta'(z)\|^2. \end{aligned}$$

Similarly, (with the role of z replaced by $z_1 - z_2$ in the above calculation), if $\eta(z_1) = \eta(z_2)$, it follows that $\eta'(z_1) = \eta'(z_2)$, for all $z_1, z_2 \in Z$. Thus, the map

$$U_0\eta(z) := \eta'(z) \quad (z \in Z)$$

defines an injective norm-preserving map from $\eta(X)$ to $\eta'(Y)$, and it is surjective by definition. Since $\overline{\eta(X)} = \mathfrak{H} \otimes_\nu \mathfrak{K}$ and $\overline{\eta'(Y)} = \mathfrak{H} \otimes'_\nu \mathfrak{K}$, then U_0 extends uniquely by boundedness to an isomorphism U from $\mathfrak{H} \otimes_\nu \mathfrak{K}$ to $\mathfrak{H} \otimes'_\nu \mathfrak{K}$. \square

DEFINITION 1.5.6. The *relative tensor product* of a right B -module \mathfrak{H} and a left B -module \mathfrak{K} relative to a faithful normal state ν on B is the Hilbert space

$$\mathfrak{H} \otimes_\nu \mathfrak{K}$$

associated to the positive sesquilinear forms defined in Lemma 1.5.5. We define $x \otimes_\nu y$ as the image of $x \otimes y$ for $x \in \mathfrak{H}$ and $y \in \mathfrak{K}$, but with either $x \in \mathfrak{D}(\mathfrak{H}, \nu)$ or $y \in \mathfrak{D}'(\mathfrak{K}, \nu)$, under the respective quotient maps.

PROPOSITION 1.5.7. Let B be a von Neumann algebra, $\nu \in \mathfrak{F}(B)$, \mathfrak{H} a right B -module and \mathfrak{K} a left B -module. If $x \in \mathfrak{H}$ and $y \in \mathfrak{K}$, with either $x \in \mathfrak{D}(\mathfrak{H}, \nu)$ or $y \in \mathfrak{D}'(\mathfrak{K}, \nu)$, then:

- (1) The relative tensor product $\mathfrak{H} \otimes_\nu \mathfrak{K}$ is a $\mathcal{B}(\mathfrak{H}_B)$ - $\mathcal{B}(B\mathfrak{K})$ bimodule with the actions given by

$$a(x \otimes_\nu y)b = (ax) \otimes_\nu (yb)$$

for all $a \in \mathcal{B}(\mathfrak{H}_B)$, $b \in \mathcal{B}(B\mathfrak{K})$.

- (2) If $a \in \mathcal{B}(\mathfrak{H}_B)$ and $b \in \mathcal{B}(B\mathfrak{K})$, then there exists a unique bounded operator $a \otimes_\nu b \in \mathcal{B}(\mathfrak{H} \otimes_\nu \mathfrak{K})$ such that

$$(a \otimes_\nu b)(x \otimes_\nu y) = (ax) \otimes_\nu (by).$$

The map

$$\mathcal{B}(\mathfrak{H}_B) \odot \mathcal{B}(B\mathfrak{K}) \rightarrow \mathcal{B}(\mathfrak{H} \otimes_\nu \mathfrak{K}) : (a, b) \mapsto a \otimes_\nu b$$

extends canonically to an injective $*$ -homomorphism.

For proof see [49, Corollary 3.4] or [81, Corollary IX.3.18].

REMARKS 1.5.8. The bimodules ${}_A\mathfrak{H}_B$ and ${}_B\mathfrak{K}_C$ are correspondences in the sense of Connes and their relative tensor product

$$({}_A\mathfrak{H}_B) \otimes_\nu ({}_B\mathfrak{K}_C)$$

is a composition of correspondences, i.e. it is an A - C bimodule.

PROPOSITION 1.5.9 (Associativity). *Let B and C be a von Neumann algebras with $\nu \in \mathfrak{F}(B)$ and $\xi \in \mathfrak{F}(C)$. If \mathfrak{H} , \mathfrak{K} and \mathfrak{L} are respectively a right B -module, a B - C bimodule and a left C -module, then*

$$(\mathfrak{H} \otimes_\nu \mathfrak{K}) \otimes_\xi \mathfrak{L} = \mathfrak{H} \otimes_\nu (\mathfrak{K} \otimes_\xi \mathfrak{L})$$

as $\mathcal{B}(\mathfrak{H}_B)$ - $\mathcal{B}({}_B\mathfrak{L})$ bimodules.

For proof see [49, Theorem 3.6] or [81, Theorem IX.3.20].

REMARKS 1.5.10. Canonical isomorphisms:

$${}_A(\mathfrak{H} \otimes_\nu L^2(B))_B \cong {}_A\mathfrak{H}_B \cong {}_A(L^2(B) \otimes_\nu \mathfrak{H})_B$$

The standard bimodule is the “identity” bimodule.

CHAPTER 2

Dynamical systems and transport plans

The mathematical formulation of the physicist's often crude experience leads in an uncanny number of cases to an amazingly accurate description of a large class of phenomena.

–Eugene Wigner, 1960.

In this chapter we introduce the main mathematical object of concern in this thesis, namely a dynamical system. Our main method of studying systems will be through *optimal transport plans* between systems on von Neumann algebras. This can be thought of as an extension of classical probability theory. A discussion of the original motivation for classical optimal transport, as well as its modern applications, can be found in the books by Villani [86, 87].

The reader is referred to [41, 42] and [43], for a noncommutative version of optimal transport as used in this thesis which is mainly based on the latter. Our approach simultaneously extends the notion of classical transport between probability measures [21, 29, 86], as well as transport between quantum states [41, 45], to optimal transport between dynamical systems on possibly different von Neumann algebras [42, 43]. Much of the framework of [41] 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.

Detailed balance is a form of microscopic reversibility and is intimately related to equilibrium [5, 26, 44, 46, 48, 64, 66]. A number of conditions called *quantum detailed balance* (QDB) for quantum Markov semigroups (QMS) have been proposed in the literature to distinguish, among invariant states, those enjoying reversibility properties. Roughly speaking, all of these conditions are based on a notion of dual or adjoint [18]. We adopt a particular formulation of QDB with respect to reversing operations, the so-called *standard quantum detailed balance* conditions, discussed and developed in [47, 48].

We start the chapter by giving a *preliminary* description of dynamical maps and the various kinds of duals of such maps in Section 2.1. This will be extended in Section 2.2 to a form general enough for our approach to Wasserstein distances. We formulate the theory of optimal transport plans in the noncommutative case in terms of von Neumann algebras in Section 2.3. In Section 2.4, we discuss how one can obtain an extended or generalized version of a property on a dynamical system

from another system. This allows us to compare a possibly complex system with a simple or well understood system via transport plans, to analyze the former and learn more about its properties. In Section 2.5 we discuss quantum detailed balance and related duals of systems.

A key notion will be that of a dual of a system, which will play a central role in the definition of the types of Wasserstein distances to be introduced in Section 3.1. We will define three kinds of such duals.

2.1. Dynamical maps

The dynamical maps in this thesis will be given by unital positive linear maps (u.p. maps, for short) between von Neumann algebras. In quantum physics one is generally interested in unital completely positive (u.c.p.) linear maps, but our mathematical framework (and indeed that of [42] and [43]) 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. We therefore need to cover merely positive maps in our framework.

A central notion for us will be that of a dual of a given dynamical map. The different kinds of duals for dynamical maps are introduced and some of their basic properties demonstrated, with special interest in modular dynamics and KMS-duals which will play an indispensable role in Chapters 3 and 4.

DEFINITION 2.1.1 (Dual of a map). Let A and B be von Neumann algebras with $\mu \in \mathfrak{F}(A)$ and $\nu \in \mathfrak{F}(B)$. Given a u.p. map $E : A \rightarrow B$ satisfying $\nu \circ E = \mu$, its *dual* (w.r.t. μ and ν) $E' : B' \rightarrow A'$ is defined by

$$(2.1.1) \quad \langle \Lambda_\mu, aE'(b')\Lambda_\mu \rangle = \langle \Lambda_\nu, E(a)b'\Lambda_\nu \rangle, \quad \forall a \in A, b' \in B',$$

where the vectors Λ_μ and Λ_ν are cyclic for A and B , respectively. We do not include μ and ν in the notation for the dual, as it will always be clear from context, and would make the notation unnecessarily cumbersome.

REMARKS 2.1.2. The existence of such duals is non-trivial, however according to [1, Proposition 3.1], the ($*$ -algebraic) dual E' exists and it is a u.p. map satisfying

$$\mu' \circ E' = \nu' \quad \text{and} \quad E'' := (E')' = E,$$

where $\mu' := \mu \circ j_A \in \mathfrak{F}(A')$ and $\nu' := \nu \circ j_B \in \mathfrak{F}(B')$. Under the given assumptions, the maps E and E' are necessarily normal, i.e., σ -weakly continuous. If E is a u.c.p. map, then so is E' . The reader can refer to [1] for the theory behind such duals, also summarized in [45, Section 2].

Note that the dual condition (2.1.1) can also be expressed as

$$(2.1.2) \quad \mu(aE'(b')) = \nu(E(a)b')$$

for all $a \in A$ and $b' = B'$, where $\mu \in \mathfrak{F}(A)$ and $\nu \in \mathfrak{F}(B)$.

DEFINITION 2.1.3. A *reversing operation* θ_μ for the pair (A, μ) , is a $*$ -anti-homomorphism $\theta_\mu : A \rightarrow A$ (i.e., θ_μ is linear, $\theta_\mu(a^*) = \theta_\mu(a)^*$, and $\theta_\mu(a_1 a_2) = \theta_\mu(a_2) \theta_\mu(a_1)$) such that

$$\theta_\mu^2 = \text{id}_A \quad \text{and} \quad \mu \circ \theta_\mu = \mu.$$

We will need an appropriate definition for reversals of a dynamical map between von Neumann algebras, which we formalize as follows.

DEFINITION 2.1.4. Let θ_μ and θ_ν be reversing operations for (A, μ) and (B, ν) , respectively. If $E : A \rightarrow B$ is a u.p. map such that $\nu \circ E = \mu$, then we define:

- (1) the *KMS-dual* of E (w.r.t. μ and ν) by

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

where E' is the dual of E .

- (2) the (θ_μ, θ_ν) -*KMS dual* of E by

$$E^{\leftarrow} := \theta_\mu \circ E^\sigma \circ \theta_\nu : B \rightarrow A,$$

in terms of the KMS-dual E^σ of E . One could write $E^{\theta_\mu, \theta_\nu}$ instead of E^{\leftarrow} , but θ_μ and θ_ν will always be clear from context.

- (3) the θ_μ -*KMS-dual* of a u.p. map $\alpha : A \rightarrow A$ such that $\mu \circ \alpha = \mu$ by

$$\alpha^{\leftarrow} := \theta_\mu \circ \alpha^\sigma \circ \theta_\mu : A \rightarrow A,$$

in terms of the KMS dual $\alpha^\sigma = j_A \circ \alpha' \circ j_A : A \rightarrow A$. The θ_μ -KMS dual is also denoted by α^θ , but the reversing operation will always be clear from context.

LEMMA 2.1.5. Consider a map E as in Definition 2.1.1. Then E has a Hilbert space representation as a contraction $K : \mathfrak{H}_\mu \rightarrow \mathfrak{H}_\nu$ defined by

$$Ka\Lambda_\mu := E(a)\Lambda_\nu, \quad \forall a \in A,$$

similarly E' is represented as the contraction $K^* : \mathfrak{H}_\nu \rightarrow \mathfrak{H}_\mu$, and E^σ is represented by the contraction $J_A K^* J_B : \mathfrak{H}_\nu \rightarrow \mathfrak{H}_\mu$.

PROOF. That K is well-defined follows from $\nu \circ E = \mu$ (which implies that $\nu(E(a)^* E(a)) \leq \nu(E(a^* a)) = \mu(a^* a)$ by Kadison's inequality). This implies that E' is represented by K^* , since

$$\begin{aligned} \langle \Lambda_\mu, aE'(b')\Lambda_\mu \rangle &= \langle \Lambda_\nu, E(a)b'\Lambda_\nu \rangle \\ \implies \langle \Lambda_\mu, E'(b')a\Lambda_\mu \rangle &= \langle \Lambda_\nu, b'E(a)\Lambda_\nu \rangle \\ \implies \langle E'(b')^* \Lambda_\mu, a\Lambda_\mu \rangle &= \langle (b')^* \Lambda_\nu, E(a)\Lambda_\nu \rangle \\ &= \langle (b')^* \Lambda_\nu, Ka\Lambda_\mu \rangle \\ &= \langle K^*(b')^* \Lambda_\nu, a\Lambda_\mu \rangle, \end{aligned}$$

for all $a \in A, b' \in B'$. Thus, $E'(b')^* \Lambda_\mu = K^*(b')^* \Lambda_\nu$ for all $b' \in B'$, from which it then follows that E' is represented by K^* . This in turn means that E^σ is represented by $J_A K^* J_B$:

$$\begin{aligned} \langle \Lambda_\mu, a E^\sigma(b) \Lambda_\mu \rangle &= \langle a^* \Lambda_\mu, J_A E' (j_B(b))^* \Lambda_\mu \rangle \\ &= \langle E' (j_B(b))^* \Lambda_\mu, J_A a^* \Lambda_\mu \rangle \\ &= \langle K^* (J_B b J_B) \Lambda_\mu, J_A a^* \Lambda_\mu \rangle \\ &= \langle a^* \Lambda_\mu, J_A K^* J_B b \Lambda_\nu \rangle \\ &= \langle \Lambda_\mu, a J_A K^* J_B b \Lambda_\nu \rangle, \end{aligned}$$

for all $a \in A, b \in B$. Thus, $E^\sigma(b) \Lambda_\mu = J_A K^* J_B b \Lambda_\nu$, for all $b \in B$. \square

PROPOSITION 2.1.6. *Let A be a von Neumann algebra with $\mu \in \mathfrak{F}(A)$, and θ_μ the reversing operation for (A, μ) .*

- (1) *For any $*$ -automorphism τ_A on A such that $\mu \circ \tau_A = \mu$, we have*

$$\tau'_A = j_A \circ \tau_A^{-1} \circ j_A,$$

where $j_A := J_A(\cdot)^* J_A$ with J_A the modular conjugation associated to (A, μ) . Furthermore,

$$\tau_A^\sigma = \tau_A^{-1}.$$

- (2) *The reversing operation θ_μ for (A, μ) is KMS-symmetric, i.e.*

$$\theta_\mu^\sigma = \theta_\mu.$$

PROOF. Consider the cyclic representation $(\mathfrak{H}_\mu, \text{id}_A, \Lambda_\mu)$ of (A, μ) .

- (1) Let U be a unitary operator on \mathfrak{H}_μ such that $U \Lambda_\mu = \Lambda_\mu$ and

$$\tau_A(a) = U a U^*, \quad \forall a \in A.$$

Then, by the definition of the dual of a map, we have

$$\begin{aligned} \langle \Lambda_\mu, a \tau'_A(a') \Lambda_\mu \rangle &= \langle \Lambda_\mu, U a U^* a' \Lambda_\mu \rangle \\ &= \langle \Lambda_\mu, a U^* a' U \Lambda_\mu \rangle, \end{aligned}$$

for all $a \in A$ and $a' \in A'$, since $U^* \Lambda_\mu = \Lambda_\mu$. Thus,

$$\tau'_A(a') = U^* a' U = j_A \circ \tau_A^{-1} \circ j_A(a'), \quad \forall a' \in A',$$

since $U J_A = J_A U$ (see [20, Corollary 2.5.32(c)]). Hence

$$\tau_A^\sigma = j_A \circ \tau'_A \circ j_A = \tau_A^{-1},$$

by the definition of the KMS-dual, and $j_A^2 = \text{id}_A$.

- (2) Let $\Theta_\mu : \mathfrak{H}_\mu \rightarrow \mathfrak{H}_\mu$ be an anti-unitary operator with $\Theta_\mu^2 = 1$ and $\Theta_\mu \Lambda_\mu = \Lambda_\mu$ such that

$$\theta_\mu(a) = \Theta_\mu a^* \Theta_\mu,$$

i.e. $\theta_\mu(a) \Lambda_\mu = \Theta_\mu a^* \Lambda_\mu$, for all $a \in A$. Then, analogous to part (1) above, the dual of θ_μ can be expressed as

$$\theta'_\mu(a') = \Theta_\mu a'^* \Theta_\mu, \quad \forall a' \in A',$$

from which we have

$$\begin{aligned}
\theta_\mu^\sigma(a)\Lambda_\mu &= j_A \circ \theta'_\mu \circ j_A(a)\Lambda_\mu \\
&= J_A \Theta_\mu J_A a^* \Lambda_\mu \\
&= J_A^2 \Theta_\mu a^* \Lambda_\mu \\
&= \Theta_\mu a^* \Lambda_\mu \\
&= \theta_\mu(a)\Lambda_\mu,
\end{aligned}$$

for all $a \in A$, since $J_A \Theta_\mu = \Theta_\mu J_A$ by [45, Proposition 6.4]. \square

PROPOSITION 2.1.7. *Let A , B and C be von Neumann algebras with $\mu \in \mathfrak{F}(A)$, $\nu \in \mathfrak{F}(B)$, and $\xi \in \mathfrak{F}(C)$. For the u.p. maps $E_1 : A \rightarrow B$ and $E_2 : B \rightarrow C$ satisfying $\nu \circ E_1 = \mu$ and $\xi \circ E_2 = \nu$, we have*

$$\begin{aligned}
(E_2 \circ E_1)' &= E_1' \circ E_2', \\
(E_2 \circ E_1)^\sigma &= E_1^\sigma \circ E_2^\sigma
\end{aligned}$$

and

$$(E_2 \circ E_1)^\leftarrow = E_1^\leftarrow \circ E_2^\leftarrow.$$

PROOF. Let (A, μ) , (B, ν) and (C, ξ) be in the cyclic representations $(\mathfrak{H}_\mu, \text{id}_A, \Lambda_\mu)$, $(\mathfrak{H}_\nu, \text{id}_B, \Lambda_\nu)$ and $(\mathfrak{H}_\xi, \text{id}_C, \Lambda_\xi)$, respectively. Then

$$\begin{aligned}
\langle \Lambda_\mu, a(E_2 \circ E_1)'(c')\Lambda_\mu \rangle &= \langle \Lambda_\xi, E_2 \circ E_1(a)c'\Lambda_\xi \rangle \\
&= \langle \Lambda_\nu, E_1(a)E_2'(c')\Lambda_\nu \rangle \\
&= \langle \Lambda_\mu, aE_1'(E_2'(c'))\Lambda_\mu \rangle,
\end{aligned}$$

for all $a \in A$ and $c' \in C'$. Thus, $(E_2 \circ E_1)' = E_1' \circ E_2'$, since Λ_μ is cyclic and separating for A . By the definition of the KMS-dual, we have $E_1^\sigma = j_A \circ E_1' \circ j_B$ and $E_2^\sigma = j_B \circ E_2' \circ j_C$, which give

$$\begin{aligned}
E_1^\sigma \circ E_2^\sigma &= j_A \circ E_1' \circ E_2' \circ j_C \\
&= j_A \circ (E_2 \circ E_1)' \circ j_C \\
&= (E_2 \circ E_1)^\sigma,
\end{aligned}$$

since $j_B \circ j_B = \text{id}_B$. Furthermore,

$$\begin{aligned}
E_1^\leftarrow \circ E_2^\leftarrow &= \theta_\mu \circ E_1^\sigma \circ E_2^\sigma \circ \theta_\xi \\
&= \theta_\mu \circ (E_2 \circ E_1)^\sigma \circ \theta_\xi \\
&= (E_2 \circ E_1)^\leftarrow,
\end{aligned}$$

since $\theta_\nu^2 = \text{id}_B$. \square

PROPOSITION 2.1.8. *Let θ_μ and θ_ν be reversing operations for (A, μ) and (B, ν) , respectively, and E a u.p. map as in Definition 2.1.1. Then*

(1) *The KMS-dual $E^\sigma = (j_B \circ E \circ j_A)'$ is a u.p. map such that*

$$\mu \circ E^\sigma = \nu \quad \text{and} \quad E^{\sigma\sigma} := (E^\sigma)^\sigma = E.$$

(2) The map $E^{\leftarrow} = (\theta_\nu \circ E \circ \theta_\mu)^\sigma$ is a u.p. map satisfying

$$\mu \circ E^{\leftarrow} = \nu \quad \text{and} \quad (E^{\leftarrow})^{\leftarrow} = E.$$

PROOF. Let (A, μ) and (B, ν) be in the cyclic representations $(\mathfrak{H}_\mu, \text{id}_A, \Lambda_\mu)$ and $(\mathfrak{H}_\nu, \text{id}_B, \Lambda_\nu)$, respectively.

(1) Since the dual $E' : B' \rightarrow A'$ of E is a u.c.p. map such that $\mu' \circ E' = \nu'$ and $(E')' = E$, then $E^\sigma = j_A \circ E' \circ j_B$ is itself u.c.p. (see [15, Proposition 2.6.4]), and

$$\mu \circ E^\sigma = \mu \circ j_A \circ E' \circ j_B = \mu' \circ E' \circ j_B = \nu' \circ j_B = \nu.$$

It follows from Lemma 2.1.5 that

$$\begin{aligned} \langle \Lambda_\mu, a' j_A \circ E' \circ j_B(b) \Lambda_\mu \rangle &= \langle a'^* \Lambda_\mu, J_A E' (j_B(b))^* \Lambda_\mu \rangle \\ &= \langle E' (j_B(b))^* \Lambda_\mu, J_A a'^* \Lambda_\mu \rangle \\ &= \langle K^* j_B(b)^* \Lambda_\nu, j_A(a') \Lambda_\mu \rangle \\ &= \langle J_B b \Lambda_\nu, K j_A(a') \Lambda_\mu \rangle \\ &= \langle J_B b \Lambda_\nu, E(j_A(a')) \Lambda_\nu \rangle \\ &= \langle E(j_A(a'))^* J_B b \Lambda_\nu, J_B \Lambda_\nu \rangle \\ &= \langle \Lambda_\nu, J_B E(j_A(a'))^* J_B b \Lambda_\nu \rangle \\ &= \langle \Lambda_\nu, j_B \circ E \circ j_A(a') b \Lambda_\nu \rangle, \end{aligned}$$

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

$$(2.1.3) \quad (j_B \circ E \circ j_A)^\sigma = j_A \circ E' \circ j_B = E^\sigma,$$

and consequently

$$(E^\sigma)^\sigma = (j_A \circ E' \circ j_B)^\sigma = j_B \circ [j_B \circ (E')' \circ j_A] \circ j_A = (E')' = E$$

since $j_A^2 = \text{id}_A$ and $j_B^2 = \text{id}_B$.

(2) Since the reversing operations θ_μ and θ_ν are KMS-symmetric, by Proposition 2.1.6(2), we have

$$E^{\leftarrow} = \theta_\mu \circ E^\sigma \circ \theta_\nu = (\theta_\nu \circ E \circ \theta_\mu)^\sigma$$

by Proposition 2.1.7. Furthermore,

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

since $\mu \circ E^\sigma = \nu$. Finally,

$$(E^{\leftarrow})^{\leftarrow} = \theta_\nu \circ (E^{\leftarrow})^\sigma \circ \theta_\mu = \theta_\nu \circ [(\theta_\nu \circ E \circ \theta_\mu)^\sigma]^\sigma \circ \theta_\mu = E,$$

since $\theta_\mu^2 = \text{id}_A$ and $\theta_\nu^2 = \text{id}_B$.

□

As a consequence of Lemma 2.1.5, we have the following result on the marginal states of a transport plan:

PROPOSITION 2.1.9. *For $\mu \in \mathfrak{F}(A)$ and $\nu \in \mathfrak{F}(B)$, consider the u.p. map $E : A \rightarrow B$ given as in Definition 2.1.1. Then*

$$\begin{aligned}\mu'(a^*a') &= \mu(a^*a), \\ \nu'(b^*b') &= \nu(b^*b), \\ \mu(a^*E'(b)) &= \nu(E(a)^*b),\end{aligned}$$

and

$$\mu'(a^*E'(b')) = \mu(E^\sigma(b)^*a),$$

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

PROOF. By Lemma 2.1.5 the maps E , E' and E^σ have Hilbert space representations given by K , K^* and $J_A K^* J_B$, respectively. It then follows that

$$\begin{aligned}\mu'(a^*a') &= \langle a' \Lambda_\mu, a' \Lambda_\mu \rangle = \langle J_A a \Lambda_\mu, J_A a \Lambda_\mu \rangle = \langle a \Lambda_\mu, a \Lambda_\mu \rangle = \mu(a^*a), \\ \nu'(b^*b') &= \langle b' \Lambda_\nu, b' \Lambda_\nu \rangle = \langle J_B b \Lambda_\nu, J_B b \Lambda_\nu \rangle = \langle b \Lambda_\nu, b \Lambda_\nu \rangle = \nu(b^*b),\end{aligned}$$

$$\begin{aligned}\mu(a^*E'(b)) &= \langle a \Lambda_\mu, E'(b) \Lambda_\mu \rangle \\ &= \langle a \Lambda_\mu, K^* b \Lambda_\nu \rangle \\ &= \langle K a \Lambda_\mu, b \Lambda_\nu \rangle \\ &= \langle E(a) \Lambda_\nu, b \Lambda_\nu \rangle \\ &= \nu(E(a)^*b),\end{aligned}$$

and

$$\begin{aligned}\mu'(a^*E'(b')) &= \langle a' \Lambda_\mu, E'(b') \Lambda_\mu \rangle \\ &= \langle J_A a \Lambda_\mu, K^* J_B b' \Lambda_\nu \rangle \\ &= \langle J_A K^* J_B b' \Lambda_\nu, a \Lambda_\mu \rangle \\ &= \langle E^\sigma(b) \Lambda_\mu, a \Lambda_\mu \rangle \\ &= \mu(E^\sigma(b)^*a),\end{aligned}$$

for all $a \in A$, $a' \in A'$, $b \in B$ and $b' \in B'$, where we have used the facts that $J_A \Lambda_\mu = \Lambda_\mu$ and $J_B \Lambda_\nu = \Lambda_\nu$ from Tomita-Takesaki theory. \square

When dynamical maps are given by the modular dynamics, we further have that the corresponding state is invariant (in the sense of (1.2.4)). In this special case, we have the following result:

PROPOSITION 2.1.10 (Modular dynamics). *Let A be a von Neumann algebra with $\mu \in \mathfrak{F}(A)$. Consider the associated modular automorphism group $\sigma^\mu = \{\sigma_t^\mu : t \in \mathbb{R}\}$ given by (1.2.3). Then*

$$(2.1.4) \quad (\sigma_t^\mu)' = \sigma_t^{\mu'} \quad \text{and} \quad (\sigma_t^\mu)^\sigma = (\sigma_t^\mu)^{-1} = \sigma_{-t}^\mu,$$

for all $t \in \mathbb{R}$, where $\mu' := \mu \circ j_A \in \mathfrak{F}(A')$.

PROOF. By Tomita-Takesaki theory we have

$$\Delta'_\mu = \Delta_\mu^{-1} \quad \text{and} \quad (\Delta'_\mu)^{it} = (\Delta_\mu^{-1})^{it} = \Delta_\mu^{-it} = (\Delta_\mu^{it})^*$$

for all $t \in \mathbb{R}$. It follows from (1.2.3) that

$$(\sigma_t^\mu)^{-1} = \Delta_\mu^{-it}(\cdot)\Delta_\mu^{it} = \sigma_{-t}^\mu,$$

for all $t \in \mathbb{R}$. By Proposition 2.1.6(1), we have

$$(\sigma_t^\mu)' = j_A \circ (\sigma_t^\mu)^{-1} \circ j_A = \Delta_\mu^{-it}(\cdot)\Delta_\mu^{it} = (\Delta'_\mu)^{it}(\cdot)(\Delta'_\mu)^{-it} = \sigma_t^{\mu'}$$

for all $t \in \mathbb{R}$. Furthermore,

$$(\sigma_t^\mu)^\sigma = j_A \circ (\sigma_t^\mu)' \circ j_A = (\sigma_t^\mu)^{-1},$$

for all $t \in \mathbb{R}$, again by Proposition 2.1.6 and since $j_A^2 = \text{id}_A$. \square

The dynamical maps introduced here will be extended in the setting of dynamical systems in the next section where instead of considering a single u.p. map at a time we consider an indexed class of all such maps on a given von Neumann algebra.

2.2. Dynamical systems

In this section we introduce dynamical systems on von Neumann algebras and their various kinds of duals, extending the notions discussed in Section 2.1.

DEFINITION 2.2.1. A *dynamical system* is given by $\mathbf{A} = (A, \alpha, \mu, k)$, where A is a von Neumann algebra, $\mu \in \mathfrak{F}(A)$ and $k = (k_1, \dots, k_d)$ with $k_1, \dots, k_d \in A$ for some $d \in \{1, 2, 3, \dots\}$, while α consists of the following: Let Υ be any set. To each $v \in \Upsilon$ corresponds a set Z_v and *generalized dynamics* α_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

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

REMARKS 2.2.2. (i) We will refer to dynamical systems simply as systems. We view Z_v as a set of “points in time” in an abstract sense. Each α_v is viewed as dynamics, so \mathbf{A} is really a set of dynamical systems on A , indexed by v , and all leaving the state μ invariant.

(ii) We do not assume any structure, for example semigroup structure, on Z_v . In part this is because we do not need any structure, but also since in applications, we want to allow for dynamics that may not have semigroup structure.

- (iii) 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 do not place any restrictions on the choice of k , for example, $k_1 = k_2$ is allowed.

We also define the dual α' , the KMS-dual α^σ and the θ_μ -KMS-dual α^\leftarrow through

$$(2.2.1) \quad \alpha'_{v,z} := (\alpha_{v,z})', \quad \alpha^\sigma_{v,z} := (\alpha_{v,z})^\sigma \quad \text{and} \quad \alpha^\leftarrow_{v,z} := (\alpha_{v,z})^\leftarrow,$$

for all $z \in Z_v$ and $v \in \Upsilon$, generalizing the dynamical maps given in Section 2.1.

DEFINITION 2.2.3 (Duals of a system). Let \mathbf{A} be a system.

- (1) The *dual of a system* \mathbf{A} is defined to be

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

where A' is the commutant of the von Neumann algebra A , $\mu' := \mu \circ j_A \in \mathfrak{F}(A')$, and $k' = (k'_1, \dots, k'_d) := (j_A(k_1^*), \dots, j_A(k_d^*))$.

- (2) The *KMS-dual* of a system \mathbf{A} is defined to be

$$\mathbf{A}^\sigma := (A, \alpha^\sigma, \mu, k).$$

Furthermore, \mathbf{A} is said to be *KMS-symmetric* if $\alpha^\sigma = \alpha$.

- (3) We say that \mathbf{A} is *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, μ) . The *reverse* of \mathbf{A} is then defined as

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

The KMS-dual of a system which will play a key role in one of the types of Wasserstein distances to be introduced in Section 3.1.

For the remainder of this chapter, we fix Υ , the Z_v 's, and d , i.e., they are the same for all systems.

REMARKS 2.2.4. The following notational convention will be used: \mathbf{A} will denote (A, α, μ, k) , as in the definition above, and similarly we write

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

Denote the collection consisting of all systems by

$$\mathfrak{A}.$$

Our Wasserstein distances will be defined on \mathfrak{A} . Notationally, however, it will be convenient to allow systems without coordinates as well (the case $d = 0$), written as (A, α, μ) , though they will not be viewed as members of \mathfrak{A} . This is needed to formulate certain conditions related to transport plans, involving modular dynamics, more conveniently in the definition at the end of this chapter.

PROPOSITION 2.2.5. *For any reversible system \mathbf{A} , we have that the duals \mathbf{A}' , \mathbf{A}^σ and \mathbf{A}^\leftarrow are themselves systems, i.e., \mathbf{A}' , \mathbf{A}^σ , $\mathbf{A}^\leftarrow \in \mathfrak{A}$, with*

$$(\mathbf{A}')' = (\mathbf{A}^\sigma)^\sigma = (\mathbf{A}^\leftarrow)^\leftarrow = \mathbf{A}.$$

Furthermore, they satisfy

$$(\mathbf{A}')^\sigma = (\mathbf{A}^\sigma)', \quad (\mathbf{A}')^\leftarrow = (\mathbf{A}^\leftarrow)', \quad \text{and} \quad (\mathbf{A}^\leftarrow)^\sigma = (\mathbf{A}^\sigma)^\leftarrow.$$

PROOF. Given a system \mathbf{A} , then $A' = J_A A J_A$ is a von Neumann algebra, and $\mu' = \mu \circ j_A \in \mathfrak{F}(A')$, by Theorem 1.2.1. By the definition of the dual map, we have

$$\mu' \circ \alpha'(a') = \langle \Lambda_\mu, \alpha'(a') \Lambda_\mu \rangle = \langle \Lambda_\mu, a' \alpha(1) \Lambda_\mu \rangle = \langle \Lambda_\mu, a' \Lambda_\mu \rangle = \mu'(a'),$$

for all $a' \in A'$, since α is unital. By the definition of KMS dual of α , we have

$$\mu \circ \alpha^\sigma = \mu \circ (j_A \circ \alpha' \circ j_A) = \mu' \circ \alpha' \circ j_A = \mu' \circ j_A = \mu,$$

and by the definition of θ -KMS dual we have

$$\mu \circ \alpha^\leftarrow = \mu \circ (\theta_{\mathbf{A}} \circ \alpha^\sigma \circ \theta_{\mathbf{A}}) = \mu \circ \alpha^\sigma \circ \theta_{\mathbf{A}} = \mu \circ \theta_{\mathbf{A}} = \mu,$$

since $\mu \circ \theta_{\mathbf{A}} = \mu$. Thus, we have \mathbf{A}' , \mathbf{A}^σ , $\mathbf{A}^\leftarrow \in \mathfrak{A}$. It is easily seen that $(\mathbf{A}')' = \mathbf{A}$, since $(\alpha')' = \alpha$. Similarly, $(\mathbf{A}^\sigma)^\sigma = \mathbf{A}$ and $(\mathbf{A}^\leftarrow)^\leftarrow = \mathbf{A}$, since $(\alpha^\sigma)^\sigma = (\alpha^\leftarrow)^\leftarrow = \alpha$, by Proposition 2.1.8.

Furthermore, we have

$$\begin{aligned} (\alpha')^\sigma &= j_A \circ (\alpha')' \circ j_A \\ &= (j_A \circ \alpha' \circ j_A)' \\ &= (\alpha^\sigma)', \end{aligned}$$

by (2.1.3). Consequently,

$$\begin{aligned} (\alpha')^\leftarrow &= \theta_{\mathbf{A}} \circ (\alpha')^\sigma \circ \theta_{\mathbf{A}} \\ &= \theta_{\mathbf{A}} \circ (\alpha^\sigma)' \circ \theta_{\mathbf{A}} \\ &= (\theta_{\mathbf{A}} \circ \alpha^\sigma \circ \theta_{\mathbf{A}})' \\ &= (\alpha^\leftarrow)' \end{aligned}$$

by Proposition 2.1.7. Similarly,

$$\begin{aligned} (\alpha^\sigma)^\leftarrow &= \theta_{\mathbf{A}} \circ (\alpha^\sigma)^\sigma \circ \theta_{\mathbf{A}} \\ &= (\theta_{\mathbf{A}} \circ \alpha^\sigma \circ \theta_{\mathbf{A}})^\sigma \\ &= (\alpha^\leftarrow)^\sigma, \end{aligned}$$

by Proposition 2.1.7. The required results then follow. \square

Given any system \mathbf{A} , the condition $\{k_1^*, \dots, k_d^*\} = \{k_1, \dots, k_d\}$ will at times become relevant. This condition will be needed in proving faithfulness of an asymmetric metric. For later convenience, we give this condition a name:

DEFINITION 2.2.6. A system \mathbf{A} is said to be *hermitian* if

$$\{k_1^*, \dots, k_d^*\} = \{k_1, \dots, k_d\}.$$

Note that the set $\{k_1, \dots, k_d\}$ is only required to be closed under the involution operation but individual elements need not be self-adjoint, i.e we may have $k_i^* \neq k_i$ for $i = 1, 2, \dots, d$.

DEFINITION 2.2.7. The *coordinate algebra* M of a system \mathbf{A} is the von Neumann subalgebra of A generated by $\{k_1, \dots, k_d\}$. Similarly, N will denote the coordinate algebra of \mathbf{B} .

Note that a hermitian system is one whose von Neumann algebra has a finite $*$ -subalgebra, while a coordinate algebra is a finitely generated von Neumann algebra of a given algebra. Thus, a coordinate algebra is hermitian.

DEFINITION 2.2.8. Two systems \mathbf{A} and \mathbf{B} are said to be *isomorphic* if there is a $*$ -isomorphism $\iota : A \rightarrow B$ such that

$$\iota \circ \alpha = \beta \circ \iota, \quad \nu \circ \iota = \mu \quad \text{and} \quad \iota(k_i) = l_i$$

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

For all intents and purposes isomorphic systems are the same, but possibly represented differently.

2.3. Transport plans between systems

In this section we formulate a noncommutative version of the optimal transport plan problem in terms of von Neumann algebras. This can be thought of as an extension of the classical probability theory, and at the same time an extension of transport between states.

We begin with a brief account of the classical optimal transport problem which is cast in terms of probability distributions by defining a transport plan and a suitable cost function. In this case a transport plan ω from one probability measure μ (on a space X) to another ν (on a space Y) is simply given by a coupling of the two measures, i.e. a probability measure on $X \times Y$ such that

$$\omega(U \times Y) = \mu(U) \quad \text{and} \quad \omega(X \times V) = \nu(V),$$

with the following interpretation: $\omega(U \times V)$ is the “amount” of probability transported from $U \subseteq X$ to $V \subseteq Y$. In particular, $\omega(U \times Y) = \mu(U)$ says that everything in U ends up in Y , while $\omega(X \times V) = \nu(V)$ says that V ends up full when X is emptied, since Y has the same total volume as X , namely 1.

The cost function is taken as the usual distance squared in \mathbb{R}^d , giving the following cost of transport from one probability measure to another on some closed subset $X = Y$ of \mathbb{R}^d :

$$(2.3.1) \quad I(\omega) = \int_{X \times X} \|x - y\|^2 d\omega(x, y)$$

where ω is a transport plan from one probability measure μ to the other ν , i.e. ω is a coupling of the two measures. The goal is then to optimize the cost of transport by finding the minimum of $I(\omega)$, for a given pair (μ, ν) , the square root of which then defines the quadratic Wasserstein distance W_2 between μ and ν , i.e.

$$(2.3.2) \quad W_2(\mu, \nu) = \inf_{\omega} I(\omega)^{1/2},$$

giving a metric on an appropriate set of probability measures. This is a specific but important case of the optimal transport problem.

We are interested in obtaining a noncommutative extension of the case where X is a bounded set, ensuring that the coordinate functions $x \mapsto x_i$, in terms of $x = (x_1, \dots, x_d)$, are bounded. We replace these coordinate functions by elements $k_1, \dots, k_d \in A$ of a von Neumann algebra A . The k_i are then bounded operators, which is why this corresponds to bounded X . In this approach the closest analogy to the classical coordinate functions would be to assume that the k_i are self-adjoint, but for our development this is not actually needed, though we do ultimately need a weaker version of this (see Definition 2.2.6) to obtain faithfulness of the Wasserstein distance (see Corollary 4.2.4).

A direct translation of the classical cost function $c(x, y) := \|x - y\|^2$ above, for the same algebra rather than different algebras, is then

$$c = \sum_{i=1}^d |k_i \otimes 1 - 1 \otimes k_i|^2 \in A \odot A,$$

where 1 denotes the unit of A and $|a|^2 := a^*a$ for a in any $*$ -algebra. The cost of transport plan ω expressed on $A \odot A$ (instead of $A \odot A'$) would then be given by

$$I(\omega) = \omega(c).$$

However, the noncommutativity of A makes this direct translation untenable. The cost will be formulated more rigorously below.

We will now make use of the assumption that the systems \mathbf{A} and \mathbf{B} are equipped with “ d -dimensional coordinate systems” expressed as $k = (k_1, \dots, k_d)$ and $l = (l_1, \dots, l_d)$ respectively, where $k_i \in A$ and $l_i \in B$ for $i = 1, 2, \dots, d$. Instead of what we have above, for the cost $I(\omega)$ for any transport plan ω from \mathbf{A} to \mathbf{B} , we *heuristically propose* to use

$$(2.3.3) \quad I(\omega) = \omega \left(\sum_{i=1}^d |k_i \otimes 1 - 1 \otimes (S_\nu l_i^* S_\nu)|^2 \right)$$

in terms of the coordinate systems of choice, in analogy to the classical transport cost for a transport plan ω between two measures on the same bounded subset X of \mathbb{R}^d . Here $S_\nu : \mathfrak{H}_\nu \rightarrow \mathfrak{H}_\nu : b\Lambda_\nu \mapsto b^*\Lambda_\nu$, $b \in B$ is the conjugate linear (and typically unbounded) operator from Tomita-Takesaki theory associated to $\nu \in \mathfrak{F}(B)$.

- REMARKS 2.3.1. (i) Note that the cost function now appears to have a dependence on ν , which is clearly different from the classical case. Notice also 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 (2.3.1) can be recovered as a special case of the form in (2.3.3), at least for the case corresponding to a bounded subset X of \mathbb{R}^d . For the case of finite dimensional or abelian von Neumann algebras, the formulation in (2.3.3) is sufficient. However, for more general von Neumann algebras S_ν can be unbounded, leading to technical complications which we can circumvent (see Section 3.1) by an alternative approach containing (2.3.3) in finite dimensional and abelian von Neumann algebras as special cases.
- (ii) As in the classical case, Wasserstein distance is obtained as the minimum of the square root of the cost. Of course, as opposed to the case of Wasserstein distance between measures on the same space X , (2.3.3) 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 inclusion of the operator S_ν ensures that we get the usual metric properties, in particular the triangle inequality and zero distance between a system and itself.

The starting point of our technical development is the definition of a *transport plan*, extending the $X \times X$ case in the classical theory.

DEFINITION 2.3.2. Given two systems **A** and **B**, we write

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

to express that $\omega \in T(\mu, \nu)$ (see Definition 1.2.3) and

$$(2.3.4) \quad \omega(\alpha_{v,z}(a) \otimes b') = \omega(a \otimes \beta'_{v,z}(b'))$$

for all $a \in A$, $b' \in B'$, $z \in Z_v$ and $v \in \Upsilon$, in which case we call ω a *transport plan from **A** to **B***.

- REMARKS 2.3.3. (i) The reason for including 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 project.

- (ii) The notion $\mathbf{A}\omega\mathbf{B}$ was introduced in [45] under the name “balance” as an extension of certain detailed balance conditions. The latter would be formulated in terms of $B = A$, with β being some variation on the dual α' of α , while ω is a specific state; this will be reviewed in Section 2.5. 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. The reader is referred to [52], for classical joining theory, and [11, 38, 39, 40] for the noncommutative version.

Both these points are relevant in this project as well. However, we take the (optimal) transport point of view in this thesis, 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 [41], specifically for modular dynamics (from Tomita-Takesaki theory), to obtain symmetry of Wasserstein metrics on states.

- (iii) If the state ω is only required to satisfy the coupling property (1.2.7), then it is called a *transport plan from μ to ν* as in Definitions 1.2.3 and 2.3.2. 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 [86].

In defining a Wasserstein distance 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 to use the full set of all allowed transport plans. But there are further refinements that can be made to this 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 as in [43], refining [42, Definition 3.5] with a corresponding change in notation and terminology.

DEFINITION 2.3.4. Let \mathbf{A} and \mathbf{B} be two systems.

- (1) The set of *transport plans* from \mathbf{A} to \mathbf{B} is denoted by

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

- (2) 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 the condition $(A, \sigma^\mu, \mu)\omega(B, \sigma^\nu, \nu)$ means

$$\omega(\sigma_t^\mu(a) \otimes b') = \omega\left(a \otimes \sigma_t^{\nu'}(b')\right), \quad \forall a \in A, b' \in B', t \in \mathbb{R},$$

and σ^μ and σ^ν denote the modular groups associated to μ and ν , respectively.

(3) The set of *KMS transport plans* from \mathbf{A} to \mathbf{B} is

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

Note that the transport plans do not depend on the coordinate systems k and l . Furthermore, we always have $\mu \odot \nu' \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$, and

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

The conditions $\mathbf{A}^{\sigma}\omega\mathbf{B}^{\sigma}$ and $(A, \sigma^{\mu}, \mu)\omega(B, \sigma^{\nu}, \nu)$ will collectively be referred to as the *modular balance condition*.

A transport plan $\omega \in T(\mu, \nu)$ from μ to ν can be represented as a channel (u.c.p. map) E_{ω} from A to B via the following:

DEFINITION 2.3.5. For any $\omega \in T(\mu, \nu)$, a *channel* $E_{\omega} : A \rightarrow B$ is defined as the unique function such that

$$(2.3.5) \quad \omega(a \otimes b') = \delta_{\nu}(E_{\omega}(a) \otimes b'), \quad \forall a \in A, b' \in B',$$

i.e. $\omega = \delta_{\nu} \circ (E_{\omega} \odot \text{id}_{B'}) : A \odot B' \rightarrow \mathbb{C}$, where δ_{ν} is given as in Proposition 1.2.5.

REMARKS 2.3.6. It is well known in quantum physics, in particular in the context of quantum information, that a transport plan corresponds to a channel, 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 [29] for the finite dimensional case, as is typically used in quantum information. A general form of this correspondence was discussed and used in [11, 45], 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 [36]. 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 reviewed in Section 3.1.

In the classical case the correspondence between couplings of probability measures and Markov operators was studied in a special case (for couplings of a measure with itself) in [21], and more generally in [13, 68], though it does not appear to be widely used in classical optimal transport.

We state the following result without proof:

THEOREM 2.3.7. *In terms of the representation machinery built in Section 1.2, in particular (1.2.16), we define a linear map*

$$(2.3.6) \quad E_{\omega} : A \rightarrow B : a \mapsto u_{\nu}^* \iota_{\mathfrak{H}_{\nu}}^* \pi_{\omega}(a \otimes 1) \iota_{\mathfrak{H}_{\nu}} u_{\nu},$$

where $\iota_{\mathfrak{H}_{\nu}} : \mathfrak{H}_{\nu} \rightarrow \mathfrak{H}_{\omega}$ is the inclusion map, and $\iota_{\mathfrak{H}_{\nu}}^* : \mathfrak{H}_{\omega} \rightarrow \mathfrak{H}_{\nu}$ its adjoint. Then E_{ω} is a well-defined normal and completely positive map satisfying the properties:

$$E_{\omega}(1) = 1, \quad \|E_{\omega}\| = 1, \quad \text{and} \quad \nu \circ E_{\omega} = \mu.$$

See [45, Theorem 3.2], for proof.

There is a one-to-one correspondence between transport plans and channels:

PROPOSITION 2.3.8. *For all $\omega \in T(\mu, \nu)$, there exists a unique u.c.p. map $E_\omega : A \rightarrow B$ with $\nu \circ E_\omega = \mu$, such that*

$$(2.3.7) \quad \omega(a \otimes b') = \delta_\nu(E_\omega(a) \otimes b'), \quad \forall a \in A, b' \in B'.$$

Conversely, for any linear map $E : A \rightarrow B$, there is a linear map $\omega_E : A \odot B' \rightarrow \mathbb{C}$ such that

$$\omega_E := \delta_\nu \circ (E \odot id_{B'}) \in T(\mu, \nu).$$

We omit the proof of this proposition. The proof can be found in [45, Proposition 3.4].

REMARKS 2.3.9. The result above provides a close connection between elements of $T(\mu, \nu)$ and channels $E : A \rightarrow B$ satisfying $\nu \circ E = \mu$. The map E_ω in this condition necessarily exists and is indeed forced to be unital and completely positive. All this is demonstrated in [45, Section 3]. The state δ_ν (see Proposition 1.2.5) 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 2.3.5 provides a generalization of the (finite dimensional) Choi-Jamiołkowski duality between channels and states as used in quantum physics [29, 56, 61], to a von Neumann algebra framework.

PROPOSITION 2.3.10. *For systems \mathbf{A} and \mathbf{B} , let $\omega \in T(\mu, \nu)$, and consider the u.c.p. map $E_\omega : A \rightarrow B$ given by Proposition 2.3.8. Then:*

- (1) *The linear functional defined by*

$$\omega' := \delta_{\mu'} \circ (E'_\omega \odot id_A) : B' \odot A \rightarrow \mathbb{C},$$

where $E'_\omega : B' \rightarrow A'$ is the dual of E_ω , satisfies

$$\omega'(b' \otimes a) = \omega(a \otimes b'), \quad \forall a \in A, b' \in B'$$

and $\omega' \in T(\nu', \mu')$.

- (2) *The linear functional $\omega^\sigma : B \odot A' \rightarrow \mathbb{C}$ defined by*

$$\omega^\sigma(b \otimes a') := \delta_\mu(E_\omega^\sigma(b) \otimes a'), \quad \forall a' \in A', b \in B,$$

where $E_\omega^\sigma := j_A \circ E'_\omega \circ j_B : B \rightarrow A$ is the KMS dual of E_ω , is a transport plan from ν to μ , i.e. $\omega^\sigma \in T(\nu, \mu)$.

- (3) *The linear functional $\omega^{\leftarrow} : B \odot A' \rightarrow \mathbb{C}$ defined by*

$$\omega^{\leftarrow}(b \otimes a') = \delta_\mu(E_\omega^{\leftarrow}(b) \otimes a'), \quad \forall a' \in A', b \in B,$$

in terms of Definition 2.3.5, i.e., $E_{\omega^{\leftarrow}} = E_\omega^{\leftarrow}$, is a transport plan from ν to μ , i.e. $\omega^{\leftarrow} \in T(\nu, \mu)$.

PROOF. For any $\omega \in T(\mu, \nu)$, there is a unique map $E_\omega : A \rightarrow B$ such that $\nu \circ E_\omega = \mu$ and satisfying (2.3.7), by Proposition 2.3.8.

- (1) By the definition of the dual of a u.p. map (see Definition 2.1.1) and Proposition 1.2.5, we have

$$\begin{aligned}
 \omega'(b' \otimes a) &= \delta_{\mu'}(E'_\omega(b') \otimes a) \\
 &= \langle \Lambda_\mu, E'_\omega(b')a\Lambda_\mu \rangle \\
 &= \langle \Lambda_\nu, E_\omega(a)b'\Lambda_\nu \rangle \\
 &= \delta_\nu(E_\omega(a) \otimes b') \\
 &= \omega(a \otimes b'),
 \end{aligned}$$

for all $a \in A$ and $b' \in B'$. In particular, we have

$$\omega'(b' \otimes 1) = \omega(1 \otimes b') = \nu'(b')$$

and

$$\omega'(1 \otimes a) = \omega(a \otimes 1) = \mu(a),$$

for all $a \in A$ and $b' \in B'$. Thus, $\omega' \in T(\nu', \mu')$.

- (2) By the definition of the KMS-dual of a map (see Definition 2.1.4 and Lemma 2.1.5), we have

$$\begin{aligned}
 \omega^\sigma(b \otimes 1) &= \delta_\mu(E_\omega^\sigma(b) \otimes 1) \\
 &= \langle \Lambda_\mu, E_\omega^\sigma(b)\Lambda_\mu \rangle \\
 &= \langle \Lambda_\mu, J_A K_\omega^* J_B b \Lambda_\nu \rangle \\
 &= \langle K_\omega^* J_B b \Lambda_\nu, \Lambda_\mu \rangle \\
 &= \langle J_B b \Lambda_\nu, K_\omega \Lambda_\mu \rangle \\
 &= \langle J_B b \Lambda_\nu, E_\omega(1)\Lambda_\nu \rangle \\
 &= \langle \Lambda_\nu, b\Lambda_\nu \rangle \\
 &= \nu(b),
 \end{aligned}$$

and

$$\begin{aligned}
 \omega^\sigma(1 \otimes a') &= \delta_\mu(E_\omega^\sigma(1) \otimes a') \\
 &= \langle \Lambda_\mu, E_\omega^\sigma(1)a'\Lambda_\mu \rangle \\
 &= \langle \Lambda_\mu, a'\Lambda_\mu \rangle \\
 &= \mu'(a'),
 \end{aligned}$$

for all $a' \in A'$ and $b \in B$. Thus, $\omega^\sigma \in T(\nu, \mu)$.

- (3) By the definition of the (θ_μ, θ_ν) -KMS dual (see Definition 2.1.4) and Proposition 2.1.8, we have

$$\begin{aligned}
 \omega^{\leftarrow}(b \otimes 1) &= \delta_\mu(E_\omega^{\leftarrow}(b) \otimes 1) \\
 &= \langle \Lambda_\mu, E_\omega^{\leftarrow}(b)\Lambda_\mu \rangle \\
 &= \mu(E_\omega^{\leftarrow}(b)) \\
 &= \nu(b)
 \end{aligned}$$

and

$$\begin{aligned}\omega^{\leftarrow}(1 \otimes a') &= \delta_{\mu}(E_{\omega}^{\leftarrow}(1) \otimes a') \\ &= \langle \Lambda_{\mu}, E_{\omega}^{\leftarrow}(1) a' \Lambda_{\mu} \rangle \\ &= \mu(a')\end{aligned}$$

for all $a' \in A'$ and $b \in B$. Thus, $\omega^{\leftarrow} \in T(\nu, \mu)$. □

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

$$(2.3.8) \quad E_{\omega} \circ \alpha_{v,z} = \beta_{v,z} \circ E_{\omega}, \quad \forall z \in Z_v, v \in \Upsilon,$$

by [45, 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_{ω} will allow us to define transport cost while avoiding the complications mentioned above, due to the unboundedness of S_{ν} (see Definition 3.1.1).

PROPOSITION 2.3.11. *For systems \mathbf{A} and \mathbf{B} , let $\omega \in T(\mu, \nu)$.*

(1) *Then*

$$(2.3.9) \quad \mathbf{A}\omega\mathbf{B} \Leftrightarrow \mathbf{B}'\omega'\mathbf{A}' \Leftrightarrow \mathbf{B}^{\sigma}\omega^{\sigma}\mathbf{A}^{\sigma},$$

where ω' and ω^{σ} are respectively defined in terms of $E_{\omega'} = E'_{\omega}$ and $E_{\omega^{\sigma}} = E^{\sigma}_{\omega}$, via the correspondence in Definition 2.3.5.

(2) *For reversible systems \mathbf{A} and \mathbf{B} , we have*

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

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. If we let $\omega \in T(\mu, \nu)$, then there is a unique map $E_{\omega} : A \rightarrow B$ such that $\nu \circ E_{\omega} = \mu$, by Proposition 2.3.8.

(1) Since $j_A^2 = \text{id}_A$ and $j_B^2 = \text{id}_B$, it follows that

$$\begin{aligned}E_{\omega^{\sigma}} \circ \beta_{v,z}^{\sigma} &= \alpha_{v,z}^{\sigma} \circ E_{\omega^{\sigma}} \Leftrightarrow E_{\omega}^{\sigma} \circ \beta_{v,z}^{\sigma} = \alpha_{v,z}^{\sigma} \circ E_{\omega}^{\sigma} \\ &\Leftrightarrow j_A \circ E'_{\omega} \circ \beta'_{v,z} \circ j_B = j_A \circ \alpha'_{v,z} \circ E'_{\omega} \circ j_B \\ &\Leftrightarrow E'_{\omega} \circ \beta'_{v,z} = \alpha'_{v,z} \circ E'_{\omega} \\ &\Leftrightarrow (E_{\omega} \circ \alpha_{v,z})' = (\beta_{v,z} \circ E_{\omega})' \\ &\Leftrightarrow E_{\omega} \circ \alpha_{v,z} = \beta_{v,z} \circ E_{\omega},\end{aligned}$$

by Proposition 2.1.7. The result then follows by (2.3.8).

(2) Since $\theta_{\mathbf{A}}^2 = \text{id}_A$ and $\theta_{\mathbf{B}}^2 = \text{id}_B$, then

$$\begin{aligned}E_{\omega^{\leftarrow}} \circ \beta_{v,z}^{\leftarrow} &= \alpha_{v,z}^{\leftarrow} \circ E_{\omega^{\leftarrow}} \Leftrightarrow \theta_{\mathbf{A}} \circ E_{\omega}^{\sigma} \circ \beta_{v,z}^{\sigma} \circ \theta_{\mathbf{B}} = \theta_{\mathbf{A}} \circ \alpha_{v,z}^{\sigma} \circ E_{\omega}^{\sigma} \circ \theta_{\mathbf{B}} \\ &\Leftrightarrow E_{\omega}^{\sigma} \circ \beta_{v,z}^{\sigma} = \alpha_{v,z}^{\sigma} \circ E_{\omega}^{\sigma} \\ &\Leftrightarrow E_{\omega} \circ \alpha_{v,z} = \beta_{v,z} \circ E_{\omega},\end{aligned}$$

by Proposition 2.1.7. The result then follows by (2.3.8).

Furthermore, if $\omega \in T(\mathbf{A}, \mathbf{B})$ for reversible \mathbf{A} and \mathbf{B} , then

$$E_\omega \circ \theta_{\mathbf{A}} = \theta_{\mathbf{B}} \circ E_\omega$$

since the reversing operations $\theta_{\mathbf{A}}$ and $\theta_{\mathbf{B}}$ are part of the dynamics; thus $\theta_{\mathbf{B}} \circ E_\omega \circ \theta_{\mathbf{A}} = E_\omega$, since $\theta_{\mathbf{B}}^2 = \text{id}_{\mathbf{B}}$. Then

$$E_\omega^{\leftarrow} = \theta_{\mathbf{A}} \circ E_\omega^\sigma \circ \theta_{\mathbf{B}} = (\theta_{\mathbf{B}} \circ E_\omega \circ \theta_{\mathbf{A}})^\sigma = E_\omega^\sigma$$

by Proposition 2.1.7, since $\theta_{\mathbf{A}}^\sigma = \theta_{\mathbf{A}}$ and $\theta_{\mathbf{B}}^\sigma = \theta_{\mathbf{B}}$. Hence $E_\omega^{\leftarrow} = E_\omega^\sigma$, from which $\omega^{\leftarrow} = \omega^\sigma$ by Proposition 2.3.8. \square

REMARKS 2.3.12. Since $(\sigma_t^\mu)^\sigma = \sigma_{-t}^\mu$, by Proposition 2.1.10, then the modular condition $(A, \sigma^\mu, \mu)\omega(B, \sigma^\nu, \nu)$ can also be written as

$$(A, \sigma^\mu, \mu)^\sigma \omega(B, \sigma^\nu, \nu)^\sigma.$$

Indeed, for all $t \in \mathbb{R}$, we have

$$\begin{aligned} (A, \sigma^\mu, \mu)^\sigma \omega(B, \sigma^\nu, \nu)^\sigma &\iff E_\omega^\sigma \circ \sigma_{-t}^\mu = \sigma_{-t}^\nu \circ E_\omega^\sigma \\ &\iff \sigma_t^\nu \circ E_\omega = E_\omega \circ \sigma_t^\mu \\ &\iff (A, \sigma^\mu, \mu)\omega(B, \sigma^\nu, \nu). \end{aligned}$$

Hence, if the modular dynamics are included in \mathbf{A} and \mathbf{B} at the same index value in Υ , then the modular condition becomes redundant in $T_\sigma(\mathbf{A}, \mathbf{B})$. Similarly, for any $*$ -automorphism τ_A of A such that $\mu \circ \tau_A = \mu$, we have $\tau_A^\sigma = \tau_A^{-1}$ by Proposition 2.1.6.

If for each pair (v, z) , it holds that $\alpha_{v,z}$ and $\beta_{v,z}$ are either both $*$ -automorphisms, or both *KMS-symmetric*, i.e., $\alpha_{v,z}^\sigma = \alpha_{v,z}$ and $\beta_{v,z}^\sigma = \beta_{v,z}$, then

$$T_\sigma(\mathbf{A}, \mathbf{B}) = T(\mathbf{A}, \mathbf{B})$$

given that the modular dynamics are included in \mathbf{A} and \mathbf{B} as above.

2.4. Extending dynamical properties by optimal transport

In this section we give a conceptual exposition of the basic features of our main mathematical framework, and motivate our approach to Wasserstein distances. We use the same notation as in previous sections, where \mathbf{A} and \mathbf{B} represent systems, but we will omit their coordinates k and l since we are not discussing Wasserstein distances in this section.

Given a property which a system may possibly 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 other words, for two systems \mathbf{A} and \mathbf{B} with \mathbf{B} satisfying some given property, the problem is then to find an $\omega \in T(\mu, \nu)$ such that $\mathbf{A}\omega\mathbf{B}$ holds, in which case \mathbf{A} satisfies a generalized extension of the property. In

particular, our goal is to define extensions of detailed balance conditions in this way. Keep in mind that \mathbf{A} is the system that we actually want to study.

Note that when ω is a product state, $\mathbf{A}\omega\mathbf{B}$ is trivial, in which case \mathbf{A} does not inherit any of the properties of \mathbf{B} in a weak form. 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 chapter. Wasserstein distances quantify deviations from detailed balance, and in Chapter 4 we establish bounds on such deviations.

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 time.

We 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

$$\langle \Lambda_\mu, aF(b')\Lambda_\mu \rangle = \langle \Lambda_\nu, E(a)b'\Lambda_\nu \rangle, \quad \forall a \in A, b' \in B'.$$

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

PROPOSITION 2.4.1. *The two basic properties satisfied by the u.p. map α in $\mathbf{A} = (A, \alpha, \mu)$, namely invariance (i.e. $\mu \circ \alpha = \mu$) and unitality, which are dual to one another, can respectively be expressed as*

$$\mathbf{A}\omega\mathbf{B} \quad \text{and} \quad \mathbf{B}\psi\mathbf{A},$$

if $\mathbf{B} = (B, \beta, \nu)$ is taken as a 1-point system (i.e. $B = \mathbb{C}$).

PROOF. Since \mathbf{B} is a 1-point system, we necessarily have that

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

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

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

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for all $a \in A$ and $b' \in B' = \mathbb{C}$, i.e., $\mu \circ \alpha = \mu$. On the other hand $\mathbf{B}\psi\mathbf{A}$ says

$$\nu(b)\mu'(a') = \nu \circ \beta(b)\mu'(a') = \psi(\beta(b) \otimes a') = \psi(b \otimes \alpha'(a')) = \nu(b)\mu' \circ \alpha'(a'),$$

for all $a' \in A'$ and $b \in B$, expressing $\mu' \circ \alpha' = \mu'$ which is dual (and equivalent) to $\alpha(1) = 1$. The latter can be seen from the following:

$$\mu' \circ \alpha'(a') = \langle \Lambda_\mu, \alpha'(a')\Lambda_\mu \rangle = \langle \Lambda_\mu, \alpha(1)a'\Lambda_\mu \rangle,$$

so $\alpha(1) = 1$ gives $\mu' \circ \alpha'(a') = \mu'(a')$. Conversely, $\mu' \circ \alpha' = \mu'$ gives

$$\langle \alpha(1)^*\Lambda_\mu, a'\Lambda_\mu \rangle = \mu'(a') = \langle \Lambda_\mu, a'\Lambda_\mu \rangle,$$

so $\alpha(1)^*\Lambda_\mu = \Lambda_\mu$, as Λ_μ is cyclic for A' . Hence $\alpha(1) = 1$, since Λ_μ is separating for A . \square

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 α . 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 Chapter 5.

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 define generalized versions of properties of \mathbf{B} in an arbitrary system \mathbf{A} . An instance of which will be given in the Section 2.5, where the property of interest is detailed balance.

PROPOSITION 2.4.2. *If \mathbf{A} is a system, then $\mathbf{A}\delta_\mu\mathbf{A}$, where δ_μ is the transport plan from \mathbf{A} to itself (see Proposition 1.2.5). Conversely, if \mathbf{A} and \mathbf{B} are two systems with $(A, \mu) = (B, \nu)$ such that $\mathbf{A}\delta_\mu\mathbf{B}$, then $\mathbf{A} = \mathbf{B}$, i.e. $\alpha = \beta$.*

PROOF. From the definition of the dual, it follows that

$$\delta_\mu(\alpha(a) \otimes a') = \mu(\alpha(a)a') = \mu(a\alpha'(a')) = \delta_\mu(a \otimes \alpha'(a'))$$

for all $a \in A$ and $a' \in A'$. Conversely, by the uniqueness of the dual, for all $a \in A$ and $a' \in A'$, we have

$$\begin{aligned} \mathbf{A}\delta_\mu\mathbf{B} &\implies \delta_\mu(a \otimes \alpha'(a')) = \delta_\mu(\alpha(a) \otimes a') = \delta_\mu(a \otimes \beta'(a')) \\ &\implies \alpha'(a') = \beta'(a') \\ &\implies \alpha' = \beta'. \end{aligned}$$

Thus, $\mathbf{A} = \mathbf{B}$. \square

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 the properties of \mathbf{B} . 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 a natural generalization of probability transfer involving 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 $\mu \circ \alpha = \mu$ 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 turn out to typically be asymmetric, since the two directions relate to different (though dual) aspects of dynamics.

For simplicity, in the examples of this thesis 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} .

2.5. Quantum detailed balance

In this section we discuss some points around quantum detailed balance (QDB) and related duals of dynamical maps. The origins of quantum detailed balance can be found in papers [5, 7, 26, 64, 66]. We focus on only one form of detailed balance, namely standard quantum detailed balance with respect to a reversing operation, as defined and discussed in [47, 48]. This provides background to how we connect detailed balance and Wasserstein metrics in Chapters 3 and 4.

We continue with the notational convention of previous sections, in which \mathbf{A} and \mathbf{B} denote dynamical systems. Note that the coordinates $k := (k_1, \dots, k_d)$ and $l := (l_1, \dots, l_d)$, where $k_i \in A$ and $l_i \in B$ for $i = 1, 2, \dots, d$, will not play a role in this section, since we do not yet consider Wasserstein distances.

We start with a brief review of classical detailed balance by giving its formulation in our framework through examples in finite dimensions. The most basic classical system satisfying detailed balance is given by the following:

EXAMPLE 2.5.1 (2-point system). Consider the 2-dimensional classical algebra B of complex-valued functions on a two point set. Note that in this case the von Neumann algebra is given by

$$B := \mathbb{C}^2 = \left\{ \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} : b_1, b_2 \in \mathbb{C} \right\}$$

consisting of “column vectors”, with pointwise (or entrywise) multiplication as its product and entrywise complex conjugation as the adjoint. The standard form (in the sense of Tomita-Takesaki theory) of B is

$$\pi(B) := \left\{ \begin{bmatrix} b_1 & 0 \\ 0 & b_2 \end{bmatrix} : b_1, b_2 \in \mathbb{C} \right\},$$

where $\pi : B \rightarrow \mathcal{B}(\mathbb{C}^2) \cong M_2(\mathbb{C})$ is a representation of B on \mathbb{C}^2 . We sometimes simply write B instead of $\pi(B)$. A faithful (and necessarily normal) state ν on B is represented by

$$\nu = [\nu_1 \ \nu_2] \quad \text{with } \nu_1, \nu_2 > 0,$$

i.e., $\nu(b) \equiv \nu b$ in terms of the usual matrix multiplication. The cyclic and separating vector for B is given by

$$\Lambda_\nu := \begin{bmatrix} \sqrt{\nu_1} \\ \sqrt{\nu_2} \end{bmatrix} \in B,$$

and

$$\nu(b) = \langle \Lambda_\nu, \pi(b)\Lambda_\nu \rangle = b_1\nu_1 + b_2\nu_2$$

for all $b \in B$. Furthermore, we have $\nu(1) = \nu_1 + \nu_2 = 1$ and

$$\nu(b^*b) = b^*b\nu = |b_1|^2\nu_1 + |b_2|^2\nu_2 \geq 0, \quad \forall b \in B.$$

Consider a Markov chain on B given by the transition matrix

$$(2.5.1) \quad O := \begin{bmatrix} \tilde{r} & r \\ s & \tilde{s} \end{bmatrix} \quad \text{where } r, s \in [0, 1] \quad \text{and } \tilde{r} := 1 - r, \quad \tilde{s} := 1 - s,$$

where the entries r, \tilde{r}, s and \tilde{s} are viewed as transition probabilities between the various pairs of pure states (namely the two points in the 2-point system), i.e. r is the probability for the transition from state 2 to 1, while s is for the transition from state 1 to 2, and so on. Note that the sum of entries in the same row is one, indicating that whenever a transition occurs the “particle” ends up in one of the two available states. The dynamics are expressed in terms of this Markov chain. In the Schrödinger picture, in which the time-evolution is carried by the states, we have

$$O(\nu) = \nu O = [\nu_1 \ \nu_2] \begin{bmatrix} \tilde{r} & r \\ s & \tilde{s} \end{bmatrix} = [(\tilde{r}\nu_1 + s\nu_2) \ (r\nu_1 + \tilde{s}\nu_2)].$$

In the Heisenberg picture, in which the time-evolution is carried by the observables, we have

$$\beta(b) = Ob = \begin{bmatrix} \tilde{r} & r \\ s & \tilde{s} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \begin{bmatrix} \tilde{r}b_1 + rb_2 \\ sb_1 + \tilde{s}b_2 \end{bmatrix}.$$

Note that $\beta(1) = 1$, since $r + \tilde{r} = s + \tilde{s} = 1$, and thus β is unital.

In terms of this, detailed balance is defined by

$$r\nu_1 = s\nu_2,$$

which says that the probability of flow from point 1 to point 2, is the same as from 2 to 1. Note that invariance, i.e. $\nu \circ \beta = \nu$, is satisfied precisely when the detailed balance condition holds: for all $b \in B$,

$$\begin{aligned} \nu \circ \beta(b) = \nu(b) &\iff 0 = \nu(O - 1)b \\ &\iff 0 = (s\nu_2 - r\nu_1)(b_1 - b_2) \\ &\iff r\nu_1 = s\nu_2. \end{aligned}$$

Hence we have a system $\mathbf{B} = (B, \beta, \nu)$. We interpret \mathbf{B} as a system with a single classical spin. For the dual $\mathbf{B}' = (B', \alpha', \nu')$ of \mathbf{B} we have $B' = B$, $\nu' = \nu$ and

$$0 = \beta(a)b - a\beta'(b) = \beta(a)b - \beta'(b)a = [\beta - \beta'](ab)$$

for all $a, b \in B$, by commutativity. It then follows that $\beta' = \beta$, thus $\mathbf{B}' = \mathbf{B}$ expressing detailed balance.

For classical algebras on a set of finite number of points we have the following:

EXAMPLE 2.5.2 (Classical Markov chains). 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 coordinate-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 $\mathfrak{H}_A = \mathbb{C}^m$, or simply letting A act coordinate-wise on \mathfrak{H}_A , so essentially we have A in standard form. In this case we have $A' = A$ and $j_A : A \rightarrow A$ is the identity map (see Examples 1.2.2 and 1.3.8), hence not relevant in this example. Similarly, we take the von Neumann algebra B of functions on n points to be in standard form on $\mathfrak{H}_B = \mathbb{C}^n$.

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

$$(2.5.2) \quad \alpha_{pq} \geq 0 \quad \text{and} \quad \sum_{q=1}^m \alpha_{pq} = 1,$$

and similarly for β . Note that α_{pq} is the probability for a transition to occur from point p to point q .

The states μ and ν 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 ν . These are assumed to be invariant, that is

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

in terms of the usual matrix multiplication, i.e., $\mu \circ \alpha = \mu\alpha$. Correspondingly α 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 (cf. Example 2.5.1).

In the current representation, the dual (from Section 2.2) of \mathbf{A} is the system $\mathbf{A}' = (A, \alpha', \mu)$ with α' given by

$$\alpha'_{pq} = \frac{\mu_q}{\mu_p} \alpha_{qp}, \quad \forall p, q = 1, \dots, m.$$

The latter follows from the requirement that $\mu(a\alpha'(b)) = \mu(\alpha(a)b)$ for all $a, b \in A$, which is equivalent to

$$\begin{aligned} 0 &= \sum_{p,q=1}^m \mu_p a_p \alpha'_{pq} b_q - \sum_{p,q=1}^m \mu_q \alpha_{qp} a_p b_q \\ &= \sum_{p,q=1}^m [\mu_p \alpha'_{pq} - \mu_q \alpha_{qp}] a_p b_q, \end{aligned}$$

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 $\beta' = \beta$.

We are interested in defining detailed balance conditions and extensions thereof for a quantum system \mathbf{A} . As was seen in the examples above, 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

$$(2.5.3) \quad \mathbf{A}' = \mathbf{A}.$$

However, in the quantum or abstract noncommutative setting, this condition no longer makes sense, as we have $\alpha' : A' \rightarrow A'$ as opposed to $\alpha : A \rightarrow A$, with $A' \neq A$. Therefore a direct mathematical translation of (2.5.3) 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, 26, 37, 44, 47, 48, 64, 66, 67, 73], 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 [73, 76].

There is in fact an alternative dual, the KMS-dual, of α , denoted by $\alpha^\sigma : A \rightarrow A$, which does map from A to A , giving us the system $\mathbf{A}^\sigma = (A, \alpha^\sigma, \mu)$. 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 to the general noncommutative framework. However, that does not necessarily mean that $\mathbf{A}^\sigma = \mathbf{A}$ is a physically sensible definition of quantum detailed balance (also see Example 2.5.5 in relation to this). Nevertheless, the KMS dual does appear in what are known as standard quantum detailed balance conditions, one of which is defined below in terms of reversals of systems.

DEFINITION 2.5.3. A reversible system \mathbf{A} is said to satisfy $\theta_{\mathbf{A}}$ -sqdb if

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

where $\mathbf{A}^\leftarrow := (A, \alpha^\leftarrow, \mu)$ is the reverse of \mathbf{A} and $\theta_{\mathbf{A}}$ is a reversing operation for (A, μ) given by Definition 2.2.3.

REMARKS 2.5.4. As in Section 2.2, one has $\alpha^{\leftarrow\leftarrow} := (\alpha^\leftarrow)^\leftarrow = \alpha$, and consequently $\mathbf{A}^{\leftarrow\leftarrow} := (\mathbf{A}^\leftarrow)^\leftarrow = \mathbf{A}$. In this respect note that

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

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.

EXAMPLE 2.5.5. Consider a system $\mathbf{A} = (M_n, \alpha, \mu)$ on M_n with α and μ represented directly on M_n instead of on the standard form. 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 (see Example 1.2.2). Assuming that μ is given by a diagonal density matrix and taking the reversing operation θ on M_n to be transposition (this is a standard choice), we consequently have $\alpha^{\leftarrow} = \alpha'$. In this case θ -sqdb is therefore expressed by

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

i.e., $\alpha' = \alpha$, emphasizing the similarity of θ -sqdb to the classical case (2.5.3). The condition $\mathbf{A}^\sigma = \mathbf{A}$ instead says $\theta \circ \alpha' \circ \theta = \alpha$. Essentially j_A and θ cancel in θ -sqdb.

REMARKS 2.5.6. For more on θ -sqdb, refer to [18, 47, 48]. Here we simply note that θ -sqdb can be expressed in terms of transport plans (or balance) as set out in [45, Corollary 6.7]. The same is in fact true of usual detailed balance of a Markov chain, as was discussed for example in [85, Section II] and [44, Section 3], though from a conceptually different point of view and without connecting it to ideas from optimal transport.

CHAPTER 3

Wasserstein distances

Ordinary language is too poor, it is too vague, to express relationships so delicate, so rich, and so precise. This, then, is a primary reason why the physicist cannot do without mathematics; it furnishes him with the only language he can speak.
– Henri Poincaré, 1913.

We intend to define Wasserstein distances from one dynamical system \mathbf{A} to another system \mathbf{B} in analogy to quadratic Wasserstein distance between probability measures on \mathbb{R}^d , while also taking the dynamics of the systems into account. Due to the dynamics and non-commutativity, such distances are typically not symmetric, i.e., the distances from \mathbf{B} to \mathbf{A} may differ than those from \mathbf{A} to \mathbf{B} . However, it will be seen that one can define various versions of these Wasserstein distances, including symmetric versions.

Classically, there are two broad approaches to Wasserstein distances between probability measures. The one is through transport plans, and the other by viewing transport as a dynamical process. In this thesis we consider a quantum extension of the transport approach, simultaneously extending the theory to distances between systems, rather than just states.

For a classical treatment of Wasserstein metrics of order 2 in terms of a dynamical formulation, see [12], and for the corresponding non-commutative version, or quantum Wasserstein metrics see [23, 24, 25]. In some other approaches to Wasserstein distances via transport plans (in the special case of states, rather than systems), $W(\mu, \mu) = 0$ and the usual triangle inequality are not obtained. See for example [54] and [36], even though the latter follows a similar approach to cost as in this thesis. It should be noted that these papers nevertheless manage to make progress on their applications, and indeed [51] has pointed out that a lack of the usual metric properties is actually of some 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]. In our approach, however, the triangle inequality holds even for Wasserstein distances between systems.

In Section 3.1 we formulate the cost of a transport plan between systems, as well as define the quadratic Wasserstein distance functions.

The rest of the chapter is dedicated to proving the metric properties of these distance functions with the triangle inequality demonstrated in Section 3.2 and symmetry in Section 3.3. We conclude the chapter with a discussion of the metric properties in Section 3.4

We continue with the notation from Sections 2.2 and 2.3, again fixing Υ , the Z_ν 's, and d for all systems to be considered.

3.1. Cost of transport

In this section we give a noncommutative formulation of the cost of a transport plan between systems, and also introduce the quadratic Wasserstein distance functions. As we only consider the quadratic case in this thesis, we henceforth simply refer to Wasserstein distances (should they not yet be shown to be metrics) and Wasserstein metrics.

A more rigorous formulation of cost for transport, containing the *ansatz* cost in (2.3.3) as a special case, is given below making use of the Choi-Jamiołkowski duality (see Proposition 2.3.8). The channel E_ω corresponding to a transport plan $\omega \in T(\mathbf{A}, \mathbf{B})$, defined in Section 2.3, allows us to define transport cost while avoiding the complications due to unboundedness of the Tomita operator S_ν :

DEFINITION 3.1.1. Let \mathbf{A} and \mathbf{B} be two systems, then the *cost* of a transport plan $\omega \in T(\mathbf{A}, \mathbf{B})$ is defined as

$$(3.1.1) \quad I_{\mathbf{A}, \mathbf{B}}(\omega) := \sum_{i=1}^d [\mu(k_i^* k_i) + \nu(l_i^* l_i) - \nu(E_\omega(k_i)^* l_i) - \nu(l_i^* E_\omega(k_i))],$$

in terms of the coordinate systems $k := (k_1, \dots, k_d)$ and $l := (l_1, \dots, l_d)$ of \mathbf{A} and \mathbf{B} , respectively.

REMARKS 3.1.2. To apply this in practice and particular examples, one should keep in mind that the k and l appearing in the cost function, and ultimately in Wasserstein distances, 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 (2.3.3) to have a sensible physical meaning.

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 (2.3.3). But unlike the latter, (3.1.1) only refers to bounded operators, thus avoiding complications even when some $S_\nu l_i^* S_\nu$'s are unbounded.

An important formula related to cost of transport, expressed in terms of the representation machinery built in Section 1.2, in particular (1.2.10) and (1.2.11), is the following:

PROPOSITION 3.1.3. For all $\omega \in T(\mu, \nu)$, $a \in A$ and $b \in B$,

$$\|\pi_\mu^\omega(a)\Omega - \pi_\nu^\omega(b)\Omega\|_\omega^2 = \mu(a^*a) + \nu(b^*b) - \nu(E_\omega(a)^*b) - \nu(b^*E_\omega(a))$$

where $\|\cdot\|_\omega$ is the norm of the Hilbert space \mathfrak{H}_ω .

PROOF. Let $\omega \in T(\mu, \nu)$, $a \in A$ and $b \in B$, then

$$\begin{aligned} \|\pi_\mu^\omega(a)\Omega - \pi_\nu^\omega(b)\Omega\|_\omega^2 &= \langle \pi_\mu^\omega(a)\Omega, \pi_\mu^\omega(a)\Omega \rangle_\omega + \langle \pi_\nu^\omega(b)\Omega, \pi_\nu^\omega(b)\Omega \rangle_\omega \\ &\quad - \langle \pi_\mu^\omega(a)\Omega, \pi_\nu^\omega(b)\Omega \rangle_\omega - \langle \pi_\nu^\omega(b)\Omega, \pi_\mu^\omega(a)\Omega \rangle_\omega. \end{aligned}$$

We evaluate each of the terms above in turn. By the coupling property of ω , we have

$$\begin{aligned} \langle \pi_\mu^\omega(a)\Omega, \pi_\mu^\omega(a)\Omega \rangle_\omega &= \langle \pi_\omega(a \otimes 1)\Omega, \pi_\omega(a \otimes 1)\Omega \rangle_\omega \\ &= \langle \Omega, \pi_\omega(a^*a \otimes 1)\Omega \rangle_\omega \\ &= \omega(a^*a \otimes 1) \\ &= \mu(a^*a), \end{aligned}$$

and

$$\begin{aligned} \langle \pi_\nu^\omega(b)\Omega, \pi_\nu^\omega(b)\Omega \rangle_\omega &= \langle \pi_\omega(1 \otimes b)\Omega, \pi_\omega(1 \otimes b)\Omega \rangle_\omega \\ &= \langle \Omega, \pi_\omega(1 \otimes b^*b)\Omega \rangle_\omega \\ &= \omega(1 \otimes b^*b) \\ &= \nu(b^*b). \end{aligned}$$

Making use of the projection P_ν of \mathfrak{H}_ω onto \mathfrak{H}_ν^ω , we have

$$\begin{aligned} \langle \pi_\mu^\omega(a)\Omega, \pi_\nu^\omega(b)\Omega \rangle_\omega &= \langle \pi_\mu^\omega(a)\Omega, P_\nu \pi_\nu^\omega(b)\Omega \rangle_\omega \\ &= \langle \pi_\mu^\omega(a)\Omega, P_\nu [u_\nu b u_\nu^*] \Omega \rangle_\omega \\ &= \langle u_\nu^* P_\nu \pi_\mu^\omega(a) u_\nu [u_\nu^* \Omega], b [u_\nu^* \Omega] \rangle_\omega \\ &= \langle u_\nu^* P_\nu \pi_\mu^\omega(a) u_\nu \Lambda_\nu, b \Lambda_\nu \rangle \\ &= \langle E_\omega(a) \Lambda_\nu, b \Lambda_\nu \rangle \\ &= \langle \Lambda_\nu, E_\omega(a)^* b \Lambda_\nu \rangle \\ &= \nu(E_\omega(a)^* b), \end{aligned}$$

by Theorem 2.3.7, from which we get

$$\begin{aligned} \langle \pi_\nu^\omega(b)\Omega, \pi_\mu^\omega(a)\Omega \rangle_\omega &= \overline{\langle \pi_\mu^\omega(a)\Omega, \pi_\nu^\omega(b)\Omega \rangle_\omega} \\ &= \overline{\nu(E_\omega(a)^* b)} \\ &= \nu(b^* E_\omega(a)). \end{aligned}$$

□

REMARKS 3.1.4. It follows that an equivalent, but more suggestive formulation of cost of transport, in terms of the cyclic representations $(\mathfrak{H}_\mu^\omega, \pi_\mu^\omega, \Omega)$ and $(\mathfrak{H}_\nu^\omega, \pi_\nu^\omega, \Omega)$ of (A, μ) and (B, ν) , respectively, inherited

as in (1.2.10) and (1.2.11) from a cyclic representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega)$ of $(A \odot B', \omega)$, is

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

where we have written

$$\pi_\mu^\omega(k)\Omega \equiv (\pi_\mu^\omega(k_1)\Omega, \dots, \pi_\mu^\omega(k_d)\Omega) \in \bigoplus_{i=1}^d \mathfrak{H}_\omega,$$

while $\|\cdot\|_{\oplus\omega}$ denotes the norm of $\bigoplus_{i=1}^d \mathfrak{H}_\omega$, i.e.

$$I_{\mathbf{A}, \mathbf{B}}(\omega) = \sum_{i=1}^d \left\| \pi_\mu^\omega(k_i)\Omega - \pi_\nu^\omega(l_i)\Omega \right\|_\omega^2.$$

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 $I_{\mathbf{A}, \mathbf{B}}(\omega)$ along with the relative tensor products. On the other hand, (3.1.1) is useful in relation to symmetry, as well as the consequences of zero Wasserstein distance in Chapter 4.

With the transport cost in hand, we can now define Wasserstein distances from one system to another. The cost $I_{\mathbf{A}, \mathbf{B}}(\omega)$ does not depend directly on the dynamical maps α and β , but they do 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. The specific distance functions we study in this thesis, will collectively be called *Wasserstein distances*.

DEFINITION 3.1.5. Given a set \mathfrak{A} of systems as in Section 2.2, we define the *Wasserstein distance* W on \mathfrak{A} by

$$(3.1.2) \quad W(\mathbf{A}, \mathbf{B}) := \inf_{\omega \in T(\mathbf{A}, \mathbf{B})} I_{\mathbf{A}, \mathbf{B}}(\omega)^{1/2},$$

the *modular Wasserstein distance* W_σ on \mathfrak{A} by

$$(3.1.3) \quad W_\sigma(\mathbf{A}, \mathbf{B}) := \inf_{\omega \in T_\sigma(\mathbf{A}, \mathbf{B})} I_{\mathbf{A}, \mathbf{B}}(\omega)^{1/2},$$

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

$$(3.1.4) \quad W_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) := \inf_{\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})} I_{\mathbf{A}, \mathbf{B}}(\omega)^{1/2},$$

for all $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, in terms of Definitions 2.3.4 and 3.1.1.

These are also called Wasserstein distances of order 2, or quadratic Wasserstein distances. Since we focus exclusively on the quadratic case in this thesis, we do not include a subscript 2 as is standard in the classical case.

DEFINITION 3.1.6. Given $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, 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 $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$. Correspondingly for W and W_{σ} .

LEMMA 3.1.7 (Existence of optimal transport plans). *Optimal transport plans always exist for the Wasserstein distances W , W_{σ} and $W_{\sigma\sigma}$.*

PROOF. We prove it for $W_{\sigma\sigma}$. The other cases are similar but simpler. Without loss (see for example [39, 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. By the definition of $W_{\sigma\sigma}$ 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 $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ due to compactness. As a result, ω 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 $i = 1, \dots, d$, where $l_i \in B$ with $l = (l_1, \dots, l_d)$ a coordinate system for \mathbf{B} , as $B' \Lambda_{\nu}$ is dense in \mathfrak{H}_{ν} . 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 using (3.1.1) and (2.3.5), we find

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

Consequently,

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

for all $\varepsilon > 0$. □

This lemma is of some independent interest, since it says that the Wasserstein distance is always reached by some transport plan. We note that optimal transport plans in general need not be unique.

EXAMPLE 3.1.8. In (3.1.1), 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 [80] and [81, Theorem IX.4.2]. Then ω_F defined from E_F through (2.3.5) 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 μ is tracial, in particular when A is abelian, in which case σ^μ is trivial and the condition $\sigma_t^\mu(F) = F$ is automatically satisfied.

We remind the reader of some terminology:

DEFINITION 3.1.9 (Metric space; metric). A *metric space* is a pair (X, d) , where X is a set and $d : X \times X \rightarrow \mathbb{R}$ is a distance function (or *metric*) on X , i.e. for all $x, y, z \in X$ we have

- (M1) $d : X \times X \rightarrow [0, \infty)$ (Non-negativity)
- (M2) $d(x, z) \leq d(x, y) + d(y, z)$ (Triangle inequality)
- (M3) $d(x, y) = d(y, x)$ (Symmetry)
- (M4) $x = y \implies d(x, y) = 0$ (Definiteness)
- (M5) $d(x, y) = 0 \implies x = y$ (Faithfulness).

The following table defines some related terminology:

	(M1)	(M2)	(M3)	(M4)	(M5)
Metric	✓	✓	✓	✓	✓
Pseudo-metric	✓	✓	✓	✓	×
Asymmetric metric	✓	✓	×	✓	✓
Asymmetric pseudometric	✓	✓	×	✓	×

The Wasserstein functions W , W_σ and $W_{\sigma\sigma}$ are real and non-negative:

PROPOSITION 3.1.10. For all $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$ and $\omega \in T(\mathbf{A}, \mathbf{B})$, we have that $I_{\mathbf{A}, \mathbf{B}}(\omega) \geq 0$. Consequently,

$$0 \leq W(\mathbf{A}, \mathbf{B}) \leq W_\sigma(\mathbf{A}, \mathbf{B}) \leq W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$$

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

PROOF. That $I_{\mathbf{A}, \mathbf{B}}(\omega) \geq 0$ follows directly from Proposition 3.1.3 and Remarks 3.1.4. Alternatively, since by Kadison's inequality $E_\omega(a^*a) \geq E_\omega(a)^*E_\omega(a)$, we have

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

for all $a \in A$ and $b \in B$. The required result then follows, since

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

□

In the rest of the sections of this chapter we proceed to prove the main metric properties of the distance functions W , W_σ and $W_{\sigma\sigma}$. The proofs are similar to those appearing in [41] and [42, Section 3] for systems on the same von Neumann algebra. Much of the framework of [41] 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.

3.2. The triangle inequality

In this section we intend to show that the Wasserstein functions W , W_σ and $W_{\sigma\sigma}$ satisfy the triangle inequality. To do this we make use of the natural bimodule structure of the GNS Hilbert spaces \mathfrak{H}_ω and \mathfrak{H}_ψ of the transport plans ω and ψ , respectively, and their relative tensor product

$$\mathfrak{H} := \mathfrak{H}_\omega \otimes_\nu \mathfrak{H}_\psi.$$

Denote the cyclic representations of $(A \odot B', \omega)$ and $(B \odot C', \psi)$ by $(\mathfrak{H}_\omega, \pi_\omega, \Omega)$ and $(\mathfrak{H}_\psi, \pi_\psi, \Psi)$, respectively. As in (1.2.10) and (1.2.11), denote the cyclic representations that the pairs (A, μ) and (B, ν) inherit by restriction from that of $(A \odot B', \omega)$ by $(\mathfrak{H}_\mu^\omega, \pi_\mu^\omega, \Omega)$ and $(\mathfrak{H}_\nu^\omega, \pi_\nu^\omega, \Omega)$, respectively. Similarly, $(\mathfrak{H}_\nu^\psi, \pi_\nu^\psi, \Psi)$ and $(\mathfrak{H}_\xi^\psi, \pi_\xi^\psi, \Psi)$ denote the cyclic representations of (B, ν) and (C, ξ) , respectively, inherited from that of $(B \odot C', \psi)$.

PROPOSITION 3.2.1. *For $\omega \in T(\mu, \nu)$, consider the cyclic representation $(\mathfrak{H}_\omega, \pi_\omega, \Omega)$ of $(A \odot B', \omega)$. Then \mathfrak{H}_ω is an A - B bimodule with the structure given by*

$$\pi_{\mathfrak{H}_\omega}(a) := \pi_\omega(a \otimes 1) \big|_{\mathfrak{H}_\mu^\omega} \quad \text{and} \quad \pi'_{\mathfrak{H}_\omega}(b) := \pi_\omega(1 \otimes j_B(b)) \big|_{\mathfrak{H}_\nu^\omega}$$

and writing

$$axb := \pi_{\mathfrak{H}_\omega}(a)\pi'_{\mathfrak{H}_\omega}(b)x = \pi_\omega(a \otimes j_B(b))x,$$

for all $a \in A$, $b \in B$ and $x \in \mathfrak{H}_\omega$.

PROOF. Since π_ω is a unital $*$ -homomorphism, it follows that the map

$$\pi_{\mathfrak{H}_\omega} : A \rightarrow \mathcal{B}(\mathfrak{H}_\omega) : a \mapsto \pi_\omega(a \otimes 1)$$

is also a unital $*$ -homomorphism, and it is normal by [11, Theorem 3.3]. Thus \mathfrak{H}_ω is a left A -module. Similarly, the map

$$\pi'_{\mathfrak{H}_\omega} : B \rightarrow \mathcal{B}(\mathfrak{H}_\omega) : b \mapsto \pi_\omega(1 \otimes j_B(b))$$

is a normal unital $*$ -anti-homomorphism, from which it follows that \mathfrak{H}_ω is a right B -module. Finally,

$$\begin{aligned} a(xb) &= \pi_{\mathfrak{H}_\omega}(a)\pi'_{\mathfrak{H}_\omega}(b)x \\ &= \pi_\omega(a \otimes 1)\pi_\omega(1 \otimes j_B(b))x \\ &= \pi_\omega(1 \otimes j_B(b))\pi_\omega(a \otimes 1)x \\ &= \pi'_{\mathfrak{H}_\omega}(b)\pi_{\mathfrak{H}_\omega}(a)x \\ &= (ax)b, \end{aligned}$$

for all $a \in A$, $b \in B$ and $x \in \mathfrak{H}_\omega$. □

The correspondence between channels and transport plans allows us to compose transport plans $\omega \in T(\mu, \nu)$ and $\psi \in T(\nu, \xi)$ to obtain a transport plan $\omega \circ \psi \in T(\mu, \xi)$ defined through

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

Of interest is how this transport plan is related to the relative tensor product of the A - B and B - C bimodules \mathfrak{H}_{ω} and \mathfrak{H}_{ψ} , respectively. So we set

$$\varphi := \omega \circ \psi$$

and consider the relative tensor product $\mathfrak{H} = \mathfrak{H}_{\omega} \otimes_{\nu} \mathfrak{H}_{\psi}$. The relative tensor product \mathfrak{H} is itself an A - C bimodule, and contains the vector

$$(3.2.1) \quad \Phi := \Omega \otimes_{\nu} \Psi$$

which can be taken as the cyclic vector in the representation $(\mathfrak{H}_{\varphi}, \pi_{\varphi}, \Phi)$ of $(A \odot C', \varphi)$. This representation can be obtained from the bimodule \mathfrak{H} using the not necessarily cyclic representation π of $A \odot C'$ defined through

$$\pi(a \otimes c')z := azj_C(c'), \quad \forall z \in \mathfrak{H}.$$

By restriction one then obtains that

$$(3.2.2) \quad \mathfrak{H}_{\varphi} := \overline{\pi(A \odot C')\Phi} \subset \mathfrak{H} \quad \text{and} \quad \pi_{\varphi}(t) := \pi(t)|_{\mathfrak{H}_{\varphi}}, \quad \forall t \in A \odot C'.$$

That this indeed provides a cyclic representation for $(A \odot C', \varphi)$, follows from [44, Corollary 5.7]. In turn this induces a cyclic representation $(\mathfrak{H}_{\mu}^{\varphi}, \pi_{\mu}^{\varphi}, \Phi)$ of (A, μ) by setting

$$(3.2.3) \quad \mathfrak{H}_{\mu}^{\varphi} := \overline{\pi_{\varphi}(A \odot 1)\Phi} \quad \text{and} \quad \pi_{\mu}^{\varphi}(a) := \pi_{\varphi}(a \otimes 1)|_{\mathfrak{H}_{\mu}^{\varphi}}, \quad \forall a \in A.$$

Similarly,

$$(3.2.4) \quad \mathfrak{H}_{\xi}^{\varphi} := \overline{\pi_{\varphi}(1 \odot C')\Phi} \quad \text{and} \quad \pi_{\xi}^{\varphi}(c') := \pi_{\varphi}(1 \otimes c')|_{\mathfrak{H}_{\xi}^{\varphi}}, \quad \forall c' \in C',$$

gives a cyclic representation $(\mathfrak{H}_{\xi}^{\varphi}, \pi_{\xi}^{\varphi}, \Phi)$ of (C', ξ') .

The main technical point in proving the triangle inequality is the following lemma, which is a key (and we presume well-known) feature of the quotient construction of the relative tensor product. An embedding is a structure-preserving map that allows one space to be represented within another; in the case of Hilbert spaces, this map is an injective isometry. In this context, the embeddings of \mathfrak{H}_{ν} into \mathfrak{H}_{ω} and \mathfrak{H}_{ψ} respectively are identified in the relative tensor product $\mathfrak{H} = \mathfrak{H}_{\omega} \otimes_{\nu} \mathfrak{H}_{\psi}$. This is precisely the reason that the relative tensor product is the natural setting to prove the triangle inequality.

LEMMA 3.2.2. *Let $\omega \in T(\mu, \nu)$, $\psi \in T(\nu, \xi)$ and $\mathfrak{H} = \mathfrak{H}_{\omega} \otimes_{\nu} \mathfrak{H}_{\psi}$. Then*

$$(3.2.5) \quad \iota_{\omega}(\pi_{\nu}^{\omega}(b)\Omega) = \iota_{\psi}(\pi_{\nu}^{\psi}(b)\Psi), \quad \forall b \in B,$$

where $\iota_{\omega} : \mathfrak{H}_{\omega} \rightarrow \mathfrak{H} : x \mapsto x \otimes_{\nu} \Psi$ and $\iota_{\psi} : \mathfrak{H}_{\psi} \rightarrow \mathfrak{H} : y \mapsto \Omega \otimes_{\nu} y$ are the embeddings of \mathfrak{H}_{ω} and \mathfrak{H}_{ψ} into \mathfrak{H} , respectively.

PROOF. Given any $b \in B$, write $x = \pi_\nu^\omega(b)\Omega \in \mathfrak{H}_\omega$ and $y = \pi_\nu^\psi(b)\Psi \in \mathfrak{H}_\psi$. From the definition of $L_\nu(x)$ (see (1.5.1)), we find that

$$L_\nu(x) = \pi_\nu^\omega(b)u_\nu$$

in terms of the unitary operator u_ν given by (1.2.12), since for any $d \in B$, using $\pi_\nu^\omega(b') = u_\nu b' u_\nu^*$, we have

$$\begin{aligned} L_\nu(x)\eta'_\nu(d) &= \pi'_{\mathfrak{H}}(d)x \\ &= \pi_\omega(1 \otimes j_B(d))x \\ &= \pi_\nu^\omega(j_B(d))\pi_\nu^\omega(b)\Omega \\ &= \pi_\nu^\omega(b)\pi_\nu^\omega(j_B(d))\Omega \\ &= \pi_\nu^\omega(b)u_\nu j_B(d)\Lambda_\nu \\ &= \pi_\nu^\omega(b)u_\nu J_B d^* \Lambda_\nu \\ &= \pi_\nu^\omega(b)u_\nu \eta'_\nu(d). \end{aligned}$$

Hence, $L_\nu(x)^*L_\nu(x) = u_\nu^*\pi_\nu^\omega(b^*b)u_\nu = b^*b$, $L_\nu(\Omega)^*L_\nu(x) = 1^*b = b$, etc. From the bilinear form used in the quotient construction of the relative tensor product (see [81, Proposition IX.3.15 and Definition IX.3.16]), and using the left B -module structure of \mathfrak{H}_ψ , one finds that

$$\begin{aligned} \|\iota_\omega(x) - \iota_\psi(y)\|_{\mathfrak{H}}^2 &= \langle \iota_\omega(x), \iota_\omega(x) \rangle - \langle \iota_\omega(x), \iota_\omega(y) \rangle - \langle \iota_\omega(y), \iota_\omega(x) \rangle \\ &\quad + \langle \iota_\omega(y), \iota_\omega(y) \rangle \\ &= \langle x \otimes_\nu \Psi, x \otimes_\nu \Psi \rangle - \langle x \otimes_\nu \Psi, \Omega \otimes_\nu y \rangle \\ &\quad - \langle \Omega \otimes_\nu y, x \otimes_\nu \Psi \rangle + \langle \Omega \otimes_\nu y, \Omega \otimes_\nu y \rangle \\ &= \langle \Psi, L_\nu(x)^*L_\nu(x)\Psi \rangle_\psi - \langle \Psi, L_\nu(x)^*L_\nu(\Omega)y \rangle_\psi \\ &\quad - \langle y, L_\nu(\Omega)^*L_\nu(x)\Psi \rangle_\psi + \langle y, L_\nu(\Omega)^*L_\nu(\Omega)y \rangle_\psi \\ &= \langle \Psi, b^*b\Psi \rangle_\psi - \langle \Psi, b^*y \rangle_\psi - \langle y, b\Psi \rangle_\psi + \langle y, y \rangle_\psi \\ &= \langle \Psi, b^*b\Psi \rangle_\psi - \langle \Psi, b^*\pi_\nu^\psi(b)\Psi \rangle_\psi \\ &\quad - \langle \pi_\nu^\psi(b)\Psi, b\Psi \rangle_\psi + \langle \pi_\nu^\psi(b)\Psi, \pi_\nu^\psi(b)\Psi \rangle_\psi \\ &= \langle \Psi, b^*b\Psi \rangle_\psi - \langle b\Psi, b\Psi \rangle_\psi - \langle \Psi, b^*b\Psi \rangle_\psi + \langle b\Psi, b\Psi \rangle_\psi \\ &= 0, \end{aligned}$$

since $\langle b^*b\Psi, \Psi \rangle_\psi = \langle \pi_\psi(b^*b \otimes 1_C)\Psi, \Psi \rangle_\psi$, etc. \square

The second fact we need is the following lemma.

LEMMA 3.2.3. *Let $\omega \in T(\mu, \nu)$, $\psi \in T(\nu, \xi)$ and $\mathfrak{H} := \mathfrak{H}_\omega \otimes_\nu \mathfrak{H}_\psi$. If $\varphi = \omega \circ \psi$ (defined via $E_\varphi = E_\psi \circ E_\omega$ as in Section 2.3), then*

$$(3.2.6) \quad \iota_\omega(\pi_\mu^\omega(a)\Omega) = \pi_\mu^\varphi(a)\Phi, \quad \forall a \in A,$$

and

$$(3.2.7) \quad \iota_\psi(\pi_\xi^\psi(c)\Psi) = \pi_\xi^\varphi(c)\Phi, \quad \forall c \in C,$$

with $\Phi = \Omega \otimes_\nu \Psi$ as in (3.2.1).

PROOF. Let $x \in \mathfrak{H}_\mu^\omega \subset \mathfrak{H}_\omega$. Then, for all $a \in A$, we have

$$\begin{aligned} \iota_\omega (\pi_\mu^\omega(a)x) &= [\pi_\mu^\omega(a)x] \otimes_\nu \Psi \\ &= [\pi_\omega(a \otimes 1)x] \otimes_\nu \Psi \\ &= ax \otimes_\nu \Psi \\ &= \pi_\varphi(a \otimes 1) (x \otimes_\nu \Psi) \\ &= \pi_\mu^\varphi(a) (x \otimes_\nu \Psi) \end{aligned}$$

by (3.2.3). In particular, we have $\iota_\omega (\pi_\mu^\omega(a)\Omega) = \pi_\mu^\varphi(a)\Phi$, for all $a \in A$.

Let $w_\xi : \mathfrak{H}_\xi^\psi \rightarrow \mathfrak{H}_\xi^\varphi$ be the unitary equivalence of the cyclic representations $(\mathfrak{H}_\xi^\psi, \pi_{\xi'}^\psi, \Psi)$ and $(\mathfrak{H}_\xi^\varphi, \pi_{\xi'}^\varphi, \Phi)$ of (C', ξ') given by $w_\xi c' \Psi := \pi_{\xi'}^\varphi(c')\Phi$, for all $c' \in C'$ (cf. (1.2.12)). Consider the modular conjugations J_C^ψ and J_C^φ associated to (ψ, Ψ) and (φ, Φ) , respectively, but restricted to the von Neumann algebra C . Then $J_C^\varphi = w_\xi J_C^\psi w_\xi^*$, from which it follows that

$$\pi_\xi^\psi = j_C^\psi \circ \pi_{\xi'}^\psi \circ j_C^\varphi$$

where $j_C^\psi := J_C^\psi(\cdot)^* J_C^\psi$ and $j_C^\varphi := J_C^\varphi(\cdot)^* J_C^\varphi$ are defined on $\mathcal{B}(\mathfrak{H}_\nu^\psi)$ and $\mathcal{B}(\mathfrak{H}_\nu^\varphi)$ respectively. Furthermore, we have

$$\begin{aligned} w_\xi \pi_{\xi'}^\psi(c') \Psi &= \pi_{\xi'}^\varphi(c') \Phi \\ &= \pi_\varphi(1 \otimes c') \Phi \\ &= \Phi j_C(c') \\ &= \Omega \otimes_\nu [\Psi j_C(c')] \\ &= \Omega \otimes_\nu [\pi_\psi(1 \otimes c') \Psi] \\ &= \Omega \otimes_\nu [\pi_{\xi'}^\psi(c') \Psi] \end{aligned}$$

for all $c' \in C'$, by (3.2.3). It follows that $w_\xi y = \Omega \otimes_\nu y$, and

$$\begin{aligned} J_C^\varphi(\Omega \otimes_\nu y) &= w_\xi J_C^\psi w_\xi^*(\Omega \otimes_\nu y) \\ &= w_\xi J_C^\psi y \\ &= \Omega \otimes_\nu J_C^\psi y \end{aligned}$$

for all $y \in \mathfrak{H}_\xi^\psi$. Consequently,

$$\begin{aligned} \iota_\psi (\pi_\xi^\psi(c)y) &= \Omega \otimes_\nu [\pi_\xi^\psi(c)y] \\ &= \Omega \otimes_\nu [J_C^\psi \pi_{\xi'}^\psi(j_C(c^*)) J_C^\psi y] \\ &= J_C^\varphi [\Omega \otimes_\nu \pi_\psi(1 \otimes j_C(c^*)) J_C^\psi y] \\ &= J_C^\varphi [\Omega \otimes_\nu (J_C^\psi y) c^*] \end{aligned}$$

for all $c \in C$ and $y \in \mathfrak{H}_\xi^\psi$. In particular, we have

$$\begin{aligned} \iota_\psi \left(\pi_\xi^\psi(c) \Psi \right) &= J_C^\varphi [\Phi c^*] \\ &= J_C^\varphi \pi_\varphi(1 \otimes j_C(c^*)) \Phi \\ &= J_C^\varphi \pi_\xi^\varphi(j_C(c^*)) J_C^\varphi \Phi \\ &= \pi_\xi^\varphi(c) \Phi, \end{aligned}$$

for all $c \in C$. □

PROPOSITION 3.2.4. *For all $\mathbf{A}, \mathbf{B}, \mathbf{C} \in \mathfrak{A}$,*

$$W_{\sigma\sigma}(\mathbf{A}, \mathbf{C}) \leq W_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) + W_{\sigma\sigma}(\mathbf{B}, \mathbf{C}).$$

Similarly for W and W_σ .

PROOF. We prove it for $W_{\sigma\sigma}$. The other cases are similar but simpler. 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 $E_{\omega \circ \psi} := E_\psi \circ E_\omega$. Since

$$\begin{aligned} E_\varphi \circ \alpha_{v,z} &= E_\psi \circ E_\omega \circ \alpha_{v,z} \\ &= E_\psi \circ \beta_{v,z} \circ E_\omega \\ &= \gamma_{v,z} \circ E_\psi \circ E_\omega \\ &= \gamma_{v,z} \circ E_\varphi, \end{aligned}$$

it follows that $\mathbf{A}\varphi\mathbf{C}$, by (2.3.8). Similarly, $\mathbf{A}^\sigma\varphi\mathbf{C}^\sigma$ and $(A, \sigma^\mu, \mu)\varphi(B, \sigma^\xi, \xi)$. Together, we get $\varphi \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{C})$. Using Remarks 3.1.4, and applying ι_ω and ι_ψ componentwise to elements of direct sums, we have

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

where we employed the triangle inequality in $\left(\bigoplus_{i=1}^d \mathfrak{H}, \|\cdot\|_{\oplus\mathfrak{H}} \right)$, applied Lemmas 3.2.2 and 3.2.3, and used the fact that ι_ω and ι_ψ preserve the inner products. 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. □

Note that the role of $\mathfrak{H}_\omega \otimes_\nu \mathfrak{H}_\psi$ is to ensure that the “middle term” coming from the difference between $\pi_\nu^\omega(l) \Omega$ and $\pi_\nu^\psi(l) \Psi$ via embedding

into $\bigoplus_{i=1}^d (\mathfrak{H}_\omega \otimes_\nu \mathfrak{H}_\psi)$, indeed disappears. Exactly this point of the triangle inequality tends to run astray in other transport plan based approaches to the Wasserstein distance. See in particular [36], which in turn built on [54]; also see [55, Footnote 4].

3.3. Symmetry

To obtain symmetry of a Wasserstein distance, we are going to use a restricted set of transport plans from one system to another. This is where the modular balance condition of the allowed transport plans becomes important. A suitable path to symmetry is provided by KMS-duals. We note that only $W_{\sigma\sigma}$ is symmetric, while W and W_σ are typically asymmetric, because KMS-duals play a key role in the proof.

Note that there is an asymmetry between $\mathbf{A}\omega\mathbf{B}$ and $\mathbf{B}\omega'\mathbf{A}$, since these conditions relate to two different properties satisfied by \mathbf{A} , namely

$$(3.3.1) \quad \mu \circ \alpha = \mu \quad \text{and} \quad \alpha(1) = 1,$$

(see Section 2.4, in particular 2.4.1). This boils down to $\mathbf{A}\omega\mathbf{B}$ being equivalent to $\mathbf{B}'\omega'\mathbf{A}'$, by Proposition 2.3.11, 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 $W(\mathbf{A}, \mathbf{B}) = W(\mathbf{B}, \mathbf{A})$.

We have the following properties of dual transport plans:

PROPOSITION 3.3.1. *Let $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$.*

(1) *For all $\omega \in T(\mathbf{A}, \mathbf{B})$, we have*

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

If, in addition, $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$ are reversible then

$$\omega \in T_\sigma(\mathbf{A}, \mathbf{B}) \iff \omega^\leftarrow \in T_\sigma(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow)$$

(2) *For all $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$, we have*

$$\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) \iff \omega' \in T_{\sigma\sigma}(\mathbf{B}', \mathbf{A}') \iff \omega^\sigma \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$$

If, in addition, $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$ are reversible then

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

PROOF. For any $\omega \in T(\mu, \nu)$, we have

$$\omega' \in T(\nu', \mu') \quad \text{and} \quad \omega^\sigma, \omega^\leftarrow \in T(\nu, \mu)$$

for all $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, by Proposition 2.3.10.

(1) It follows from Proposition 2.1.8 that

$$\begin{aligned}
E_\omega^\sigma \circ (\sigma_t^\nu)^\sigma &= (\sigma_t^\mu)^\sigma \circ E_\omega^\sigma \iff (E_\omega \circ \sigma_t^\mu)^\sigma = (\sigma_t^\nu \circ E_\omega)^\sigma \\
&\iff E_\omega \circ \sigma_t^\mu = \sigma_t^\nu \circ E_\omega \\
&\iff (E_\omega \circ \sigma_t^\mu)' = (\sigma_t^\nu \circ E_\omega)' \\
&\iff E_\omega' \circ (\sigma_t^\nu)' = (\sigma_t^\mu)' \circ E_\omega' \\
&\iff E_\omega' \circ \sigma_t^{\nu'} = \sigma_t^{\mu'} \circ E_\omega',
\end{aligned}$$

for all $t \in \mathbb{R}$, where the last equivalence follows by Proposition 2.1.10. Thus, for all $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, we have

$$\omega \in T_\sigma(\mathbf{A}, \mathbf{B}) \iff \omega' \in T_\sigma(\mathbf{B}', \mathbf{A}') \iff \omega^\sigma \in T_\sigma(\mathbf{B}^\sigma, \mathbf{A}^\sigma)$$

by Propositions 2.2.5, and 2.3.11(1). For reversible systems $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, we further have

$$\omega \in T_\sigma(\mathbf{A}, \mathbf{B}) \iff \omega^{\leftarrow} \in T_\sigma(\mathbf{B}^{\leftarrow}, \mathbf{A}^{\leftarrow}),$$

by Proposition 2.3.11(2).

(2) The following equivalence relations hold

$$\mathbf{A}^\sigma \omega \mathbf{B}^\sigma \iff (\mathbf{B}^\sigma)' \omega' (\mathbf{A}^\sigma)' \iff (\mathbf{B}')^\sigma \omega' (\mathbf{A}')^\sigma$$

and

$$\mathbf{A}^\sigma \omega \mathbf{B}^\sigma \iff (\mathbf{B}^\sigma)^\sigma \omega^\sigma (\mathbf{A}^\sigma)^\sigma \iff \mathbf{B} \omega^\sigma \mathbf{A},$$

for all $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$, by Propositions 2.3.11 and 2.2.5. Hence,

$$\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) \iff \omega' \in T_{\sigma\sigma}(\mathbf{B}', \mathbf{A}') \iff \omega^\sigma \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{A}),$$

by the definition of KMS-duals and Proposition 2.3.10. For reversible systems $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, we further have that $\omega^{\leftarrow} = \omega^\sigma$, again by Proposition 2.3.11. The required result then follows. \square

PROPOSITION 3.3.2. *For $\omega \in T(\mathbf{A}, \mathbf{B})$, the following statements are equivalent:*

- (1) $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$.
- (2) $K_\omega \Delta_\mu^{it} = \Delta_\nu^{it} K_\omega, \forall t \in \mathbb{R}$.
- (3) $K_\omega J_A = J_B K_\omega$.
- (4) $\mu(a E_\omega^\sigma(b)) = \nu(E_\omega(a)b) \forall a \in A, b \in B$.

PROOF. Let (A, μ) and (B, ν) be in standard form on Hilbert spaces \mathfrak{H}_μ and \mathfrak{H}_ν , respectively. For $\omega \in T(\mu, \nu)$, denote by K_ω the Hilbert space representation of the unique map E_ω such that $\nu \circ E_\omega = \mu$ as in Lemma 2.1.5.

(1) \implies (2): By (2.3.8), we have $E_\omega \circ \sigma_t^\mu = \sigma_t^\nu \circ E_\omega$, for all $t \in \mathbb{R}$, since $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$. Then

$$\begin{aligned} K_\omega \Delta_\mu^{it} a \Lambda_\mu &= K_\omega \sigma_t^\mu(a) \Lambda_\mu \\ &= E_\omega(\sigma_t^\mu(a)) \Lambda_\nu \\ &= \sigma_t^\nu(E_\omega(a)) \Lambda_\nu \\ &= \Delta_\nu^{it} E_\omega(a) \Lambda_\nu \\ &= \Delta_\nu^{it} K_\omega a \Lambda_\mu \end{aligned}$$

for all $a \in A$ and $t \in \mathbb{R}$, by Lemma 2.1.5. Hence $K_\omega \Delta_\mu^{it} = \Delta_\nu^{it} K_\omega$, for all $t \in \mathbb{R}$, since Λ_μ is cyclic and separating for A .

(2) \implies (3): If $K_\omega \Delta_\mu^{it} = \Delta_\nu^{it} K_\omega$, for all $t \in \mathbb{R}$, then $K_\omega \Delta_\mu^{1/2} = \Delta_\nu^{1/2} K_\omega$ by [78, E. 9.23]. Then, for all $a \in A$,

$$\begin{aligned} K_\omega J_A a \Lambda_\mu &= K_\omega J_A S_\mu a^* \Lambda_\mu \\ &= K_\omega \Delta_\mu^{1/2} a^* \Lambda_\mu \\ &= \Delta_\nu^{1/2} K_\omega a^* \Lambda_\mu \\ &= \Delta_\nu^{1/2} E_\omega(a)^* \Lambda_\nu \\ &= \Delta_\nu^{1/2} S_\nu E_\omega(a) \Lambda_\nu \\ &= J_B E_\omega(a) \Lambda_\nu \\ &= J_B K_\omega a \Lambda_\mu, \end{aligned}$$

since $S_\mu = J_A \Delta_\mu^{1/2}$ and $J_A^2 = 1$. Hence $K_\omega J_A = J_B K_\omega$, since Λ_μ is cyclic and separating for A .

(3) \implies (4): If $K_\omega J_A = J_B K_\omega$, then

$$J_A K_\omega^* = J_A K_\omega^* J_B^2 = J_A (J_B K_\omega)^* J_B = J_A (K_\omega J_A)^* J_B = K_\omega^* J_B$$

since $J_A^2 = 1$ and $J_B^2 = 1$. It then follows that

$$E_\omega^\sigma(b) \Lambda_\mu = J_A K_\omega^* J_B b \Lambda_\nu = K_\omega^* b \Lambda_\nu = E_\omega'(b) \Lambda_\mu,$$

for all $b \in B$, by Lemma 2.1.5. Then, by (2.1.2), we get

$$\nu(E_\omega(a)b) = \mu(aE_\omega'(b)) = \mu(aE_\omega^\sigma(b))$$

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

(4) \implies (1): For all $a \in A$ and $b \in B$, we have

$$\mu(aE_\omega^\sigma(b)) = \nu(E_\omega(a)b) = \mu(aE_\omega'(b)),$$

by hypothesis and the definition of E_ω' (see (2.1.2)). From which it follows that $E_\omega^\sigma(b) \Lambda_\mu = E_\omega'(b) \Lambda_\mu$, for all $b \in B$, since $\mu \in \mathfrak{F}(A)$. Thus

$E_\omega^\sigma = E'_\omega$, since Λ_μ is cyclic and separating for A . Then

$$\begin{aligned} E_\omega^\sigma \circ (\sigma_t^\nu)^\sigma &= E'_\omega \circ \sigma_{-t}^\nu \\ &= \left(\sigma_{-t}^\nu \circ E_\omega \right)' \\ &= \left(E_\omega \circ \sigma_{-t}^{\mu'} \right)' \\ &= \sigma_{-t}^\mu \circ E'_\omega \\ &= (\sigma_t^\mu)^\sigma \circ E_\omega^\sigma, \end{aligned}$$

by Propositions 2.1.10 and 2.1.7. Hence $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$. \square

The basic properties of duals given in Propositions 2.1.9 and 3.3.2, allow us to prove the following lemma in terms of the KMS transport plans of Definition 3.1.5, which subsequently leads to symmetry of $W_{\sigma\sigma}$.

LEMMA 3.3.3. *For any $\mu \in \mathfrak{F}(A)$ and $\nu \in \mathfrak{F}(B)$, we have*

$$\|\pi_\mu^\omega(a)\Omega_\omega - \pi_\nu^\omega(b)\Omega_\omega\|_\omega = \|\pi_\nu^{\omega^\sigma}(b)\Omega_{\omega^\sigma} - \pi_\mu^{\omega^\sigma}(a)\Omega_{\omega^\sigma}\|_{\omega^\sigma}$$

for all $a \in A$, $b \in B$ and $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$, where $\omega^\sigma \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$ is determined by $E_{\omega^\sigma} = E_\omega^\sigma$. For emphasis we have written Ω_ω for the cyclic vector appearing in a cyclic representation associated to ω , and similarly for ω^σ .

PROOF. For any $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$, we have that $\omega^\sigma \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$ by Proposition 3.3.1. It therefore follows from Propositions 3.1.3, 2.1.9 and 3.3.2 that

$$\begin{aligned} \|\pi_\mu^\omega(a)\Omega_\omega - \pi_\nu^\omega(b)\Omega_\omega\|_\omega^2 &= \mu(a^*a) + \nu(b^*b) - \nu(E_\omega(a)^*b) - \nu(b^*E_\omega(a)) \\ &= \nu(b^*b) + \mu(a^*a) - \mu(E_\omega^\sigma(b)^*a) - \mu(a^*E_\omega^\sigma(b)) \\ &= \nu(b^*b) + \mu(a^*a) - \mu(E_{\omega^\sigma}(b)^*a) - \mu(a^*E_{\omega^\sigma}(b)) \\ &= \|\pi_\nu^{\omega^\sigma}(b)\Omega_{\omega^\sigma} - \pi_\mu^{\omega^\sigma}(a)\Omega_{\omega^\sigma}\|_{\omega^\sigma}^2 \end{aligned}$$

for all $a \in A$, $b \in B$. \square

A transport plan has the same cost as its duals:

PROPOSITION 3.3.4. *For systems \mathbf{A} and \mathbf{B} , let $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$. Then*

$$(3.3.2) \quad I_{\mathbf{A}, \mathbf{B}}(\omega) = I_{\mathbf{B}', \mathbf{A}'}(\omega') = I_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}(\omega^\sigma),$$

where $\omega' \in T_\sigma(\mathbf{B}', \mathbf{A}')$ and $\omega^\sigma \in T_\sigma(\mathbf{B}^\sigma, \mathbf{A}^\sigma)$. For reversible systems \mathbf{A} and \mathbf{B} , we have

$$I_{\mathbf{A}, \mathbf{B}}(\omega) = I_{\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow}(\omega^\leftarrow),$$

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

PROOF. Given any $\omega \in T(\mathbf{A}, \mathbf{B})$, then

$$\omega \in T_\sigma(\mathbf{A}, \mathbf{B}) \iff \omega' \in T_\sigma(\mathbf{B}', \mathbf{A}') \iff \omega^\sigma \in T_\sigma(\mathbf{B}^\sigma, \mathbf{A}^\sigma)$$

for all $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, by Proposition 3.3.1. Furthermore,

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

by Propositions 2.1.9 and 3.3.2. Similarly, $I_{\mathbf{B}^{\sigma}, \mathbf{A}^{\sigma}}(\omega^{\sigma}) = I_{\mathbf{A}, \mathbf{B}}(\omega)$.

For reversible \mathbf{A} and \mathbf{B} , we have that $\omega \in T_{\sigma}(\mathbf{A}, \mathbf{B})$ if and only if $\omega^{\leftarrow} \in T_{\sigma}(\mathbf{B}^{\leftarrow}, \mathbf{A}^{\leftarrow})$, by Proposition 3.3.1. Similar to above, it follows that $I_{\mathbf{B}^{\leftarrow}, \mathbf{A}^{\leftarrow}}(\omega^{\leftarrow}) = I_{\mathbf{A}, \mathbf{B}}(\omega)$. \square

PROPOSITION 3.3.5. *For all $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, we have*

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

PROOF. It follows from Lemma 3.3.3 and Proposition 3.1.3, that for each $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ there is an $\omega^{\sigma} \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$ such that

$$I_{\mathbf{A}, \mathbf{B}}(\omega) = I_{\mathbf{B}, \mathbf{A}}(\omega^{\sigma}),$$

while $(\omega^{\sigma})^{\sigma} = \omega$ because $(E_{\omega}^{\sigma})^{\sigma} = E_{\omega}$, giving a one-to-one correspondence between $T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ and $T_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$. The required symmetry $W_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) = W_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$, for all $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, then follows from Definition 3.1.5 of $W_{\sigma\sigma}$, since we retain equality in taking the infima over $T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ and $T_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$ on the left and right, respectively. \square

3.4. Metric properties of Wasserstein distances

Zero cost between a dynamical system and itself can always be attained by using a maximally entangled state as the transport plan.

PROPOSITION 3.4.1. *For the Wasserstein functions W , W_{σ} and $W_{\sigma\sigma}$, in Definition 3.1.5, we have*

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

for all $\mathbf{A} \in \mathfrak{A}$.

PROOF. 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 (2.3.8). Consequently

$$W(\mathbf{A}, \mathbf{A}) = W_{\sigma}(\mathbf{A}, \mathbf{A}) = W_{\sigma\sigma}(\mathbf{A}, \mathbf{A}) = I_{\mathbf{A}, \mathbf{A}}(\delta_{\mu}) = 0$$

by (3.1.1). \square

That cost, and consequently distances, between a system and itself is zero 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 3.4.2. Consider the standard form of M_n as described in Example 1.3.8. Note that we can respectively identify $A \odot A'$ with $M_n \otimes_s M_n$ and $\pi(a) \otimes \pi'(b)$ with $a \otimes_s b$, via the normal representations π and π' . Furthermore, the latter mutually commute since

$$\begin{aligned} \pi(a)\pi'(b^\top)X &= \pi(a)j_A(\pi(b))X \\ &= j_A(\pi(b))\pi(a)X \\ &= \pi'(b^\top)\pi(a)X, \end{aligned}$$

i.e. $(aX)b^\top = a(Xb^\top)$, for all $a, b \in M_n$, emphasizing the bimodule structure inherent to our setting. 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 μ and μ' , 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 $\Lambda_\mu \in \mathfrak{H}_A$ is a pure state of the composite system, reducing to μ and μ' respectively, and in this sense we view δ_μ as a maximally entangled state of μ and μ' .

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

$$\begin{aligned} S_\mu^* \pi(a)^* S_\mu \pi(b) \Lambda_\mu &= S_\mu^* \pi((ba)^*) \Lambda_\mu \\ &= \pi(\rho_\mu b a \rho_\mu^{-1}) \Lambda_\mu \\ &= \rho_\mu b a \rho_\mu^{-1/2} \\ &= \rho_\mu (b a \rho_\mu^{1/2}) \rho_\mu^{-1} \\ &= [\rho_\mu \otimes_s \rho_\mu^{-1}] (b a \rho_\mu^{1/2}) \\ &= \Delta_\mu (b a \rho_\mu^{1/2}) \\ &= b a \rho_\mu^{1/2} \\ &= b \rho_\mu^{1/2} (\rho_\mu^{-1/2} a \rho_\mu^{1/2}) \\ &= \pi'((\rho_\mu^{-1/2} a \rho_\mu^{1/2})^\top) \pi(b) \Lambda_\mu \end{aligned}$$

(see Example 1.2.2), and 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.

THEOREM 3.4.3. *The functions W and W_σ are asymmetric pseudometrics, while $W_{\sigma\sigma}$ is a pseudometric.*

PROOF. That W is real and non-negative follows from Proposition 3.1.10. Furthermore, W satisfies the triangle inequality and is definite, i.e. $W(\mathbf{A}, \mathbf{A}) = 0$, for all $\mathbf{A} \in \mathfrak{A}$, by Propositions 3.2.4 and 3.4.1. Thus, W is an asymmetric pseudometric. Similarly, W_σ and $W_{\sigma\sigma}$ are asymmetric pseudometrics. Moreover, $W_{\sigma\sigma}$ is symmetric, by Proposition 3.3.5, thus it is in fact a pseudometric. \square

The remaining metric property, faithfulness, namely when 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 the next chapter (see Corollary 4.2.4). In the sequel we study relevant properties of these Wasserstein pseudometrics and take initial steps in showing how the general theory of these pseudometrics can be used to study the structure and properties of systems. This is what we turn to next.

CHAPTER 4

Properties and implications of Wasserstein distances

Our experience hitherto justifies us in believing that nature is the realization of the simplest conceivable mathematical ideas.
 – Albert Einstein, 1954.

In this chapter 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 (Section 4.1). 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 addition (Section 4.2) 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 chapters, again fixing Υ , the Z_v 's, and d for all systems to be considered.

4.1. Bounds on deviation from detailed balance

The Wasserstein pseudometrics W_σ and $W_{\sigma\sigma}$ have the following symmetries with respect to the three types of duals of systems introduced in Section 2.2 and discussed in Chapter 3.

THEOREM 4.1.1. *For all $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, 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 the usual symmetric property of $W_{\sigma\sigma}$ (see Theorem 3.4.3).

PROOF. Given any $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$, we have $\omega' \in T_\sigma(\mathbf{B}', \mathbf{A}')$ and $\omega^\sigma \in T_\sigma(\mathbf{B}^\sigma, \mathbf{A}^\sigma)$ such that

$$I_{\mathbf{A}, \mathbf{B}}(\omega) = I_{\mathbf{B}', \mathbf{A}'}(\omega') = I_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}(\omega^\sigma),$$

by Proposition 3.3.4. Consequently, by the definition of W_σ , we have

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

since we retain the equalities in taking the infima over the sets $T_\sigma(\mathbf{A}, \mathbf{B})$, $T_\sigma(\mathbf{B}', \mathbf{A}')$ and $T_\sigma(\mathbf{B}^\sigma, \mathbf{A}^\sigma)$, respectively (as in the proof of Proposition 3.3.5). For reversible $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$, we have $I_{\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow}(\omega^\leftarrow) = I_{\mathbf{A}, \mathbf{B}}(\omega)$. Thus, $W_\sigma(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow) = W_\sigma(\mathbf{A}, \mathbf{B})$.

The case of $W_{\sigma\sigma}$ is very similar. For instance, if $\omega \in T(\mathbf{A}, \mathbf{B})$ and $\mathbf{A}, \mathbf{B} \in \mathfrak{A}$ are reversible, 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 Proposition 3.3.5, $W_{\sigma\sigma}(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow) = W_{\sigma\sigma}(\mathbf{A}^\leftarrow, \mathbf{B}^\leftarrow)$. Similarly for the other two dualities. \square

This result along with the basic metric properties in Theorem 3.4.3, 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.

For the next result, recall Definition 2.2.3(3), and Definition 2.5.3.

COROLLARY 4.1.2. *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 Proposition 3.2.4 and Theorem 4.1.1)

$$\begin{aligned} W_\sigma(\mathbf{A}, \mathbf{A}^\leftarrow) &\leq W_\sigma(\mathbf{A}, \mathbf{B}) + W_\sigma(\mathbf{B}, \mathbf{A}^\leftarrow) \\ &= W_\sigma(\mathbf{A}, \mathbf{B}) + W_\sigma(\mathbf{B}^\leftarrow, \mathbf{A}^\leftarrow) \\ &= W_\sigma(\mathbf{A}, \mathbf{B}) + W_\sigma(\mathbf{A}, \mathbf{B}) \\ &= 2W_\sigma(\mathbf{A}, \mathbf{B}), \end{aligned}$$

by Theorem 4.1.1. Similarly for the other cases. \square

REMARKS 4.1.3. 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 \mathbf{A} is a hermitian system whose von Neumann algebra A is generated by the coordinate system k , i.e. $\{k_1^*, \dots, k_d^*\} = \{k_1, \dots, k_d\}$, as can be seen from [42, Theorems 3.9 and 3.10] and [41, Section 6] as well as the arguments used there. Those papers do not explicitly cover W_σ as defined in this thesis. Similarly for the other cases in the corollary

above. For W_σ and $W_{\sigma\sigma}$ we in fact discuss this from a more general point of view in Section 4.2 (Theorem 4.2.2 and Corollary 4.2.4).

Since we do not have corresponding symmetries for W (from the proof of Theorem 4.1.1 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 4.1.4. Applying the corollary when \mathbf{B} is classical, i.e., B is abelian, we take the reversing operation of \mathbf{B} 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 2.5), which generalizes detailed balance of a Markov chain (see Examples 2.5.1 and 2.5.2). 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 the 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_σ can be stated as

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

We note that W is not symmetric in general (see [42, §5.2 and 5.3] and [43, §4.3]), 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 which are 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.

4.2. Zero Wasserstein distance and common structure

In order to shed light on issues regarding the structure of a system \mathbf{A} , we turn to the implications of zero Wasserstein distance in relation to common structure in the two systems. Our basic result in this regard is stated as Theorem 4.2.2 below. This in fact boils down to a generalization of the faithfulness of an (asymmetric) metric d , namely the property that $d(x, y) = 0$ implies $x = y$, which was not discussed in the previous chapter. 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_σ and $W_{\sigma\sigma}$.

This is intimately related to the coordinates of a system, in particular the corresponding coordinate algebra (Definition 2.2.7), and the hermitian condition (Definition 2.2.6) of a system will also become relevant. In [41, 42] the latter was needed as part of the proof of faithfulness of an asymmetric metric. This will now be obtained in a generalized form for W_σ and $W_{\sigma\sigma}$.

We need the following lemma extending a basic technical point from [41, Lemma 6.3].

LEMMA 4.2.1. *Consider systems \mathbf{A} and \mathbf{B} , with \mathbf{A} hermitian. Let M and N be the coordinate algebras of \mathbf{A} and \mathbf{B} respectively (see Definition 2.2.7). 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_ω 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 (3.1.5),

$$\begin{aligned} & \mu(k_i^* k_i) + \nu(l_i^* l_i) - \nu(E_\omega(k_i)^* l_i) - \nu(l_i^* E_\omega(k_i)) \\ &= \nu(|l_i - E_\omega(k_i)|^2) + \nu(E_\omega(|k_i|^2) - |E_\omega(k_i)|^2) \\ &= 0, \end{aligned}$$

for all $i = 1, \dots, d$, due to $I_{\mathbf{A}, \mathbf{B}}(\omega) = 0$. Thus

$$\nu(|l_i - E_\omega(k_i)|^2) = 0 \quad \text{and} \quad \nu(E_\omega(|k_i|^2) - |E_\omega(k_i)|^2) = 0$$

for all $i = 1, \dots, d$, since $E_\omega(|k_i|^2) \geq |E_\omega(k_i)|^2$ by Kadison's inequality. Since ν is faithful, the former implies that

$$(4.2.1) \quad E_\omega(k_i) = l_i$$

while the latter implies that

$$E_\omega(k_i^* k_i) = E_\omega(k_i)^* E_\omega(k_i)$$

for all $i = 1, \dots, d$.

Setting

$$A_\omega := \{a \in A : E_\omega(a^* a) = E_\omega(a)^* E_\omega(a)\}$$

it follows from [28, Theorem 3.1] that A_ω is a (norm closed) subalgebra of A and that

$$(4.2.2) \quad A_\omega = \{a_2 \in A : E_\omega(a_1 a_2) = E_\omega(a_1) E_\omega(a_2) \text{ for all } a_1 \in A\}.$$

Since \mathbf{A} is hermitian, we have $k_1, \dots, k_d, k_1^*, \dots, k_d^* \in A_\omega$, so A_ω contains the unital $*$ -algebra M_0 generated by $\{1_A, k_1, \dots, k_d\}$. Moreover, since E_ω is positive and therefore preserves the involution, we see from (4.2.2) that $E_\omega|_{M_0} : M_0 \rightarrow N$ is a unital $*$ -homomorphism. As E_ω is normal

(i.e., σ -weakly continuous) and M_0 is σ -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 σ -weakly continuous by [20, Theorem 2.4.2]. \square

Note that this lemma is applicable when $W(\mathbf{A}, \mathbf{B}) = 0$, due to the existence of an optimal transport plan in Theorem 3.1.7, which indeed led to $\mathbf{A} = \mathbf{B}$ for the case of $A = B$ and $k = l$ in [42, 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_σ 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 2.2.1. 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 (see Definition 2.2.8).

THEOREM 4.2.2. *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*

$$(4.2.3) \quad E_\omega \circ \alpha|_M = \beta \circ \iota_{\mathbf{A},\mathbf{B}}$$

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

PROOF. By Proposition 3.1.7 there is an optimal transport plan $\omega \in T_\sigma(\mathbf{A}, \mathbf{B})$ such that $W_\sigma(\mathbf{A}, \mathbf{B}) = I_{\mathbf{A},\mathbf{B}}(\omega)^{1/2} = 0$, from which it follows that $W_\sigma(\mathbf{B}^\sigma, \mathbf{A}^\sigma) = I_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}(\omega^\sigma)^{1/2} = 0$ by Theorem 4.1.1. Since $I_{\mathbf{A},\mathbf{B}}(\omega) = I_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}(\omega^\sigma) = 0$, by Lemma 4.2.1, we have normal unital $*$ -homomorphisms

$$\iota_{\mathbf{A},\mathbf{B}} := E_\omega|_M : M \rightarrow N \quad \text{and} \quad \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} := E_\omega^\sigma|_N : N \rightarrow M,$$

necessarily uniquely determined by

$$\iota_{\mathbf{A},\mathbf{B}}(k_i) = l_i \quad \text{and} \quad \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}(l_i) = k_i$$

for all $i = 1, \dots, d$. 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:

$$\iota_{\mathbf{A},\mathbf{B}} \circ \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}(l_i) = l_i \quad \text{and} \quad \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} \circ \iota_{\mathbf{A},\mathbf{B}}(k_i) = k_i$$

for all $i = 1, \dots, d$, meaning that

$$\iota_{\mathbf{A},\mathbf{B}} \circ \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} = \text{id}_{N_0} \quad \text{and} \quad \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} \circ \iota_{\mathbf{A},\mathbf{B}} = \text{id}_{M_0},$$

where M_0 and N_0 are the unital $*$ -algebras generated by $\{1_A, k_1, \dots, k_d\}$ and $\{1_B, l_1, \dots, l_d\}$, respectively. Thus, $\iota_{\mathbf{A},\mathbf{B}} \circ \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} = \text{id}_N$ and $\iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma} \circ \iota_{\mathbf{A},\mathbf{B}} = \text{id}_M$, by σ -weak continuity. 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 the definition of $T_\sigma(\mathbf{A}, \mathbf{B})$; see (2.3.8) and Definition 2.3.4. \square

In particular (4.2.3) tells us (by applying $\iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma}$ from the right) that

$$(4.2.4) \quad \beta|_N = E_\omega \circ \alpha|_M \circ \iota_{\mathbf{B}^\sigma, \mathbf{A}^\sigma},$$

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 $W_\sigma(\mathbf{A}, \mathbf{B}) = 0$.

Below we show how isomorphic systems can be identified inside \mathbf{A} and \mathbf{B} in Theorem 4.2.2 when additional assumptions are made. In particular, in Theorem 4.2.2 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 4.2.3. *Assuming that $\alpha(M) \subset M$, then in addition to Theorem 4.2.2'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 4.2.2 and $\iota_{\mathbf{A}, \mathbf{B}} := E_\omega|_M$ in its proof. Keep in mind that $\nu \circ \iota_{\mathbf{A}, \mathbf{B}} = \nu \circ E_\omega|_M = \mu|_M$. \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 former 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 the properties and behaviour of \mathbf{A} are consequently reflected in that of \mathbf{B} . Theorem 4.2.2 can be viewed as a weaker version of this situation.

To show explicitly how Theorem 4.2.2 relates to the faithfulness of an asymmetric metric, we state the following special case of this corollary:

COROLLARY 4.2.4. *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 4.2.2 and Corollary 4.2.3 is not symmetric, as may be expected from the lack of symmetry of the asymmetric pseudometric W_σ . 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 α , given β , simply because by definition we always have $W_{\sigma}(\mathbf{A}, \mathbf{B}) \leq W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$.

COROLLARY 4.2.5. *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. By Proposition 3.3.5 $W_{\sigma\sigma}$ is symmetric, and therefore it follows that $W_{\sigma\sigma}(\mathbf{A}, \mathbf{B}) = W_{\sigma\sigma}(\mathbf{B}, \mathbf{A}) = 0$. Thus $W_{\sigma}(\mathbf{A}, \mathbf{B}) = W_{\sigma}(\mathbf{B}, \mathbf{A}) = 0$, since $0 \leq W_{\sigma}(\mathbf{A}, \mathbf{B}) \leq W_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$ by Proposition 3.1.10. As in the proof of Theorem 4.1.1, for any optimal $\omega \in T_{\sigma\sigma}(\mathbf{A}, \mathbf{B})$, we have that $\omega^{\sigma} \in T_{\sigma\sigma}(\mathbf{B}, \mathbf{A})$ with $I_{\mathbf{A}, \mathbf{B}}(\omega) = I_{\mathbf{B}, \mathbf{A}}(\omega^{\sigma}) = 0$. So ω^{σ} is indeed optimal. Now we can simply apply Theorem 4.2.2 to both directions. \square

More generally, for any optimal transport plan, including 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 4.2.2 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 [33, Appendix V.B] and [45, 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) ω from \mathbf{A} to \mathbf{B} or ψ 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 α and the transport plan ω determines the behaviour of β on $E_{\omega}(A)$. The role of different optimal transport plans, when not unique, may also be of interest.

CHAPTER 5

Examples

How is it possible, with a finite number of symbols and small number of rules of manipulation, to create infinitely many thoughts?
 – Noam Chomsky, 2022.

We now clarify our transport approach to Wasserstein distances further by illustrating its main features with finite dimensional systems. In this context the transfer of probabilities are easy to follow, making the setup in Section 2.4 particularly transparent. We also illustrate how extended or refined detailed balance conditions are obtained, and find their various formulations.

Section 5.1 treats simple conceptual points used in the examples, in terms of classical systems, each on a finite number of points. A very specialized case of this is treated in Section 5.2, in which explicit calculations can be performed and simple formulas for appropriately chosen Wasserstein distances are obtained. Section 5.3 focusses on transport between a spin 1/2 (quantum) system and a single classical spin system, with special interest in detailed balance conditions and a Wasserstein distance.

5.1. Extending probability transfer to or from a point

As in Example 2.5.2, consider two classical systems $\mathbf{A} = (A, \alpha, \mu)$ and $\mathbf{B} = (B, \beta, \nu)$ whose dynamics are given by classical Markov chains on m and n point sets, respectively. We assume that \mathbf{B} satisfies detailed balance, i.e., $\beta' = \beta$. The total transfer of probability from the whole of \mathbf{A} to a single point q in \mathbf{A} , can be written as

$$(5.1.1) \quad \sum_{p=1}^m \mu_p \alpha_{pq} = \mu_q,$$

which simply expresses the invariance $\mu\alpha = \mu$. On the other hand, the transfer of probability from a single point p in \mathbf{A} to the whole of \mathbf{A} , is

$$(5.1.2) \quad \sum_{q=1}^m \mu_p \alpha_{pq} = \mu_p,$$

which expresses $\alpha(1_m) = 1_m$, where 1_m is the column with 1 as all m entries. In Section 2.4 we pointed out that $\mathbf{A}\omega\mathbf{B}$ generalizes the condition (5.1.1), 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 $\mu\alpha = \mu$. Similarly, $\mathbf{B}\psi\mathbf{A}$ was interpreted as a refinement of unitality. This will now be seen concretely for the current classical systems.

A coupling ω from μ to ν 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 ω . Note that in this finite context, the coupling ω says exactly that the portion ω_{pr} of the probability μ_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 ω 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

$$(5.1.3) \quad \sum_{p=1}^m \omega_{pr} \alpha_{pq} = \sum_{s=1}^n \omega_{qs} \beta'_{sr} = \sum_{s=1}^n \omega_{qs} \frac{\nu_r}{\nu_s} \beta_{rs},$$

which when summed over r gives exactly (5.1.1). Hence (5.1.3) is clearly a refinement of (5.1.1).

Essentially the probability μ_p of p in \mathbf{A} is split into n ‘‘compartments’’ having probabilities $\omega_{p1}, \dots, \omega_{pn}$ respectively, with the transition probability α_{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 α , is then required to be given by the total transport by β' from q ’s compartments to point r in \mathbf{B} .

Paraphrasing this, the transport from r to q by α , is equal to the transport from q to r by β' . The analogy with detailed balance is clear.

In this way α is required in some measure to adhere to rules laid down by β . In the one extreme case where

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

no restrictions are placed on α by $\mathbf{A}\omega\mathbf{B}$. In the other extreme, with $(A, \mu) = (B, \nu)$ and ω the diagonal measure associated to μ , 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 $\alpha(1_m) = 1_m$, 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

$$(5.1.4) \quad \sum_{r=1}^n \psi_{rp} \beta_{rs} = \sum_{q=1}^m \psi_{sq} \alpha'_{qp} = \sum_{q=1}^m \psi_{sq} \frac{\mu_p}{\mu_q} \alpha_{pq},$$

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} , which indeed simply expresses (5.1.2). In the paraphrased form as above, (5.1.4) says that the transport from p to s by β , is equal to the transport from s to p by α' . 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 ω' , which in this context is simply the reverse of a transport plan ω from \mathbf{A} to \mathbf{B} , namely

$$\omega' = [\omega'_{11} \quad \cdots \quad \omega'_{n1} \quad \cdots \quad \omega'_{1m} \quad \cdots \quad \omega'_{nm}],$$

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

$$(5.1.5) \quad \sum_{q=1}^m \omega_{qs} \frac{\mu_p}{\mu_q} \alpha_{pq} = \sum_{r=1}^n \omega_{pr} \beta_{rs}.$$

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 $\mathbf{B}'\omega'\mathbf{A}'$, rather than to $\mathbf{B}\omega'\mathbf{A}$ (see Proposition 2.3.11). 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 $W(\mathbf{A}, \mathbf{B}) = W(\mathbf{B}, \mathbf{A})$.

5.2. An explicit example

In order to do explicit calculations easily, we consider the example in the previous section 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 section, 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 α_{pq} refer to the points of its 4-point set $\{1, 2\} \times \{1, 2\}$ labelled 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:

$$\beta = \begin{bmatrix} \tilde{r} & r \\ s & \tilde{s} \end{bmatrix}, \quad \text{with } r, s \in [0, 1] \quad \text{and } \tilde{r} = 1 - r, \quad \tilde{s} = 1 - s.$$

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

$$(5.2.1) \quad l = l_1 = l_2 = \frac{1}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

for \mathbf{B} . This will define the Wasserstein distances from \mathbf{A} to \mathbf{B} , and from \mathbf{B} to \mathbf{A} ; see Section 2.3.

We assume that the cost ωc_{AB} for a transport plan $\omega \in T(\mathbf{A}, \mathbf{B})$ is given as in (2.3.3) 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 section we often write row matrices as tuples to clearly delineate the entries). This cost 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 $\{2, 4\}$ to the set $\{1, 3\}$ 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 ω from μ to ν 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 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 in (5.1.3), expressed by

$$\begin{aligned} (\mu_1\alpha_{12} + \mu_3\alpha_{32}) + (-\gamma_1\alpha_{12} + \gamma_2\alpha_{22} - \gamma_3\alpha_{32} + \gamma_4\alpha_{42}) &= \mu_2s + \gamma_2(\tilde{r} - s) \\ (\mu_1\alpha_{14} + \mu_3\alpha_{34}) + (-\gamma_1\alpha_{14} + \gamma_2\alpha_{24} - \gamma_3\alpha_{34} + \gamma_4\alpha_{44}) &= \mu_4s + \gamma_4(\tilde{r} - s) \end{aligned}$$

and

$$\begin{aligned} (\mu_2\alpha_{21} + \mu_4\alpha_{41}) + (\gamma_1\alpha_{11} - \gamma_2\alpha_{21} + \gamma_3\alpha_{31} - \gamma_4\alpha_{41}) &= \mu_1r + \gamma_1(\tilde{r} - s) \\ (\mu_2\alpha_{23} + \mu_4\alpha_{43}) + (\gamma_1\alpha_{13} - \gamma_2\alpha_{23} + \gamma_3\alpha_{33} - \gamma_4\alpha_{43}) &= \mu_3r + \gamma_3(\tilde{r} - s), \end{aligned}$$

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

$$(5.2.2) \quad \mu_1\alpha_{12} + \mu_3\alpha_{32} = \mu_2s, \quad \mu_1\alpha_{14} + \mu_3\alpha_{34} = \mu_4s$$

and

$$(5.2.3) \quad \mu_2\alpha_{21} + \mu_4\alpha_{41} = \mu_1r, \quad \mu_2\alpha_{23} + \mu_4\alpha_{43} = \mu_3r,$$

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 (5.2.2) and (5.2.3). To see this, a simple definition of the deviation from this optimal form can for example be taken as

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

from which we clearly see that

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

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 γ_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 α' instead of α , 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 Chapter 4).

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 ω from ν to μ 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 (5.2.2) and (5.2.3). On the other hand, for zero transport cost from \mathbf{B} to \mathbf{A} , the condition $\mathbf{B}\omega'\mathbf{A}$ is expressed by

$$(5.2.4) \quad \alpha_{12} + \alpha_{14} = \alpha_{32} + \alpha_{34} = r \quad \text{and} \quad \alpha_{21} + \alpha_{23} = \alpha_{41} + \alpha_{43} = s.$$

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, μ) 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 α_{pq} 's. In other words, there are \mathbf{A} and \mathbf{B} such that

$$(5.2.5) \quad W(\mathbf{A}, \mathbf{B}) = 0 \quad \text{and} \quad W(\mathbf{B}, \mathbf{A}) \neq 0,$$

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

$$(5.2.6) \quad W(\mathbf{A}, \mathbf{B}) \neq 0 \quad \text{and} \quad W(\mathbf{B}, \mathbf{A}) = 0.$$

For example, in the case $\alpha_{pq} > 0$ for all p and q , transform α 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 α_{pq} 's are left unchanged. Then, for small enough $|\varepsilon|$, (2.5.2), (5.1.1) and (5.2.4) are preserved, but (5.2.3) is 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 ω and ω' (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} .

5.3. 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 Section 5.2. 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 2.5.5), 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 θ , \mathbf{A} satisfies θ -sqdb (Example 2.5.5 gives a definition sufficient for this example) for any values of η, φ , and λ . 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 Section 2.2) for \mathbf{A} as the Pauli spin matrices,

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

and again using (5.2.1) for \mathbf{B} , also setting $l_3 = l$, then via (2.3.3) and (3.1.2) for $d = 3$, the condition $W(\mathbf{A}, \mathbf{B}) < 1$ implies that $r + s > 0$ and

$$(5.3.1) \quad \lambda \sin \eta + \tilde{\lambda} \sin \varphi = 0.$$

In fact, if $\mathbf{A}\omega\mathbf{B}$ for $\omega \neq \mu \otimes \nu$, and we assume $r + s > 0$, then (5.3.1) 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 (5.3.1), 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 α 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 (5.3.1) 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 μ 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 .

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