

LECTURE NOTE ON QUANTUM GRAPHS

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1. INTRODUCTION

1.1. The origin story. The idea of quantum graphs grew out of two separate theories, quantum information theory and the theory of operator algebras, independently and about the same time around 2010.

Quantum graphs in quantum information theory are motivated by the notion of confusability graphs and zero-error capacity for communication channels in the framework of classical information theory, due to Shannon [Sha56]. In this theory, a communication channel F has an input set I , we get a graph Γ_F with the vertex set I , and edges connecting the pairs of inputs that can be confusable under F (they possibly have the same outputs). One central problem is to estimate the *zero-error capacity* (or the *Shannon capacity*) of F , which counts the growth rate of the maximal empty subgraphs in the graph products Γ_F^k , which measures the rate of transmission without confusion under the iterated channels F^k on input sets I^k (the set of words of length k).

In quantum information theory, we consider a *quantum channel*, implemented by a map $N: M_{d_1} \rightarrow M_{d_2}$ of the form

$$N(\rho) = K_1 \rho K_1^* + \cdots + K_n \rho K_n^*$$

for some matrices $K_i \in M_{d_2 \times d_1}$ satisfying

$$K_1^* K_1 + \cdots + K_n^* K_n = I_{d_1}.$$

Duan [Dua09] found out that the subspace

$$S = \text{span}\{K_i^* K_j \mid i, j = 1, \dots, n\} \subset M_{d_1}$$

serves as an analogue of the confusability graph, which can capture the number of input states which remain orthogonal after applying N .

Quantum graphs in the theory of operator algebras are motivated by the paradigm of quantized sets. This is motivated by the duality between (classical) spaces and commutative operator algebras, that can be stated in several different ways to make it precise. From this viewpoint, general noncommutative algebras (of operators on a Hilbert space H) can be regarded as the algebra of functions on a hypothetical ‘quantized’ space, much like the mathematical foundation of quantum mechanics where we represent observables on a quantum mechanical system by self-adjoint operators on a Hilbert space.

Developing this paradigm, Weaver [Wea12] conceived that if $M \subset \mathcal{B}(H)$ is such an operator algebra representing a quantized set X , then a ‘quantum relation’ on X should be given by a certain subspace $S \subset \mathcal{B}(H)$ closed under composition by the commutant $M' \subset \mathcal{B}(H)$, which is the algebra of operators on H commuting with the elements of M . He undertook a systematic study to translate conditions about relations into those on S . Among others, this led to the formulation of unoriented quantum graphs (with normalization about self-loops at vertices) as *operator system bimodules*, i.e., the subspaces of $\mathcal{B}(H)$ as above that contain the identity transform id_H and are closed under the adjoint operation.

1.2. What can we do with quantum graphs? A first milestone in the theory of quantum graphs in quantum information theory was due to Duan–Severini–Winter [DSW13], which gave an estimate on the capacity of quantum channels (which are difficult to compute) in terms of an invariant for quantum graphs defined by Semi-Definite Programming (which are easier to compute), analogous to the celebrated result of Lovász [Lov06] for the zero-error capacity of classical communication channels.

Once we have quantum graphs, one natural thing to do is to relate them with analogues of graph homomorphisms. This leads to several flavors of quantum homomorphisms between quantum graphs. One way to model this is through completely positive maps between operator algebras. Another closely related approach is through homomorphisms into amplified algebras.

In fact, even in the case of classical graphs, the corresponding analogue of ‘isomorphisms’ leads to a generalization of automorphism group of a graph represented by noncommutative algebras, called quantum groups. This leads to a intriguing family of Hopf algebras defined through combinatorial structures. Acknowledgement. This lecture note grew out of the graduate course I taught at the University of Oslo in the spring of 2024, and the participants in this course helped me greatly to prepare this note.

2. CONVENTION

We denote a complex Hilbert space by H . We represent the inner product of its vectors as $\langle v, w \rangle$. Our convention is that this is conjugate linear in v and linear in w , so that

$$\langle \alpha_1 v_1 + \alpha_2 v_2, \beta_1 w_1 + \beta_2 w_2 \rangle = \sum_{i,j=1}^2 \overline{\alpha_i} \beta_j \langle v_i, w_j \rangle$$

holds. When v is a vector in H , we write v^* to denote the linear functional

$$H \rightarrow \mathbb{C}, \quad w \mapsto \langle v, w \rangle.$$

For example, if H is the column vector space $\mathbb{C}^d$ and v is its element with components $\alpha_1, \dots, \alpha_d$, then v^* is the row vector with components $\overline{\alpha_1}, \dots, \overline{\alpha_d}$.

We denote the space of bounded linear transforms on H by $\mathcal{B}(H)$. We mostly consider finite dimensional Hilbert spaces, so the boundedness condition is not essential. However, we use this conventional notation to emphasize an extra structure for operators on Hilbert spaces, namely, the *adjoint operation* $T \mapsto T^*$. It is an conjugate linear map acting on $\mathcal{B}(H)$ characterized by

$$\langle Tv, w \rangle = \langle v, T^*w \rangle \quad (v, w \in H).$$

We then have $(T_1 T_2)^* = T_2^* T_1^*$. When v_1 and v_2 are vectors in H , we write $v_1 v_2^*$ to denote the rank 1 operator on H given by

$$w \mapsto \langle v_2, w \rangle v_1.$$

Note that we have $(v_1 v_2^*)^* = v_2 v_1^*$.

We also use diagrammatic notation for linear maps between tensor powers of H inspired by tensor network. We represent a map $T \in \mathcal{B}(H^{\otimes a}, H^{\otimes b})$ by a box marked by the symbol T , with a strands sticking out to the bottom and b strands to the top. The composition of maps (when they make sense) is represented by stacking such diagrams vertically, while tensor product is represented by arranging them horizontally. For example, given $S, T \in \mathcal{B}(H)$, their composition and tensor product are represented as in Figure 1. We will also vertically flip the diagram to represent the adjoint operation, as in Figure 2.

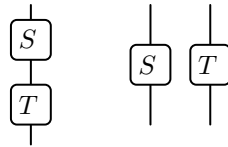


FIGURE 1. Diagrammatic presentation of ST and $S \otimes T$

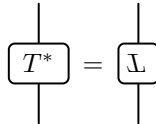


FIGURE 2. Diagrammatic presentation of adjoint

When d is a nonnegative integer, we denote the space of d -by- d square complex matrices by M_d . We denote the identity matrix of size d by $I_d \in M_d$. We frequently identify M_d with $\mathcal{B}(\mathbb{C}^d)$.

3. QUANTUM GRAPHS THROUGH ADJACENCY MATRIX OPERATORS

3.1. First definitions. In this section, we introduced basic concepts behind quantum graphs in order to set up the ground for the entire course. First, let us introduce algebraic systems representing finite quantum sets. See Remark 3.4 for more on this viewpoint.

Convention 3.1. Throughout the lecture we use the symbol B to denote a *finite-dimensional C^* -algebra*. By the structure theory of C^* -algebras, it can be written as a multimatrix algebra,

$$(3.1) \quad B \simeq \bigoplus_{k=1}^n M_{d_k}.$$

Its product operation is given by the matrix multiplication in each summand. In particular, the multiplicative unit is given by

$$1_B = I_{d_1} \oplus I_{d_2} \oplus \cdots \oplus I_{d_n}.$$

Besides the algebra structure, we consider the involution $a \mapsto a^*$ on B , which is given by conjugate transpose of matrices on each summand of (3.1).

Definition 3.2. A *faithful positive functional* on B is a linear functional $\psi: B \rightarrow \mathbb{C}$ such that $\psi(a^*a) \geq 0$ holds for all $a \in B$ (*positivity*), and $\psi(a^*a) = 0$ holds if and only if $a = 0$ holds (*faithfulness*). If, in addition, the normalization condition $\psi(1_B) = 1$ holds, we say that ψ is a *faithful state* on B .

Example 3.3. The standard choice for a faithful positive functional on a finite dimensional C^* -algebra B is

$$\psi_{\text{std}} = \sum_{k=1}^n d_k \text{Tr}_{M_{d_k}}$$

in terms of the decomposition (3.1).

Positive functionals are crucial ingredients to relate C^* -algebras to Hilbert spaces. Namely, given a positive functional ψ on B , we can define a Hermitian inner product on B by

$$\langle a, b \rangle = \psi(a^*b).$$

With this structure, we obtain a (finite-dimensional) Hilbert space. This is the *Gelfand–Naimark–Segal (GNS) construction*.

To avoid confusion, we write this Hilbert space as $L^2(B, \psi)$, and write its element corresponding to an element $a \in B$ as $\Lambda_\psi(a)$. We thus have $L^2(B, \psi) = \{\Lambda_\psi(a) \mid a \in B\}$, and the inner product

$$\langle \Lambda_\psi(a), \Lambda_\psi(b) \rangle = \psi(a^*b).$$

The map

$$\Lambda_\psi: B \rightarrow L^2(B, \psi), \quad a \mapsto \Lambda_\psi(a)$$

is often called the *GNS map*. As we are working with faithful positive functionals, this map is a linear isomorphism of complex vector spaces.

Each element $a \in B$ defines a linear transform $\pi_\psi(a)$ on $L^2(B, \psi)$ given by

$$\pi_\psi(a)\Lambda_\psi(b) = \Lambda_\psi(ab).$$

This defines a *unitary representation* of B on $L^2(B, \psi)$, in the sense that we have

$$\pi_\psi(a_1)\pi_\psi(a_2) = \pi_\psi(a_1a_2), \quad \pi_\psi(a^*) = \pi_\psi(a)^*.$$

Remark 3.4. The above construction also makes sense for infinite dimensional C^* -algebras, and possibly non-faithful positive functionals, which will be used later. In a quantum mechanical setting, given a Hilbert space H representing the system, we are often interested in finding a system of observables $X_0, X_1, \dots$ represented by self adjoint operators on H , and a state represented by a unit vector $\xi \in H$. We can instead consider a (universal) algebra $\mathcal{A}$ generated by elements $x_0, x_1, \dots$ subject to some algebraic relations, and look for a positive functional ψ on $\mathcal{A}$. By the GNS construction, we obtain operators $X_i = \pi_\psi(x_i)$ and a vector $\xi = \Lambda_\psi(1)$ (suitably normalized).

In most part of this course, we fix ψ . If the choice of ψ is understood, we simply write $L^2(B)$, $\Lambda(a)$, $\pi(a)$, etc., instead of $L^2(B, \psi)$, $\Lambda_\psi(a)$, $\pi_\psi(a)$, etc.

Next, let us consider some maps between the tensor products GNS Hilbert spaces induced by the algebra structure of B . The map $\Lambda \otimes \Lambda$ defines a linear isomorphism between $B \otimes B$ and $L^2(B) \otimes L^2(B)$. Thus, the multiplication map

$$m: B \otimes B \rightarrow B$$

may be regarded as a operator

$$L^2(B) \otimes L^2(B) \rightarrow L^2(B), \quad \Lambda(a) \otimes \Lambda(b) \mapsto \Lambda(ab).$$

Similarly, the multiplicative unit $1_B \in B$ induces a linear map

$$\eta: \mathbb{C} \rightarrow B, \quad \lambda \mapsto \lambda 1_B.$$

Again we write the induced map $\mathbb{C} \rightarrow L^2(B)$ by the same symbol η . We denote these structure maps diagrammatically as in Figure 3.

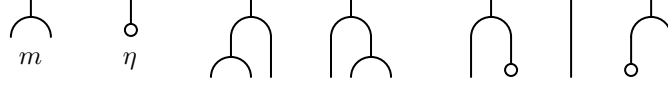


FIGURE 3. Structure maps of (B, ψ)

We are now ready to define quantum graphs. We follow the formalism of [MRV18], and define them through an analogue of adjacency matrices for graphs.

Definition 3.5. A *quantum adjacency matrix operator* on (B, ψ) is an operator $A \in \mathcal{B}(L^2(B))$ such that:

- (1) $A = A^*$ (A is self-adjoint);
- (2) $m(A \otimes A)m^* = A$ (A is *convolution idempotent*);
- (3) $(\text{id} \otimes \eta^* m)(\text{id} \otimes A \otimes \text{id})(m^* \eta \otimes \text{id}) = A$; and
- (4) $m(A \otimes \text{id})m^* = \text{id}$.

Here, id denotes the identity map of $L^2(B)$. See Figure 4 for the diagrammatic representation of these conditions. An (unoriented) *quantum graph* is given by a triple (B, ψ, A) as above.

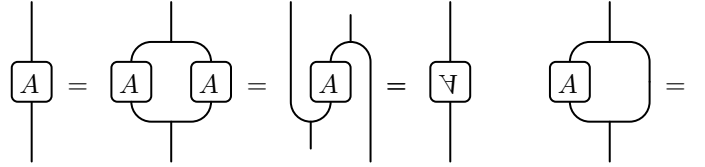


FIGURE 4. Quantum adjacency matrix

3.2. Normalized choice of functional. Depending on the context, there are often preferred choice of positive functionals on the C^* -algebras at hand. For example, if the algebra is the matrix algebra M_d , the obvious choice is the usual trace Tr . In general, the choice from Example 3.3 is a convenient choice. Analyzing why this convention works, we arrive at the following concept.

Definition 3.6. A positive functional ψ on B is said to be a δ -form, for a positive real number δ , if mm^* is a scalar multiple of identity on $L^2(B)$, and

$$(3.2) \quad \eta^* mm^* \eta = \delta \text{id}_{\mathbb{C}}$$

holds. Here, the adjoints m^* and η^* of m and η are computed with respect to the GNS inner product.

This concept originally came from the theory of compact quantum groups and their actions on C^* -algebras. In that context, the functional ψ is often assumed to be a state. Then the above condition is equivalent to

$$mm^* = \delta \text{id}_{L^2(B)}.$$

As we will see later (Proposition 4.3), in general mm^* is a B -bimodule endomorphism of $L^2(B)$. Taking the eigendecomposition of this endomorphism, we get subbimodules. Thus, ψ is a δ -form if and only if this manipulation does not give you any nontrivial submodules.

Proposition 3.7. The functional ψ_{std} from Example 3.3 is a δ -form with $\delta = \dim B$.

Proof. We first need to compute the effect of m^* . Let us take a decomposition (3.1). Let $E_{i,j}^{(k)} \in M_{d_k}$, with $i, j = 1, \dots, d_k$, be the matrix units for each direct summand. Thus, the multiplication map $m: B \otimes B \rightarrow B$ gives

$$m(\Lambda(E_{i,j}^{(k)}) \otimes \Lambda(E_{i',j'}^{(k')})) = \delta_{kk'} \delta_{ji'} \Lambda(E_{ij'}^{(k)}),$$

while the GNS inner product for ψ_{std} is given by

$$\langle \Lambda(E_{i,j}^{(k)}), \Lambda(E_{i',j'}^{(k')}) \rangle = \delta_{(i,j,k),(i',j',k')} d_k.$$

From the requirement

$$\langle m^*(\Lambda(E_{ij}^{(k)})), \Lambda(E_{il}^{(k)}) \otimes \Lambda(E_{lj}^{(k)}) \rangle = \langle \Lambda(E_{ij}^{(k)}), m(\Lambda(E_{il}^{(k)}) \otimes \Lambda(E_{lj}^{(k)})) \rangle = \psi_{\text{std}}(E_{ii}^{(k)}) = d_k,$$

we get

$$m^*(\Lambda(E_{ij}^{(k)})) = d_k^{-1} \sum_l \Lambda(E_{il}^{(k)}) \otimes \Lambda(E_{lj}^{(k)}).$$

From this we obtain

$$mm^*(\Lambda(E_{ij}^{(k)})) = d_k^{-1} d_k \Lambda(E_{ij}^{(k)}) = \Lambda(E_{ij}^{(k)}),$$

hence $mm^* = \text{id}$. Combined with $\eta(1) = 1_B$ and $\eta^* = \psi_{\text{std}}$, we get the equality (3.2) for $\delta = \sum_k d_k^2$. $\square$

Remark 3.8. When B is the matrix algebra M_d , any positive faithful functional on B is a δ -form. (The value of δ depends on the functional.)

Remark 3.9. When we rescale the positive functional and take $\psi' = r\psi$ with $r > 0$, the adjoint of the multiplication map transforms as

$$m_{\psi'}^* = r^{-1} m_{\psi}^*.$$

3.3. Classical graphs as quantum graphs. Let us compare the usual graphs with the concept of quantum graphs as we defined in Definition 3.5. Thus, we want a finite dimensional C^* -algebra, a positive functional, and a linear map on the C^* -algebra, from a graph.

The first step is to find the C^* -algebra. Given a finite V , consider the algebra of complex functions on V , that is,

$$C(V) = \{f: V \rightarrow \mathbb{C}\} \simeq \mathbb{C}^{|V|}.$$

The product is given by pointwise multiplication, and the involution f^* is given by complex conjugate, $f^*(v) = \overline{f(v)}$. Note that B has a basis $(\delta_v)_{v \in V}$, where δ_v denotes the Dirac delta function at the vertex v . We will see that, given a finite graph Γ with vertex set V , the adjacency matrix of Γ corresponds to a quantum adjacency matrix on $B = C(V)$.

As for the positive functional, we take the convention from Example 3.3, so that we have

$$\psi_{\text{std}}(f) = \sum_{v \in V} f(v).$$

Then the GNS inner product is given by

$$\langle \Lambda(\delta_v), \Lambda(\delta_w) \rangle = \delta_{v,w}.$$

Next let us work out the conditions for quantum adjacency matrix. Now, the maps η and η^* can be written as

$$\eta: \mathbb{C} \rightarrow L^2(B), \quad \lambda \mapsto \lambda \Lambda(1_V) = \lambda \sum_v \delta_v, \quad \eta^*: L^2(B) \rightarrow \mathbb{C}, \quad \Lambda(f) \mapsto \psi_{\text{std}}(f),$$

while m is given by

$$m: L^2(B) \otimes L^2(B) \rightarrow L^2(B), \quad \Lambda(\delta_v) \otimes \Lambda(\delta_w) \mapsto \delta_{v,w} \Lambda(\delta_v).$$

Lemma 3.10. *The map $m^*: L^2(B) \rightarrow L^2(B) \otimes L^2(B)$ can be written as*

$$\Lambda(\delta_v) \mapsto \Lambda(\delta_v) \otimes \Lambda(\delta_v).$$

Proof. The proof is a particular case of the one for Proposition 3.7, but let us present it again for this particular setting. From the above form of m , we have

$$\langle m^* \Lambda(\delta_v), \Lambda(\delta_{v'}) \otimes \Lambda(\delta_{w'}) \rangle = \langle \Lambda(\delta_v), m(\Lambda(\delta_{v'}) \otimes \Lambda(\delta_{w'})) \rangle = \langle \Lambda(\delta_v), \delta_{v',w'} \Lambda(\delta_{v'}) \rangle = \delta_{v,v'} \delta_{v',w'}.$$

The only possible solution for $m^* \Lambda(\delta_v)$ satisfying this condition is $\delta_v \otimes \delta_v$. $\square$

Corollary 3.11. *We have*

$$m^* \eta(\lambda) = \lambda \sum_{v \in V} \Lambda(\delta_v) \otimes \Lambda(\delta_v).$$

Given a linear transform $X \in \mathcal{B}(L^2(B))$, we represent it as the matrix $(X_{vw})_{v,w \in V}$ for the basis $\Lambda(\delta_v)_{v \in V}$. In other words, we put

$$X_{vw} = \langle \Lambda(\delta_v), X \Lambda(\delta_w) \rangle,$$

so that we have

$$X \Lambda(\delta_w) = \sum_v X_{vw} \Lambda(\delta_v).$$

Now, we can implement the Schur product (componentwise product) of matrices using m and m^* , as follows.

Proposition 3.12. *Consider two transforms $X, Y \in \mathcal{B}(L^2(B))$. We then have*

$$m(X \otimes Y) m^* = Z,$$

where Z is the transform whose matrix presentation is given by

$$Z_{uv} = X_{uv} Y_{uv} \quad (u, v \in V).$$

Proof. It's enough to prove $m(X \otimes Y) m^* \Lambda(\delta_v) = Z \Lambda(\delta_v)$ for all $v \in V$. We proceed by direct computation.

First, as we computed in Lemma 3.10, we have

$$m^*(\Lambda(\delta_v)) = \Lambda(\delta_v) \otimes \Lambda(\delta_v).$$

Applying $X \otimes Y$ to this tensor product yields

$$(X \otimes Y)(\Lambda(\delta_v) \otimes \Lambda(\delta_v)) = X \Lambda(\delta_v) \otimes Y \Lambda(\delta_v).$$

We can expand each factor as

$$X \Lambda(\delta_v) = \sum_w X_{wv} \Lambda(\delta_w), \quad Y \Lambda(\delta_v) = \sum_{w'} Y_{w'v} \Lambda(\delta_{w'}),$$

then applying the multiplication map m to the tensor product, we have

$$m \left(\sum_w X_{wv} \Lambda(\delta_w) \otimes \sum_{w'} Y_{w'v} \Lambda(\delta_{w'}) \right) = \sum_w X_{wv} Y_{wv} \Lambda(\delta_w).$$

This final expression is precisely $\sum_w Z_{wv} \Lambda(\delta_w)$, with Z_{wv} as in the assertion. $\square$

Proposition 3.13. *For $B = C(V)$ and $\psi = \psi_{\text{std}}$, a quantum adjacency matrix operator $A \in \mathcal{B}(L^2(B))$ is an operator that satisfies the following conditions:*

- $A_{vw} \in \{0, 1\}$ for all $v, w \in V$;
- $A_{vw} = A_{wv}$ for all $v, w \in V$;
- $A_{vv} = 1$ for all $v \in V$.

Proof. First, condition 2 in Definition 3.5 together with Proposition 3.12 with $X = Y = A$, implies $A_{vw}^2 = A_{vw}$. This forces A_{vw} to be either 0 or 1.

Focusing on condition 3, we consider

$$(m^* \eta \otimes \text{id})(\lambda \otimes e_w) = \lambda \sum_v e_v \otimes e_v \otimes e_w,$$

where $e_w = \Lambda(\delta_w)$ and $\lambda \in \mathbb{C}$. Applying $(\text{id} \otimes A \otimes \text{id})$, we obtain

$$\lambda \sum_v e_v \otimes \sum_u A_{uv} e_u \otimes e_w = \lambda \sum_{u,v} e_v \otimes A_{uv} e_u \otimes e_w.$$

We then apply $\text{id} \otimes \eta^* m$ to get

$$\lambda \sum_{u,v} e_v \otimes A_{uv} (\eta^* m(e_u \otimes e_w)) = \lambda \sum_{u,v} e_v \otimes A_{uv} (\eta^*(\delta_{u,w} e_u)).$$

This can be further computed as

$$\sum_{u,v} e_v \otimes A_{uv} \delta_{u,w} \psi(e_u) = \lambda \sum_{u,v} e_v \otimes A_{wv} \delta_{u,w} = \lambda \sum_v A_{wv} e_v$$

up to $L^2(B) \otimes \mathbb{C} \simeq L^2(B)$. Since this should match

$$Ae_w = \sum_v A_{vw}e_v,$$

we obtain $A_{vw} = A_{wv}$.

Since we have a real symmetric matrix, we also have condition 1.

Finally, using Proposition 3.12 again for $X = A$ and $Y = \text{id}$, we get the equivalence between $A_{vv} = 1$ for $v \in V$ and condition 4 in Definition 3.5. $\square$

These conditions describe an undirected graph whose vertex set is V , which has

- at most one edge between any two distinct vertices $v, w \in V$; and
- exactly one loop at each vertex v .

The last condition is just a normalization condition, and without losing information, we can consider graphs *without* loops at vertices, i.e., the simple graphs. That is, $A - \text{id}_B$ would correspond to the adjacency matrix of such a graph.

4. FIRST EXAMPLES OF NON-CLASSICAL QUANTUM GRAPHS

We have seen that classical graphs can be regarded as quantum graphs. Let us present some non-classical examples.

4.1. Complete and empty quantum graphs. Let us fix a finite dimensional C^* -algebra B and a positive faithful functional ψ .

Definition 4.1. The *complete quantum graph* on (B, ψ) is given by the following quantum adjacency matrix:

$$A(\Lambda_\psi(a)) = \psi(a)\Lambda_\psi(1_B).$$

In other words, A is the rank 1 operator $\eta\eta^*$.

The diagram manipulation in Figure 5 checks the conditions in Definition 3.5.

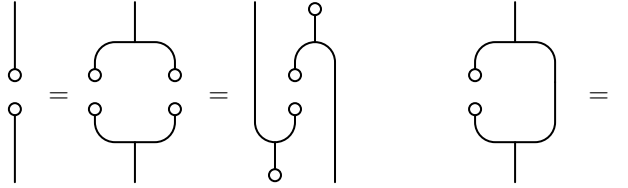


FIGURE 5. Complete quantum graph

Definition 4.2. The *empty quantum graph* on (B, ψ) is given by the following quantum adjacency matrix:

$$A = (mm^*)^{-1}.$$

To check that this choice is indeed a quantum adjacency matrix, we need the following key fact about finite dimensional C^* -algebras.

Proposition 4.3. *We have*

$$m^*m = (\text{id} \otimes m)(m^* \otimes \text{id}) = (m \otimes \text{id})(\text{id} \otimes m^*),$$

where id denotes the identity map of $L^2(B)$.

Proof. Consider $L^2(B) \otimes L^2(B)$ as a B -bimodule, where the left action of B is given by the left multiplication on the first factor (which is π_ψ), and the right action is given by the right multiplication on the second factor. Writing down the structures at hand, we have

$$a(\Lambda(b) \otimes \Lambda(c)) = \Lambda(ab) \otimes \Lambda(c), \quad (\Lambda(b) \otimes \Lambda(c))a = \Lambda(b) \otimes \Lambda(ca),$$

and

$$\langle a\Lambda(x), \Lambda(y) \rangle = \psi(x^*a^*y) = \langle \Lambda(x), a^*\Lambda(y) \rangle.$$

We claim that

$$(4.1) \quad m^*(\Lambda(a)) = am^*(\Lambda(1)) = m^*(\Lambda(1))a$$

holds for all $a \in B$. This means that $\Lambda(1)$ is a central vector, i.e., the effect of left and right actions of B agree on it.

Let us use this to compute the inner product of terms in (4.1) with a generic vector $\Lambda(b) \otimes \Lambda(c)$. As for the first term, we have

$$\langle m^*(\Lambda(a)), \Lambda(b) \otimes \Lambda(c) \rangle = \langle \Lambda(a), m(\Lambda(b) \otimes \Lambda(c)) \rangle = \langle \Lambda(a), \Lambda(bc) \rangle = \psi(a^*bc).$$

As for the second term, we have

$$\langle am^*(\Lambda(1)), \Lambda(b) \otimes \Lambda(c) \rangle = \langle m^*(\Lambda(1)), a^*\Lambda(b) \otimes \Lambda(c) \rangle = \langle m^*(\Lambda(1)), \Lambda(a^*b) \otimes \Lambda(c) \rangle.$$

This can be further computed as

$$\langle \Lambda(1), m(\Lambda(a^*b) \otimes \Lambda(c)) \rangle = \langle \Lambda(1), \Lambda(a^*bc) \rangle = \psi(a^*bc),$$

hence giving the same inner product as the first one.

Before computing the third one, we note that there is an algebra automorphism σ of B satisfying

$$(4.2) \quad \psi(ab) = \psi(b\sigma(a)).$$

(See below for the existence of such σ .) That implies

$$\langle \Lambda(x)a, \Lambda(y) \rangle = \psi(a^*xy) = \psi(x^*y\sigma(a^*)) = \langle \Lambda(x), \Lambda(y)\sigma(a^*) \rangle.$$

Now, for the third term of (4.1), we have

$$\langle m^*(\Lambda(1))a, \Lambda(b) \otimes \Lambda(c) \rangle = \langle m^*(\Lambda(1)), \Lambda(b) \otimes \Lambda(c)\sigma(a^*) \rangle,$$

which can be computed as

$$\psi(bc\sigma(a^*)) = \psi(a^*bc).$$

This again recovers the above inner products from the first and the second terms.

Now we are ready to prove the claim. Given $a, b \in B$, by applying (4.1) to ab and b , we get

$$m^*(\Lambda(ab)) = (ab)m^*(\Lambda(1)) = am^*(\Lambda(b)).$$

This says that we have

$$m^*m = (m \otimes \text{id})(\text{id} \otimes m^*).$$

A similar argument gives the equality with $(\text{id} \otimes m)(m^* \otimes \text{id})$. (Alternatively, we can also take the adjoint of the above equality.) $\square$

Remark 4.4. The above says that m^* is a homomorphism of B -bimodules. With such bimodule map $B \rightarrow B \otimes B$ with coassociativity and a map $B \rightarrow \mathbb{C}$ behaving as counit, we say that B is a *Frobenius algebra*.

Let's now prove the existence of σ as in (4.2). Observe that the bilinear form on B defined as

$$\Psi(a, b) = \psi(ab)$$

is non-degenerate. This means that, for a fixed a , if we consider the linear form on B given by

$$(4.3) \quad b \mapsto \psi(ab),$$

there must be a uniquely defined element $\sigma(a) \in B$ such that the linear form

$$b \mapsto \psi(b\sigma(a))$$

agrees with (4.3). The uniqueness implies that σ is an algebra automorphism, i.e., we have $\sigma(ab) = \sigma(a)\sigma(b)$.

One important consequence of the above proposition is that η^*m and $m^*\eta$ form a solution to the *conjugate equation* for $L^2(B, \psi)$, in the following sense.

Proposition 4.5. *We have*

$$(\text{id} \otimes \eta^*m)(m^*\eta \otimes \text{id}) = \text{id},$$

where id denotes the identity map of $L^2(B, \psi)$.

Proof. We can combine Proposition 4.3 with the unit condition for m and η , see Figure 6. $\square$

Proposition 4.6. *The operator $A = (mm^*)^{-1}$ on B is a quantum adjacency matrix operator.*

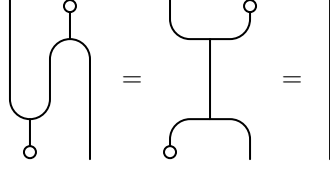


FIGURE 6. Checking the conjugate equation

Proof. By construction A is self adjoint. Let us check the other conditions using Proposition 4.3.

In order to check condition 2 in Definition 3.5, we can instead verify

$$(mm^*)m(A \otimes A)m^*(mm^*) = mm^*.$$

Proposition 4.3 implies

$$(mm^*)m(\text{id} \otimes A) = m,$$

see Figure 7 for diagrammatic calculus. A similar argument gives

$$(A \otimes \text{id})m^*(mm^*) = m^*,$$

hence we get the claim. Condition 4 can be checked in a similar way.

To check condition 3, we can instead check

$$(\text{id} \otimes \eta^* m)(\text{id} \otimes A \otimes mm^*)(m^* \eta \otimes \text{id}) = \text{id}.$$

By Proposition 4.3, we have

$$\eta^* m(mm^* \otimes \text{id}) = \eta^* m(\text{id} \otimes mm^*),$$

see Figure 8 for the diagrammatic calculus. This implies the claim. $\square$

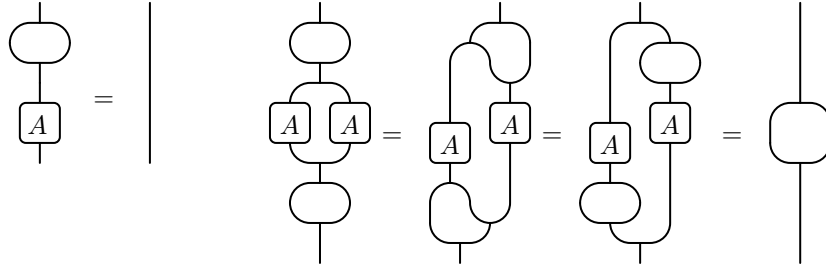


FIGURE 7. Convolution idempotent condition for the empty quantum graph

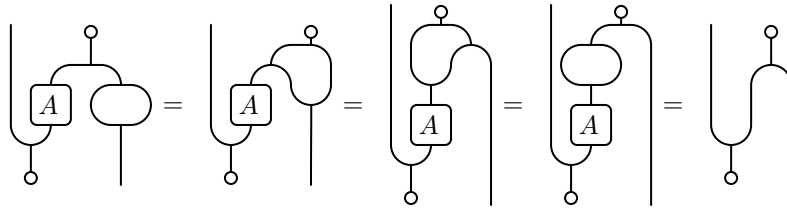


FIGURE 8. Symmetry conditions for the empty quantum graph

4.2. More on the automorphism σ . There is a more concrete presentation of σ based on the decomposition (3.1). If we restrict ψ to a direct summand M_{d_k} , for any $a \in M_{d_k}$, we have $\psi|_{M_{d_k}}(a) = \text{Tr}(Q_k a)$, where Q_k is a positive semi-definite matrix in M_{d_k} . (Existence and uniqueness of such Q_k follows from nondegeneracy of the trace pairing. The positivity follows from $\text{Tr}(Q_k a^* a) = \psi(a^* a) \geq 0$.) Since ψ is faithful, Q_k must be invertible. We then see that $\sigma^{(k)}(a) = Q_k a Q_k^{-1} \in M_{d_k}$ satisfies

$$\text{Tr}(Q_k ab) = \text{Tr}(\sigma^{(k)}(a) Q_k b) = \text{Tr}(Q_k b \sigma^{(k)}(a)).$$

Thus, $Q = \bigoplus_k Q_k \in B$ implements σ as $\sigma(a) = Q a Q^{-1}$ for $a \in B$.

The effect of multiplication by σ can be presented using the structure morphisms of B as follows.

Proposition 4.7. *We have*

$$\Lambda(\sigma(a)) = (\text{id} \otimes \eta^* m)(\text{id} \otimes \Lambda(a) \otimes \text{id}) m^* \eta, \quad \Lambda(\sigma^{-1}(a)) = (\eta^* m \otimes \text{id})(\text{id} \otimes \Lambda(a) \otimes \text{id}) m^* \eta.$$

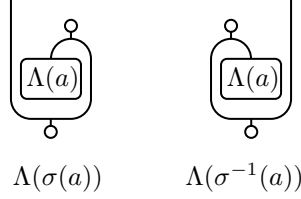


FIGURE 9. The actions of σ and σ^{-1}

Proof. The operations defined by left hand side are inverse to each other. We thus need to check that the candidate for $\Lambda(\sigma(a))$ satisfies the defining condition (4.2). We can manipulate this as in as in Figure 10 using Proposition 4.5. $\square$

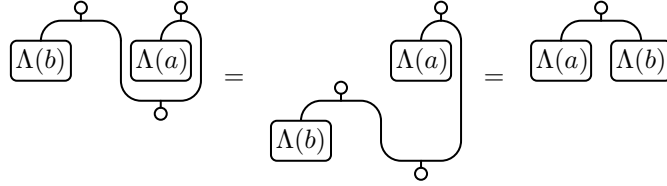


FIGURE 10. Exchanging a and b inside ψ up to the effect of σ

4.3. Quantum graphs from commutative groups. One rich source of quantum graph is the 2-cocycle deformation of groups. Let us explain a class of examples in this paradigm, based on the idea of Cayley graphs of commutative groups.

Definition 4.8. Let G be a finite group, and X be a subset of G . The *Cayley graph* $\text{Cay}(G, X)$ is constructed as follows:

- The vertex set is the group G itself.
- An edge from the vertex g to vertex h exists if and only if gh^{-1} is in X .

If an X is closed under inverse operation, we can represent the Cayley graph $\text{Cay}(G, X)$ as an undirected graph. Note that $\text{Cay}(G, X)$ has loops at each vertex if and only if the unit element e_G is in X . For our considerations, G is often chosen to be the finite-dimensional vector space over a finite field, denoted as $\mathbb{F}_p^d$.

By our discussion in Section 3.3, we have a quantum graph on the commutative algebra $C(G)$ corresponding to $\text{Cay}(G, X)$. Our goal is to deform $C(G)$ into a noncommutative algebra B and, through this transformation, derive a quantum adjoint matrix that corresponds to $\text{Cay}(G, X)$.

Definition 4.9. Let G be a finite commutative group. The *dual group* of G , denoted as $\hat{G}$, is defined as $\text{Hom}(G, \mathbb{T})$, where $\mathbb{T}$ is the unit circle of the complex plane,

$$\mathbb{T} = \{z \in \mathbb{C} \mid |z| = 1\},$$

with multiplicative group structure.

Remark 4.10. There exists an isomorphism between $\hat{G}$ and G , although it is not canonical. Specifically, when G is the cyclic group $\mathbb{Z}/n$, an element $\phi \in \hat{G}$ can be characterized by its value on the generator $[1] \in G$. Indeed, $\xi = \phi([1])$ must satisfy $\xi^n = 1$, and any such ξ leads to a well-defined ϕ by $\phi([k]) = \xi^k$. As the group of n -th roots of unit (in $\mathbb{C}$) is cyclic of order n , we have $\hat{G} \simeq G$. The general case is a direct product of this correspondence.

Definition 4.11. Let H be a group. Its group ring $\mathbb{C}[H]$ is defined as the space of formal linear combinations of the elements of H ,

$$\mathbb{C}[H] = \left\{ \sum_{h \in H} \alpha_h \cdot h \mid \alpha_h \in \mathbb{C} \right\},$$

together with the convolution product rule:

$$\left(\sum_{h \in H} \alpha_h \cdot h\right) \left(\sum_{k \in H} \beta_k \cdot k\right) = \sum_{h, k \in H} \alpha_h \beta_k \cdot (hk).$$

Proposition 4.12. *Let G be a finite commutative group. The algebra $C(G)$ is isomorphic to $\mathbb{C}[\hat{G}]$.*

Proof Sketch. This means that $C(G)$ is linearly spanned by the elements $\phi \in \hat{G}$, with the multiplication of the group $\hat{G}$ corresponding to the product as functions on G . To see that $C(G)$ is linearly spanned by the ϕ , one can look at translation actions by $g \in G$. These form a commuting family of linear transforms on $C(G)$, hence one can take the simultaneous eigendecomposition. The eigenvectors are precisely the elements $\phi \in \hat{G}$. $\square$

Up to the above identification, the standard positive functional on $C(G)$,

$$\psi_{\text{std}}: C(G) \rightarrow \mathbb{C}, \quad \psi_{\text{std}}(f) = \sum_{g \in G} f(g),$$

becomes a functional on $\mathbb{C}[\hat{G}]$ given by

$$(4.4) \quad \psi_{\text{std}}\left(\sum_{\phi \in \hat{G}} \alpha_{\phi} \cdot \phi\right) = |G| \alpha_e.$$

Definition 4.13. Let H be a group (which will be $\hat{G}$ in our case). A *2-cocycle* on H is a function

$$\omega: H \times H \rightarrow \mathbb{T}$$

satisfying

$$\omega(h_1 h_2, h_3) \omega(h_1, h_2) = \omega(h_1, h_2 h_3) \omega(h_2, h_3).$$

Such a 2-cocycle is *normalized* if it satisfies

$$\omega(h, e) = \omega(e, h) = \omega(h, h^{-1}) = 1.$$

We may assume 2-cocycles to be normalized without losing generality, which we tacitly assume in the following. (Any 2-cocycle is cohomologous to a normalized one.)

Definition 4.14. Let H be a group, and ω be a 2-cocycle on H . The *twisted group ring*, denoted as $\mathbb{C}_{\omega}[H]$, is the ring with the same underlying linear space as $\mathbb{C}[H]$, but with the product

$$m_{\omega}(h_1, h_2) = \omega(h_1, h_2)(h_1 h_2).$$

The associativity condition for the above product follows from the 2-cocycle condition. As we assume that ω is normalized, the unit element e_H is still the multiplicative unit of $\mathbb{C}_{\omega}[H]$.

Example 4.15. Consider $H = \mathbb{Z}_2^2$, and the 2-cocycle ω defined by

$$\omega(h, h') = (-1)^{h_1 h'_2 + h_2 h'_1},$$

where we write the components of h as h_1, h_2 . Then the twisted group algebra $\mathbb{C}_{\omega}[H]$ is isomorphic to M_2 . (Concretely, we can use the Pauli matrices to write this isomorphism.) Generally, for $H = \mathbb{Z}_n^2$, given an n -th root of unity ξ , we have a 2-cocycle defined by

$$\omega(h, h') = \xi^{h_1 h'_2 - h_2 h'_1}.$$

When ξ is a primitive n -th root of unity, we have $\mathbb{C}_{\omega}[H] \simeq M_n$.

An analogue of (4.4),

$$\psi_{\text{std}}\left(\sum_h \alpha_h \cdot h\right) = |H| \alpha_e$$

still gives a positive faithful functional on $\mathbb{C}_{\omega}[H]$. (One way to see this is by representing $\mathbb{C}_{\omega}[H]$ on $\ell^2(H)$ by $\pi(h)\delta_k = \omega(h, k)\delta_{hk}$, and compare ψ_{std} with the vector functional for $\sqrt{|H|}\delta_e$.) Let us identify m^* for this choice of functional.

Proposition 4.16. *The adjoint m^* on $L^2(\mathbb{C}_{\omega}[H], \psi_{\text{std}})$ is given by*

$$m^*(\Lambda(h)) = \frac{1}{|H|} \sum_{k \in H} \overline{\omega(k^{-1}, kh)} \Lambda(k^{-1}) \otimes \Lambda(kh).$$

Proof. We need to check the condition

$$\langle m^*(\Lambda(a)), \Lambda(b) \otimes \Lambda(c) \rangle = \langle \Lambda(a), \Lambda(b \cdot_\omega c) \rangle \quad (a, b, c \in \mathbb{C}_\omega[H])$$

for the right hand side of the claim. We can directly check it using

$$\langle \Lambda(h), \Lambda(k) \rangle = |H| \delta_{k,h},$$

and the product rule in $\mathbb{C}_\omega[H]$. $\square$

Remark 4.17. The above implies that mm^* is the identity map on $L^2(\mathbb{C}_\omega[H], \psi_{\text{std}})$. That is, ψ_{std} is a δ -form with $\delta = |H|$.

Now, let us consider Cayley graphs of commutative groups G with respect to subsets X . To match our convention of quantum graphs, we assume that X contains the unit of G , and is invariant under the inverse map. The (quantum) adjacency matrix of $\text{Cay}(G, X)$ is given by

$$A\delta_h = \sum_{x \in X} \delta_{xh}.$$

In other words, if λ_x denotes the (left) translation operator $\delta_h \mapsto \delta_{xh}$ (equivalently, $(\lambda_g f)(h) = f(g^{-1}h)$), we have

$$A = \sum_{x \in X} \lambda_x.$$

Since G is commutative, A commutes with any λ_g for $g \in G$. In particular, A is diagonalized by the joint eigenvectors of the λ_g .

Recall that the characters $\phi \in \hat{G}$ provide a complete system of eigenvectors, since we have

$$(\lambda_g \phi)(h) = \phi(g^{-1}h) = \overline{\phi(g)} \phi(h),$$

meaning that $\overline{\phi(g)}$ is the eigenvalue of λ_g on ϕ . Therefore, we have $A\phi = \alpha_\phi \phi$ for some real number α_ϕ . Proposition 4.16 for $H = \hat{G}$ and trivial ω implies that, condition 2 in Definition 3.5 is equivalent to

$$\sum_{\phi'} \alpha_{\phi'^{-1}} \alpha_{\phi'} \phi = |G| \alpha_\phi.$$

Similarly, condition 3 is equivalent to $\alpha_{\phi^{-1}} = \alpha_\phi$, and condition 4 is equivalent to $\sum_\phi \alpha_\phi = |G|$.

Proposition 4.18. *Let ω be a 2-cocycle on $\hat{G}$, and let $(\alpha_\phi)_\phi$ be the numbers parametrized by $\phi \in \hat{G}$, satisfying the conditions as above. Then the map*

$$A: L^2(\mathbb{C}_\omega[\hat{G}]) \rightarrow L^2(\mathbb{C}_\omega[\hat{G}]), \quad \Lambda(\phi) \mapsto \alpha_\phi \Lambda(\phi)$$

is a quantum adjacency matrix operator for $(\mathbb{C}_\omega[\hat{G}], \psi_{\text{std}})$.

Proof. Again we can use Proposition 4.16 to translate the conditions for $(\alpha_\phi)_\phi$ to the conditions in Definition 3.5. $\square$

Example 4.19. Consider the group $G = \mathbb{Z}_2^2$ and its subset $X = \{[0, 0], [0, 1], [1, 0]\}$. Let us identify $\hat{G}$ with G as in Remark 4.10. The eigenvalues of A are

$$\alpha_{[0,0]} = 3, \quad \alpha_{[1,0]} = \alpha_{[0,1]} = 1, \quad \alpha_{[1,1]} = -1.$$

Take the 2-cocycle ω on $\hat{G}$ as in Example 4.15, so that we have $\mathbb{C}_\omega[\hat{G}] \simeq M_2$. This one is neither the complete graph (which has just one eigenvalue for a δ -form) nor the empty quantum graph (which has rank 1) from Section 4.1.

5. QUANTUM GRAPHS THROUGH OPERATOR BIMODULES

Let us present another way to understand quantum graphs, based on the idea of *operator bimodules*. Historically, this was the first way the quantum graphs were conceived, independently by Duan [Dua09] (for matrix algebras) in quantum information theory and Weaver [Wea12] (for von Neumann algebras) in operator algebras. One feature of this approach is that the quantum graphs are defined independent of positive functionals, but instead using (unitary and faithful) representations of C^* -algebras, i.e., realization of B as subalgebras of $\mathcal{B}(H)$.

5.1. Quantum graphs as bimodules. Suppose that B is faithfully represented on a finite dimensional Hilbert space $H \simeq \mathbb{C}^N$, that is, we have an injective $*$ -homomorphism $\pi: B \rightarrow \mathcal{B}(H) \simeq M_N$. Let $\pi(B)'$ denote the *commutant* of $\pi(B)$ in $\mathcal{B}(H)$, which is the subalgebra of $\mathcal{B}(H)$ defined as

$$\pi(B)' = \{T \in \mathcal{B}(H) \mid \forall a \in B: \pi(a)T = T\pi(a)\}.$$

It is again a finite-dimensional C^* -algebra. Indeed, if T_1 and T_2 are in $\pi(B)'$, their product satisfies $\pi(a)T_1T_2 = T_1T_2\pi(a)$ for $a \in B$ by

$$\pi(a)T_1T_2 = T_1\pi(a)T_2 = T_1T_2\pi(a),$$

and we can check that T_1^* is also in $\pi(B)'$ using

$$(T_1\pi(a))^* = \pi(a)^*T_1^* = \pi(a^*)T_1^*$$

and a similar formula for $(\pi(a)T_1)^*$.

Definition 5.1 ([Wea12]). Let π be a faithful representation of B as above. A *quantum relation* on (B, π) is a subspace $S \subset \mathcal{B}(H)$ such that $\pi(B)'S\pi(B)' = S$. In other words, S is a $\pi(B)'$ -bimodule.

Here, $\pi(B)'S\pi(B)'$ denotes the linear span of the operators of the form $\pi(a)T\pi(b)$ for $a, b \in B$ and $T \in S$.

Definition 5.2. A *quantum graph* on (B, π) is a quantum relation on (B, π) satisfying the following conditions:

- (1) S is *reflexive*: $\pi(B)' \subset S$, or equivalently, $\text{id}_H \in S$; and
- (2) S is *symmetric*: $S = S^*$, that is, for any $T \in S$, we have $T^* \in S$.

The above conditions say that S is an *operator system* in $\mathcal{B}(H)$. Thus, we can say that the quantum graphs on (B, π) are operator systems which are in addition a bimodule for the commutant C^* -algebra for B .

Remark 5.3. Note that this definition makes sense when B and H are allowed to be infinite dimensional. In this case, we should assume that S is closed in a suitable topology, such as the topology of pointwise convergence as linear transforms on H (either with respect to the norm topology or the weak topology on H).

We will later develop methods to translate between quantum graphs (B, ψ, A) as previously described and quantum graphs (B, π, S) described above. We will now illustrate how the complete and empty graphs from Section 4.1 look under the bimodule approach, saving the proofs for later.

Example 5.4 (cf. Definition 4.1). Recall that for (B, ψ) the complete quantum graph is defined by the quantum adjacency matrix $A = \eta\eta^*$. Under the bimodule approach, this corresponds to $S = \mathcal{B}(H)$, the biggest possible bimodule.

Example 5.5 (cf. Definition 4.2). Recall that the empty graph is given by $A = (mm^*)^{-1}$. Under the bimodule approach, this corresponds to $S = \pi(B)'$, the smallest possible operator system bimodule.

5.2. Comparison for different representations. The above definitions depend on the choice of faithful representation π . However, when π and π' are two different faithful representations of B , there is a one-to-one correspondence between quantum relations S for (B, π) and quantum relations S' for (B, π') . To see that, let us first give a concrete presentation of π and $\pi(B)'$ based on the decomposition (3.1).

Let N be the dimension of target Hilbert space H , so that π can be considered as a homomorphism $B \rightarrow M_N$. Each direct summand M_{d_k} in the decomposition $B = \bigoplus_{k=1}^n M_{d_k}$ will act on some subspace of $\mathbb{C}^N$ with some multiplicity, say m_k . This means that π is of the form

$$X_1 \oplus X_2 \oplus \dots \oplus X_n \mapsto (X_1 \otimes I_{m_1}) \oplus \dots \oplus (X_n \otimes I_{m_n}),$$

where $N = d_1m_1 + \dots + d_nm_n$. Since π is faithful, we have $m_k > 0$ for all k . In particular, $\pi(B)$ becomes the subalgebra $\bigoplus_{k=1}^n (M_{d_k} \otimes I_{m_k})$ of M_N . Then the commutant becomes

$$\pi(B)' = \bigoplus_{k=1}^n (I_{d_k} \otimes M_{m_k}) \simeq \bigoplus_{k=1}^n M_{m_k}.$$

We obtain a similar description for the representation π' on H' . Thus, if m'_k is the multiplicity of M_{d_k} under π' , the target space has dimension $N' = d_1m'_1 + \dots + d_nm'_n$, and we can write

$$\pi'(B)' = \bigoplus_{k=1}^n (I_{d_k} \otimes M_{m'_k}) \simeq \bigoplus_{k=1}^n M_{m'_k}.$$

Now consider

$$K = \bigoplus_{k=1}^n I_{d_k} \otimes M_{m'_k \times m_k} \subset \mathcal{B}(H, H').$$

Given a quantum relation $S \subset \mathcal{B}(H)$ for (B, π) , we set $S' = KSK^* \subset \mathcal{B}(H')$. As we have $\pi'(B)'K\pi(B)' = K$, we get $\pi'(B)'S'\pi'(B)' = S'$, hence S' becomes a $\pi'(B)'$ -bimodule, i.e., a quantum relation on (B, π') . From the above presentations of $\pi(B)'$ and $\pi'(B)'$, we have

$$K^*K = \pi(B)', \quad KK^* = \pi'(B)'.$$

This implies that the correspondence $S \leftrightarrow S'$ between the quantum relations for (B, π) and those for (B, π') is bijective.

Moreover, this correspondence maps quantum graphs to quantum graphs. To be precise, if $S^* = S$ holds, then by definition of S' we get $S'^* = S'$. Similarly, if id_H is in S , then we have $KK^* \subset S'$, which contains $\text{id}_{H'}$.

5.3. Bimodules from classical graphs. Next, let us explain how to package the classical graphs in the bimodule formalism. As before, let V be a finite set, and consider $B = C(V)$ (complex valued functions on V). As a representation we take

$$\pi: B \rightarrow \mathcal{B}(\ell^2(V))$$

given by pointwise multiplication, that is, $\pi(f)\delta_v = f(v)\delta_v$. We then have the following structural result for the commutant.

Proposition 5.6. *We have $\pi(B)' = \pi(B)$, that is, $\pi(B)$ is a maximal abelian subalgebra of $\mathcal{B}(\ell^2(V))$.*

Proof. As usual, let us represent the elements of $\mathcal{B}(\ell^2(V))$ with respect to the basis $(\delta_v)_{v \in V}$ of $\ell^2(V)$. Then $\pi(B)$ corresponds to the algebra of all diagonal matrices. Now, the only matrices that commute with all diagonal matrices are the diagonal matrices themselves. $\square$

Proposition 5.7. *Any quantum relation for (B, π) is of the form*

$$S_E = \{(X_{vw})_{v,w \in V} \in M_V \mid \forall (v, w) \notin E: X_{vw} = 0\}$$

for some subset $E \subset V \times V$.

Proof. Given a quantum relation $S \subset \mathcal{B}(\ell^2(V))$, set

$$E_S = \{(v, w) \in V \times V \mid \exists X \in S: X_{vw} \neq 0\}.$$

We have $S_{E_S} \supset S$ from the definition, so it remains to prove the converse inclusion.

Using $\pi(B)'S\pi(B)' = S$, we see that S is spanned by the elements $\pi(\delta_v)T\pi(\delta_w)$ for $v, w \in V$ and $T \in S$. We have $(v, w) \in E_S$ if and only if this is nonzero for some T . We thus have $S_{E_S} \subset S$. $\square$

Corollary 5.8. *Any quantum graph on (B, π) is of the form S_E , where $E \subset V \times V$ is the edge set for some undirected graph with loops at the vertices $v \in V$.*

Proof. We first check that there are loops at the vertices, that is, $(v, v) \in E_S$ for $v \in V$. By definition we have $\pi(B)' \subset S$, and we now have $\pi(B)' = \pi(B)$. The element $\pi(\delta_v) \in \pi(B)$, corresponds to the diagonal matrix whose only nonzero entry is 1 at the position v , and this implies $(v, v) \in E_S$.

Next let us check that the graph is undirected, that is, $(v, w) \in E$ if and only if $(w, v) \in E$. Assuming $(v, w) \in E_S$, we can find $T \in S$ such that $T_{vw} \neq 0$. Since we have $S = S^*$, the adjoint T^* is also in S . Now, $T_{vw}^* = \overline{T_{vw}} \neq 0$ implies $(w, v) \in E_S$. $\square$

5.4. Correspondence between quantum adjacency matrices and operator system bimodules.

Let us explain how to obtain a quantum graph on (B, π) , i.e., an operator system bimodule as in Definition 5.2, from a quantum graph on (B, ψ) given by a quantum adjacency matrix as in Definition 3.5. Here we closely follow [Daw22].

We denote the *opposite algebra* of B by B^{op} , and denote the element of B^{op} corresponding to $a \in B$ by a^{op} . Thus, as a set we have $B^{\text{op}} = \{a^{\text{op}} \mid a \in B\}$, with the C^* -algebra structure

$$a^{\text{op}}b^{\text{op}} = (ba)^{\text{op}}, \quad (a^{\text{op}})^* = (a^*)^{\text{op}}.$$

We consider the “flip” operator Σ on $B \otimes B^{\text{op}}$ defined by

$$\Sigma(a \otimes b^{\text{op}}) = b \otimes a^{\text{op}}.$$

Next, let $\Psi: \mathcal{B}(L^2(B, \psi)) \rightarrow B \otimes B^{\text{op}}$ be the linear extension of the map

$$\Lambda(b)\Lambda(a)^* \mapsto a^* \otimes b^{\text{op}}.$$

This is a linear bijection.

Finally, we need the automorphism σ satisfying $\psi(ab) = \psi(b\sigma(a))$ as in the proof of Proposition 4.3, and its natural extension to one-parameter automorphism group. Recall that there is a positive invertible element $Q \in B$ such that $\sigma(a) = QaQ^{-1}$, see Section 4.2. We then put $\sigma_z(a) = Q^{iz}aQ^{-iz}$ for $z \in \mathbb{C}$. Thus, σ_{-i} agrees with the above automorphism σ , while we also have the additivity of parameters $\sigma_z(\sigma_w(a)) = \sigma_{z+w}(a)$. We also consider the automorphism σ_z^{op} on B^{op} given by $\sigma_z^{\text{op}}(a^{\text{op}}) = (\sigma_z(a))^{\text{op}}$.

Now, we can express various operations on linear transforms in terms of $B \otimes B^{\text{op}}$, as follows.

Proposition 5.9. *For any $A, A_1, A_2 \in \mathcal{B}(L^2(B, \psi))$, the following equalities hold:*

- (1) $\Psi(A^*) = \Sigma(\Psi(A)^*) = (\Sigma(\Psi(A)))^*$;
- (2) $\Psi((\text{id} \otimes \eta^* m)(\text{id} \otimes A \otimes \text{id})(m^* \eta \otimes \text{id})) = (\text{id}_B \otimes \sigma_{-i}^{\text{op}})(\Sigma(\Psi(A)))$;
- (3) $\Psi((\eta^* m \otimes \text{id})(\text{id} \otimes A \otimes \text{id})(\text{id} \otimes m^* \eta)) = (\sigma_i \otimes \text{id}_{B^{\text{op}}})(\Sigma\Psi(A))$; and
- (4) $\Psi(m(A_1 \otimes A_2)m^*) = \Psi(A_2)\Psi(A_1)$.

Proof. Since $\mathcal{B}(L^2(B, \psi))$ is spanned by the operators $\Lambda(b)\Lambda(a)^*$ for $a, b \in B$, it suffices to check each claim for the case $A = \Lambda(b)\Lambda(a)^*$.

Claim 1: We have $(\Lambda(b)\Lambda(a)^*)^* = \Lambda(a)\Lambda(b)^*$. We then compute

$$\Psi((\Lambda(b)\Lambda(a)^*)^*) = b^* \otimes a^{\text{op}} = \Sigma\Psi(\Lambda(b)\Lambda(a)^*)^*.$$

Similarly, $(a^*)^{\text{op}} = (a^*)^{\text{op}}$ gives the equality with $(\Sigma(\Psi(A)))^*$.

Claim 2: By construction we have $(\text{id}_B \otimes \sigma_{-i}^{\text{op}})(\Sigma(\Psi(\Lambda(b)\Lambda(a)^*))) = b \otimes \sigma_{-i}(a^*)^{\text{op}}$. Thus, the claim is equivalent to

$$\langle \Lambda(x), (\text{id} \otimes \eta^* m)(\text{id} \otimes \Lambda(b)\Lambda(a)^* \otimes \text{id})(m^* \eta \otimes \text{id})\Lambda(y) \rangle = \langle \Lambda(x), \Lambda(\sigma_{-i}(a^*))\Lambda(b^*)^*\Lambda(y) \rangle \quad (x, y \in B).$$

On one hand, the right side is equal to

$$\langle \Lambda(b^*), \Lambda(y) \rangle \langle \Lambda(x), \Lambda(\sigma_{-i}(a^*)) \rangle = \psi(by)\psi(x^*\sigma_{-i}(a^*)).$$

On the other, the calculations in Figure 11 then show that the left side is equal to $\overline{\psi(xa)}\psi(by)$. By

$$\overline{\psi(xa)} = \overline{\text{Tr}(Qxa)} = \text{Tr}(a^*x^*Q) = \text{Tr}(Qx^*Qa^*Q^{-1}) = \psi(x^*\sigma_{-i}(a^*)),$$

we get the desired equality.

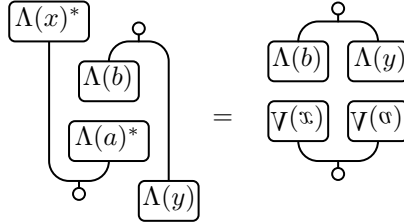


FIGURE 11. Diagrammatic calculus of $\langle \Lambda(x), (\text{id} \otimes \eta^* m)(\text{id} \otimes \Lambda(b)\Lambda(a)^* \otimes \text{id})(m^* \eta \otimes \text{id})\Lambda(y) \rangle$

Claim 3: This is similar to Claim 2.

Claim 4: For $a_1, b_1, a_2, b_2, c \in B$, we compute

$$m(\Lambda(b_1)\Lambda(a_1)^* \otimes \Lambda(b_2)\Lambda(a_2)^*)m^*\Lambda(c) = \langle \Lambda(a_1a_2), \Lambda(c) \rangle \Lambda(b_1b_2),$$

see Figure 12. This means

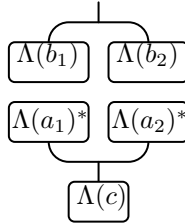


FIGURE 12. Diagrammatic presentation of $m(\Lambda(b_1)\Lambda(a_1)^* \otimes \Lambda(b_2)\Lambda(a_2)^*)m^*\Lambda(c)$

$$m(\Lambda(b_1)\Lambda(a_1)^* \otimes \Lambda(b_2)\Lambda(a_2)^*)m^* = \Lambda(b_1b_2)\Lambda(a_1a_2)^*$$

We then have

$$\Psi(\Lambda(b_1 b_2) \Lambda(a_1 a_2)^*) = (a_1 a_2)^* \otimes (b_1 b_2)^{\text{op}} = a_2^* a_1^* \otimes b_2^{\text{op}} b_1^{\text{op}},$$

which is indeed equal to $\Psi(\Lambda(b_2) \Lambda(a_2)^*) \Psi(\Lambda(b_1) \Lambda(a_1)^*)$. $\square$

Now we are ready to transform the conditions for quantum adjacency matrices to the ones for elements in $B \otimes B^{\text{op}}$.

Theorem 5.10. *The map*

$$\Psi_{0,1/2} = (\text{id}_B \otimes \sigma_{i/2}^{\text{op}}) \Psi: \mathcal{B}(L^2(B, \psi)) \rightarrow B \otimes B^{\text{op}}$$

gives a bijective correspondence between the sets

$$\{A \in \mathcal{B}(L^2(B, \psi)) \mid A = A^* = m(A \otimes A)m^* = (\text{id} \otimes \eta^* m)(\text{id} \otimes A \otimes \text{id})(m^* \eta \otimes \text{id})\}$$

and

$$\{e \in B \otimes B^{\text{op}} \mid e = e^* = e^2 = \Sigma e, \forall z \in \mathbb{C}: e = (\sigma_z \otimes \sigma_z^{\text{op}})(e)\}.$$

Proof. Let us record the direct consequences of Proposition 5.9 for $\Psi_{0,1/2}$. First, since $\sigma_{i/2}^{\text{op}}$ is an automorphism of B^{op} , claim 4 of Proposition 5.9 implies that we have

$$(5.1) \quad \Psi_{0,1/2}(m(A_1 \otimes A_2)m^*) = (\text{id}_B \otimes \sigma_{i/2}^{\text{op}})(\Psi(A_2)\Psi(A_1)) = \Psi_{0,1/2}(A_2)\Psi_{0,1/2}(A_1).$$

Next, item 2 of Proposition 5.9 gives

$$\Psi_{0,1/2}((\text{id} \otimes \eta^* m)(\text{id} \otimes A \otimes \text{id})(m^* \eta \otimes \text{id})) = (\sigma_{-i/2} \otimes \sigma_{-i/2}^{\text{op}}) \Sigma \Psi_{0,1/2}(A)$$

for general A . Moreover, we have

$$(5.2) \quad \sigma_{i/2}(a)^* = (Q^{-1/2} a Q^{1/2})^* = Q^{1/2} a^* Q^{-1/2} = \sigma_{-i/2}(a^*),$$

which together with item 1 of Proposition 5.9 gives

$$(5.3) \quad \Psi_{0,1/2}(A^*) = (\sigma_{i/2} \otimes \sigma_{i/2}^{\text{op}}) \Sigma \Psi_{0,1/2}(A)^*.$$

Now, let us write $e = \Psi_{0,1/2}(A)$, and work out how the conditions for these sets correspond to each other. First, (5.1) implies that $A = m(A \otimes A)m^*$ holds if and only if $e = e^2$ holds. Moreover, in view of (5.3), $A = A^*$ is equivalent to

$$(5.4) \quad e = (\sigma_{i/2} \otimes \sigma_{i/2}^{\text{op}}) \Sigma(e^*),$$

while $A = (\text{id} \otimes \eta^* m)(\text{id} \otimes A \otimes \text{id})(m^* \eta \otimes \text{id})$ is equivalent to

$$(5.5) \quad e = (\sigma_{-i/2} \otimes \sigma_{-i/2}^{\text{op}}) \Sigma(e).$$

If these are equal, then (5.2) implies that $\Sigma(e)$ is invariant under the involution $*$. Of course, the latter property is equivalent to $e = e^*$. Once we know this, we also get

$$e = (\sigma_i \otimes \sigma_i^{\text{op}})(e) = (Q^{-1} \otimes Q^{\text{op}})e(Q \otimes (Q^{-1})^{\text{op}}).$$

Then we see that e commutes with $f(Q^{-1} \otimes Q^{\text{op}})$ for any (complex) analytic function $f(t)$ in one real variable. In particular, $f(x) = x^{iz}$ gives us $e = (\sigma_z \otimes \sigma_z^{\text{op}})(e)$. The equality at $z = 1/2$, together with (5.5), implies $e = \Sigma(e)$.

Conversely, suppose that e agrees with e^* , $\Sigma(e)$, and $(\sigma_z \otimes \sigma_z^{\text{op}})(e)$ for $z \in \mathbb{C}$. Then equalities (5.4) and (5.5) hold, which implies $A = A^*$ and $A = (\text{id} \otimes \eta^* m)(\text{id} \otimes A \otimes \text{id})(m^* \eta \otimes \text{id})$ respectively. $\square$

Given a faithful representation $\pi: B \rightarrow \mathcal{B}(H)$, we now want to relate $e \in B \otimes B^{\text{op}}$ as described above to a operator system bimodule $S \subset \mathcal{B}(H)$. As an intermediate step, we relate e to a subspace V of $H \otimes H^*$.

The representation π gives rise to the representation $\pi^{\text{op}}: B^{\text{op}} \rightarrow \mathcal{B}(H^*)$ by $\pi^{\text{op}}(a^{\text{op}})v^* = v^* \pi(a)$ which in turn gives a representation $\pi \otimes \pi^{\text{op}}: B \otimes B^{\text{op}} \rightarrow \mathcal{B}(H \otimes H^*)$. By $e = e^2 = e^*$, the operator $(\pi \otimes \pi^{\text{op}})(e)$ is an orthogonal projection on $H \otimes H^*$, and it defines a subspace $V = (\pi \otimes \pi^{\text{op}})(e)(H \otimes H^*)$.

Now, the space $\mathcal{B}(H)$ (together with the Hilbert–Schmidt inner product) is isomorphic to $H \otimes H^*$ via the map $wv^* \mapsto w \otimes v^*$. Under this correspondence, the above representation $\pi \otimes \pi^{\text{op}}$ becomes the action of $B \otimes B^{\text{op}}$ on $\mathcal{B}(H)$ given by $(a \otimes b^{\text{op}})T = \pi(a)T\pi(b)$. Now, the subspace V can be regarded as a subspace S_0 of $\mathcal{B}(H)$.

To see that S_0 is a $\pi(B)'$ -bimodule, observe that $(\pi \otimes \pi^{\text{op}})(B \otimes B^{\text{op}})' = \pi(B)' \otimes \pi^{\text{op}}(B^{\text{op}})'$. This implies $(\pi(B)' \otimes \pi^{\text{op}}(B^{\text{op}})')V = V$, which translates to $\pi(B)'S_0\pi(B)' = S_0$.

Next consider the antilinear operator $J_0: H \otimes H^* \rightarrow H \otimes H^*$ defined by $v \otimes w^* \mapsto w \otimes v^*$, which corresponds to the adjoint operation on $\mathcal{B}(H)$. We then have

$$(\pi \otimes \pi^{\text{op}})(\Sigma e^*) = J_0(\pi \otimes \pi^{\text{op}})(e)J_0,$$

which implies

$$V = (\pi \otimes \pi^{\text{op}})(e)(H \otimes H^*) = (\pi \otimes \pi^{\text{op}})(\Sigma e^*)(H \otimes H^*) = J_0(\pi \otimes \pi^{\text{op}})(e)(H \otimes H^*) = J_0(V).$$

This means that S_0 is self adjoint.

Moreover, we can use

$$(\pi \otimes \pi^{\text{op}})(\sigma_{-i} \otimes \sigma_{-i}^{\text{op}})(e) = (\pi(Q) \otimes \pi^{\text{op}}((Q^{-1})^{\text{op}}))(\pi \otimes \pi^{\text{op}})(e)(\pi(Q^{-1}) \otimes \pi^{\text{op}}(Q^{\text{op}}))$$

and $e = (\sigma_{-i} \otimes \sigma_{-i}^{\text{op}})(e)$, combined with a similar argument as above to get

$$V = (\pi(Q) \otimes \pi^{\text{op}}((Q^{-1})^{\text{op}}))V.$$

This corresponds to

$$S_0 = \pi(Q)S_0\pi(Q^{-1}).$$

So far our construction of S_0 does not give an operator system, that is, we still do not know if $\text{id}_H \in S_0$ holds. As it turns out, the best we can hope for is $\pi(Q^{-1/2})$ to be in S_0 from the outstanding condition from Definition 3.5, namely, $m(A \otimes \text{id})m^* = \text{id}$.

Lemma 5.11. *For $a, b, c \in B$, we have*

$$(m(\Lambda(b)\Lambda(a)^* \otimes \text{id})m^*)(\Lambda(c)) = \Lambda(ba^*c).$$

Proof. Take an orthonormal basis $(\Lambda(x_i))_{i=1}^n$ of $L^2(B, \psi)$, so that $\sum_{i=1}^n \Lambda(x_i)\Lambda(x_i)^*$ represents the identity map on $L^2(B, \psi)$. We then compute

$$\begin{aligned} (m(\Lambda(b)\Lambda(a)^* \otimes \text{id})m^*)(\Lambda(c)) &= \sum_{i=1}^n (m(\Lambda(b) \otimes \Lambda(x_i))(\Lambda(a)^* \otimes \Lambda(x_i)^*)m^*)(\Lambda(c)) \\ &= \sum_{i=1}^n \Lambda(bx_i)(m(\Lambda(a) \otimes \Lambda(x_i)))^*\Lambda(c). \end{aligned}$$

Using the inner product, this can be expanded as

$$\sum_{i=1}^n \langle \Lambda(ax_i), \Lambda(c) \rangle \Lambda(bx_i) = \sum_{i=1}^n \langle \pi(a)\Lambda(x_i), \Lambda(c) \rangle \Lambda(bx_i) = \pi(b) \sum_{i=1}^n \langle \Lambda(x_i), \pi(a^*)\Lambda(c) \rangle \Lambda(x_i),$$

which is indeed equal to $\pi(b)\pi(a^*)\Lambda(c) = \Lambda(ba^*c)$. $\square$

We are now ready to characterize the final property of quantum adjacency matrices.

Proposition 5.12. *Let A be an element of the subset of $\mathcal{B}(L^2(B, \psi))$ from Theorem 5.10. Moreover, let $\pi: B \rightarrow \mathcal{B}(H)$ be a faithful representation, and let $S_0 \subset \mathcal{B}(H)$ be the $\pi(B)'$ -bimodule subspace given by the above correspondence. Then $m(A \otimes \text{id})m^* = \text{id}$ holds if and only if $\pi(Q^{-1/2}) \in S_0$ holds.*

Proof. Write $A = \sum_j \Lambda(b_j)\Lambda(a_j)^*$ for $a_j, b_j \in B$. By Lemma 5.11, we have

$$m(A \otimes \text{id})m^* = \sum_j \pi(b_j a_j^*).$$

Now, pick an orthonormal basis $(v_i)_i$ of H , and set $\hat{1} = \sum_i v_i \otimes v_i^* \in H \otimes H^*$.

Up to the unitary isomorphism between $H \otimes H^*$ and $\mathcal{B}(H)$ with the Hilbert–Schmidt inner product, the vector $\hat{1}$ corresponds to id_H in $\mathcal{B}(H)$. Thus, the vector $(\pi(a) \otimes \pi^{\text{op}}(b^{\text{op}}))\hat{1}$ corresponds to $\pi(a)\text{id}_H\pi(b) = \pi(a)\pi(b)$ in $\mathcal{B}(H)$. Thus, $\sum_j \pi(b_j a_j^*) = \text{id}$ holds if and only if

$$(5.6) \quad \sum_j (\pi(a_j) \otimes \pi^{\text{op}}((b_j^*)^{\text{op}}))\hat{1} = \hat{1}$$

holds.

We now check that this is equivalent to $\pi \otimes \pi^{\text{op}}(e)$ preserving the vector $u = (\text{id}_H \otimes \pi^{\text{op}}(Q^{-1/2}))\hat{1}$. The latter is equivalent to $u \in \pi \otimes \pi^{\text{op}}(e)(H \otimes H^*)$, or equivalently, to $\pi(Q^{-1/2}) \in S_0$.

Using $e = e^*$ and $\sigma_{i/2}(b)^* = \sigma_{-i/2}(b^*)$, we have

$$\begin{aligned} e = \Psi_{0,1/2}(A) &= \sum_j a_j^* \otimes (\sigma)_{i/2}^{\text{op}}(b_j^{\text{op}}) = \sum_j a_j \otimes (\sigma)_{-i/2}^{\text{op}}((b_j^*)^{\text{op}}) \\ &= \sum_j a_j \otimes (Q^{1/2} b_j^* Q^{-1/2})^{\text{op}} = (1 \otimes (Q^{-1/2})^{\text{op}}) \left(\sum_j a_j \otimes (b_j^*)^{\text{op}} \right) (1 \otimes (Q^{1/2})^{\text{op}}). \end{aligned}$$

Thus, (5.6) holds if and only if

$$(\pi \otimes \pi^{\text{op}})(e)(\text{id}_H \otimes \pi^{\text{op}}(Q^{-1/2}))\hat{1} = (\text{id}_H \otimes \pi^{\text{op}}(Q^{-1/2}))\hat{1}$$

holds, which, as explained, is equivalent to $\pi(Q^{-1/2}) \in S_0$. $\square$

Summarizing the above construction, when A is a quantum adjacency matrix for (B, ψ) as in Definition 3.5,

$$S_{\pi, \psi, A} = \pi(Q^{1/4})S_0\pi(Q^{1/4}) = \pi(Q^{1/2})S_0$$

is an operator system $\pi(B)'$ -bimodule inside $\mathcal{B}(H)$, satisfying an extra condition $\pi(Q)S\pi(Q^{-1}) = S$.

So far we started with a quantum adjacency matrix A for (B, ψ) , and obtained an operator system $S_{\pi, \psi, A}$ which is a quantum graph on (B, π) (satisfying an extra consistency condition for $\pi(Q)$).

If we have an operator system bimodule S , we can reverse the above process. To be precise, fix a positive faithful functional ψ on B , and take the corresponding positive element Q . Suppose that $S = \pi(Q)S\pi(Q)^{-1}$ holds. Then we get a quantum adjacency matrix A for (B, ψ) , by first taking $S_0 = \pi(Q^{-1/2})S$, and considering the subspace $V \subset H \otimes H^*$ corresponding to S_0 . The condition $\pi(B)'S_0\pi(B)' = S_0$ translates to $V = \pi(B)' \otimes \pi^{\text{op}}(B^{\text{op}})'V$, hence V can be written as $E(H \otimes H^*)$ for some orthogonal projection $E \in (\pi(B)' \otimes \pi^{\text{op}}(B^{\text{op}})')' = \pi(B) \otimes \pi^{\text{op}}(B^{\text{op}})$. This means we have a projection $e \in B \otimes B^{\text{op}}$ such that $E = \pi \otimes \pi^{\text{op}}(e)$. The self-adjointness $S_0 = S_0^*$ implies that $J_0V = V$, which translates to $e = \Sigma e$. Similarly, the invariance $S_0 = \pi(Q)S_0\pi(Q^{-1})$ implies that e is invariant under $\sigma_z \otimes \sigma_z^{\text{op}}$. Then Theorem 5.10 gives an operator $A \in \mathcal{B}(L^2(B, \psi))$ satisfying most of the conditions in Definition 3.5. Moreover, Proposition 5.12 gives the remaining condition.

Let us record the correspondence between two approaches to quantum graphs we have worked out.

Theorem 5.13. *Let B be a finite-dimensional C^* -algebra, ψ be a positive faithful functional, and $\pi: B \rightarrow \mathcal{B}(H)$ be a faithful representation of B . There is a bijective correspondence between the set of quantum adjacency matrices on (B, ψ) and the set of subspaces $S \subset \mathcal{B}(H)$ satisfying the following conditions:*

- (1) $\text{id}_H \in S$, $S = S^*$ (S is an operator system);
- (2) $\pi(B)'S\pi(B)' = S$ (S is a bimodule over the commutant $\pi(B)'$); and
- (3) $\pi(Q)S\pi(Q^{-1}) = S$.

Remark 5.14. As a corollary, when we take another *tracial* positive faithful functional ψ_0 on B , we obtain an injective map from the set of quantum adjacency matrices on (B, ψ) to the corresponding one for (B, ψ_0) , which at the level of operator system bimodules means removing condition 3 above.

Example 5.15. The case of $B = M_2$ and arbitrary ψ was classified in [Mat22].

6. QUANTUM CONFUSABILITY GRAPHS FOR QUANTUM CHANNELS

6.1. Quantum channels and unital completely positive maps. Let N be a quantum channel, which is given as a *trace preserving completely positive map* $\mathcal{B}(H_I) \rightarrow \mathcal{B}(H_O)$ for some finite dimensional Hilbert spaces H_I and H_O , respectively representing the input and output systems. Such maps are characterized by the existence of the *Kraus decomposition*, that is, we can write N as

$$N(\rho) = \sum_{i=1}^n K_i \rho K_i^* \quad (\rho \in \mathcal{B}(H_I)),$$

where the K_i are elements of $\mathcal{B}(H_I, H_O)$ satisfying $\sum_{i=1}^n K_i^* K_i = \text{id}_{H_I}$. Then, as we indicated in Section 1, we get an analogue of the confusability graph by taking $S \subset \mathcal{B}(H_I)$, the linear span of the operators $K_i^* K_j$ for $i, j = 1, \dots, n$.

By construction S is closed under taking adjoints. Moreover, it contains $\text{id}_I = \sum_i K_i^* K_i$, hence it is an operator system. Taking $B = \mathcal{B}(H_I)$ and considering the tautological representation $\pi: B \rightarrow \mathcal{B}(H_I)$ (which has the trivial commutant $\mathbb{C}\text{id}_I$), we get an example of quantum graph on (B, π) .

This construction works great for maps between matrix algebras, we would however like to generalize this to maps between finite dimensional C^* -algebras, in particular for unital completely positive maps between finite dimensional C^* -algebras.

Definition 6.1. A linear map $\theta: B \rightarrow C$ between C^* -algebras is said to be *completely positive* when its amplifications $\theta \otimes \text{id}_n: B \otimes M_n \rightarrow C \otimes M_n$ map positive elements to positive elements for every $n \geq 1$. If, in addition, θ is unital ($\theta(1_B) = 1_C$), then we say that θ is *unital completely positive*.

The $*$ -homomorphisms and positive functionals are completely positive, as in the next propositions.

Proposition 6.2. If $\theta: B \rightarrow C$ is a $*$ -homomorphism between C^* -algebras, then it is unital completely positive.

Proof. Fix $n \geq 1$ and let $x \in B \otimes M_n$. Since $\theta \otimes \text{id}_n$ is a $*$ -homomorphism we get that

$$(\theta \otimes \text{id}_n)(x^*x) = (\theta \otimes \text{id}_n)(x)^*(\theta \otimes \text{id}_n)(x),$$

hence $\theta \otimes \text{id}_n$ is positive. $\square$

Proposition 6.3. If $\psi: B \rightarrow \mathbb{C}$ is a positive functional on a C^* -algebra, then it is completely positive.

Proof. Given a Hilbert space H and $v \in H$, let us denote the map

$$\mathcal{B}(H) \rightarrow \mathbb{C}, \quad T \mapsto \langle v, Tv \rangle$$

as Ψ_v . To check that the map $\psi \otimes \text{id}_n: B \otimes M_n \rightarrow M_n$ is positive, it is enough to see that

$$\Psi_v((\psi \otimes \text{id}_n)(x)) = \langle v, (\psi \otimes \text{id}_n)(x)v \rangle$$

is nonnegative for all $v \in \mathbb{C}^n$.

Consider the GNS space $L^2(B, \psi)$ associated to (B, ψ) , and put $\Omega = \Lambda_\psi(1)$. (Since we do not assume ψ to be faithful, H might become a quotient space of B , but this does not matter in this proof.) Then we have

$$\psi(a) = \Psi_\Omega(\pi(a)),$$

and similarly, $\Psi_v((\psi \otimes \text{id}_n)(x))$ for $x \in B \otimes M_n$ can be presented as

$$\langle v, (\Psi_\Omega \pi \otimes \text{id}_n)(x)v \rangle = \langle \Omega \otimes v, (\pi \otimes \text{id}_n)(x)\Omega \otimes v \rangle.$$

If x is of the form y^*y , then we get

$$\langle \Omega \otimes v, (\pi \otimes \text{id}_n)(y^*y)\Omega \otimes v \rangle = \langle (\pi \otimes \text{id}_n)(y)(\Omega \otimes v), (\pi \otimes \text{id}_n)(y)(\Omega \otimes v) \rangle \geq 0,$$

proving the positivity of $(\pi \otimes \text{id}_n)(x)$. $\square$

For matrix algebras, the unital completely positive maps are dual to quantum channels as in the next proposition. Thus, they capture essentially same structure for matrices, but as we will see later, unital completely positive maps are better suited for general C^* -algebras without prescribed positive functionals.

Proposition 6.4. Let $N: \mathcal{B}(H_I) \rightarrow \mathcal{B}(H_O)$ be a quantum channel. Consider the dual map $N^t: \mathcal{B}(H_O) \rightarrow \mathcal{B}(H_I)$ characterized by

$$\text{Tr}_I(xN^t(y)) = \text{Tr}_O(N(x)y)$$

for $x \in \mathcal{B}(H_I)$ and $y \in \mathcal{B}(H_O)$. Then N^t is a unital completely positive map.

Proof. Note that N^t is uniquely defined by the above formula because the trace pairing is nondegenerate on matrix algebras.

To show that N^t is unital, it is sufficient to show that $\text{Tr}_I(xN^t(I_O)) = \text{Tr}_I(x)$ holds for every $x \in \mathcal{B}(H_I)$. Since N is a quantum channel, it preserves the trace. We can then compute

$$\text{Tr}_I(xN^t(I_O)) = \text{Tr}_O(N(x)I_O) = \text{Tr}_O(N(x)) = \text{Tr}_I(x),$$

proving the claim.

Let us look at the amplification of N^t . We claim that $N^t \otimes \text{id}_n = (N \otimes \text{id}_n)^t$ holds. Using the identification $\mathcal{B}(H) \otimes M_n \simeq \mathcal{B}(H \otimes \mathbb{C}^n)$, we can derive this by checking

$$\text{Tr}_{I^n}(x(N^t \otimes \text{id}_n)(y)) = \text{Tr}_{I^n}(x(N \otimes \text{id}_n)^t(y)) \quad (x \in \mathcal{B}(H_I \otimes \mathbb{C}^n), y \in \mathcal{B}(H_O \otimes \mathbb{C}^n)).$$

By linearity, it is enough to check this equality for simple tensors. Thus, for $x \in \mathcal{B}(H_I)$, $y \in \mathcal{B}(H_O)$, and $a, b \in M_n$ we calculate as

$$\text{Tr}_{I^n}((x \otimes a)(N^t \otimes \text{id}_n)(y \otimes b)) = \text{Tr}_{I^n}((x \otimes a)(N^t(y) \otimes b)) = \text{Tr}_{I^n}(xN^t(y) \otimes ab),$$

which is equal to $\text{Tr}_I(xN^t(y)) \text{Tr}_n(ab)$. Using $\text{Tr}_I(xN^t(y)) = \text{Tr}_O(N(x)y)$, we can write it as

$$\text{Tr}_{O^n}(N(x)y \otimes ab) = \text{Tr}_{O^n}((N(x) \otimes a)(y \otimes b)) = \text{Tr}_{O^n}((N \otimes \text{id}_n)(x \otimes a)(y \otimes b)).$$

Since the last one term can be written as $\text{Tr}_{I^n}((x \otimes a)(N \otimes \text{id}_n)^t(y \otimes b))$, we get the claim.

We are going to check that the positivity of N implies the positivity of N^t . This is enough to get the complete positivity of N^t , by the following argument. Since N is completely positive, the amplification $N \otimes \text{id}_n$ is positive. Then we will get the positivity of $(N \otimes \text{id}_n)^t = N^t \otimes \text{id}_n$, completing the proof.

Now, let $y \in \mathcal{B}(H_O)$ be a positive element. To see that $N^t(y)$ is positive, it is sufficient to check if $\text{Tr}_I(xN^t(y))$ is positive for arbitrary positive $x \in \mathcal{B}(H_I)$. This is indeed the case, since $\text{Tr}_I(xN^t(y)) = \text{Tr}_O(N(x)y)$ is positive from the positivity of $N(x)$ and y . $\square$

6.2. Stinespring dilation. Unital completely positive maps into matrix algebras can be factorized into a homomorphism and projection to a corner, in the following sense. Let H and K be Hilbert spaces. Suppose that $\pi: C \rightarrow \mathcal{B}(K)$ is a $*$ -representation, and $V: H \rightarrow K$ is an isometry. Then $\theta(x) = V^*\pi(x)V$ defines a map $C \rightarrow \mathcal{B}(H)$. This is positive by $\theta(y^*y) = V^*\pi(y)^*\pi(y)V$, but it is moreover unital completely positive. Indeed, the amplification of θ can be presented as

$$(\theta \otimes \text{id}_n)(x) = (V \otimes \text{id}_{\mathbb{C}^n})^*(\pi \otimes \text{id}_n)(V \otimes \text{id}_{\mathbb{C}^n}),$$

which is again positive, and we also have $\theta(1) = V^*V = \text{id}_H$. The data (K, π, V) is called a *Stinespring dilation* of θ .

Theorem 6.5. *Let C be a C^* -algebra, H be a Hilbert space, and $\theta: C \rightarrow \mathcal{B}(H)$ be a unital completely positive map. Then there is a Stinespring dilation for θ .*

Proof sketch. We may realize K as a quotient of the tensor product $C \otimes H$, with the inner product defined on simple tensors by

$$\langle x \otimes w_1, y \otimes w_2 \rangle_K = \langle w_1, \theta(x^*y)w_2 \rangle_H.$$

The fact that this has the required positivity for arbitrary tensors follows from the complete positivity of θ .

We then define $V: H \rightarrow K$ by $Vw = 1 \otimes w$, and $\pi: C \rightarrow \mathcal{B}(K)$ by $\pi(x)y \otimes w = xy \otimes w$. We can compute the adjoint of V as

$$\langle V^*(x \otimes w_1), w_2 \rangle = \langle x \otimes w_1, 1 \otimes w_2 \rangle = \langle w_1, \theta(x^*)w_2 \rangle = \langle \theta(x)w_1, w_2 \rangle,$$

hence we have $V^*(x \otimes w) = \theta(x)w$. This implies $V^*\pi(x)Vw = \theta(x)w$, as desired.

Finally, taking $x = 1$ shows that V is an isometry, since θ is unital. $\square$

The above construction has a special feature, namely, the (closed) span of $\pi(x)Vw$ for $x \in C$ and $w \in H$ is equal to K . We say such a model is *minimal*. In general, when (K, π, V) is a Stinespring dilation of θ , we get a minimal model $(\hat{K}, \hat{\pi}, \hat{V})$ by taking

$$\hat{K} = \text{span}\{\pi(x)Vw \in K \mid x \in C, w \in H\},$$

setting $\hat{V}$ to be V as a map $H \rightarrow \hat{K}$, and taking $\hat{\pi}(x)$ to be the restriction of $\pi(x)$ on $\hat{K}$.

Minimal models are universal in the following sense.

Proposition 6.6. *Let C be a finite dimensional C^* -algebra, H be a finite dimensional Hilbert space and $\theta: C \rightarrow \mathcal{B}(H)$ be a unital completely positive map. Let (K, π, V) be a minimal Stinespring dilation of θ . When (K', π', V') is another Stinespring dilation, there exists a unique isometry $u: K \rightarrow K'$ such that $uV = V'$ and $u\pi(x) = \pi'(x)u$ hold for every $x \in C$.*

Moreover, we have a $$ -homomorphism $\rho: \theta(C)' \rightarrow \mathcal{B}(K)$ characterized by*

$$(6.1) \quad \rho(y)\pi(x)Vw = \pi(x)Vyw \quad (y \in \theta(C)', x \in C, w \in H).$$

Proof. The uniqueness of u follows from the requirement

$$u\pi(x)Vw = \pi'(x)uVw = \pi'(x)V'w.$$

The computation

$$\langle \pi(x)Vw_1, \pi(y)Vw_2 \rangle = \langle w_1, V^*\pi(x^*y)Vw_2 \rangle = \langle w_1, \theta(x^*y)w_2 \rangle = \langle \pi'(x)V'w_1, \pi'(y)V'w_2 \rangle$$

shows that u is a well-defined isometry.

It remains to establish the existence of ρ . Again the requirement in the claim forces how $\rho(y)$ should act, so we need to check that it is well-defined. Consider a vector $v = \sum_{i=1}^n \pi(x_i)Vw_i$ in K . We then have

$$\langle \rho(y)v, \rho(y)v \rangle = \sum_{i,j} \langle \pi(x_i)Vyw_i, \pi(x_j)Vyw_j \rangle = \sum_{i,j} \langle w_i, y^*V^*\pi(x_i^*x_j)Vyw_j \rangle.$$

The summands are equal to $\langle w_i, y^*\theta(x_i^*x_j)yw_j \rangle$.

Now, the matrix $[\theta(x_i^*x_j)]_{i,j}$ is a positive element of $M_n(\mathcal{B}(K)) \simeq \mathcal{B}(K) \otimes M_n$, since it can be regarded as the image of the positive element $[x_i^*x_j]_{i,j} \in M_n(C)$ under the amplified map $\theta \otimes \text{id}_n$. Since y commutes with $V^*\pi(x_i^*x_j)V = \theta(x_i^*x_j)$, we have the inequality

$$[y^*\theta(x_i^*x_j)y]_{i,j} \leq \|y\|^2 [\theta(x_i^*x_j)]_{i,j}$$

in $M_n(\mathcal{B}(K))$. (You can take the square root T of $[\theta(x_i^*x_j)]_{i,j}$, which still commutes with y , and use the estimate $y^*T^2y = Ty^*yT \leq \|y\|^2 T^2$.) This implies that

$$\sum_{i,j} \langle w_i, y^*\theta(x_i^*x_j)yw_j \rangle \leq \|y\|^2 \sum_{i,j} \langle w_i, \theta(x_i^*x_j)w_j \rangle,$$

which means $\langle \rho(y)v, \rho(y)v \rangle \leq \|y\|^2 \|v\|^2$. This shows that $\rho(y)$ is well-defined as an operator on K .

By a formal argument we get $\rho(y_1)\rho(y_2) = \rho(y_1y_2)$. Moreover,

$$\langle \rho(y)\pi(x_1)Vw_1, \pi(x_2)Vw_2 \rangle = \langle \pi(x_1)Vyw_1, \pi(x_2)Vw_2 \rangle = \langle w_1, y^*\theta(x_1^*x_2)w_2 \rangle$$

implies that $\rho(y)^* = \rho(y^*)$, hence ρ is a $*$ -homomorphism. $\square$

Remark 6.7. As a particular consequence, minimal Stinespring dilation of θ is unique up to unitary equivalence. We may also extend the representation ρ of $\theta(C)'$ to the underlying space if we allow it to be non-unital. (That is, $\rho(\text{id}_H)$ would be the projection onto the direct summand $\hat{K}$ for a general Stinespring dilation as we described above.)

6.3. Quantum confusability graphs. The analogue of confusability graph for quantum channels can be generalized to the following construction. To be precise, given a quantum channel $N: \mathcal{B}(H_I) \rightarrow \mathcal{B}(H_O)$, as described before, we first consider its dual map $N^t: \mathcal{B}(H_O) \rightarrow \mathcal{B}(H_I)$ which is a unital completely positive map. Then the next theorem gives a quantum graph for $\mathcal{B}(H_I)$ and its tautological representation that recovers the quantum graph associated with N in terms of its Kraus decomposition.

Theorem 6.8. *Let B and C be finite dimensional C^* -algebras, $\pi_0: B \rightarrow \mathcal{B}(H)$ be a $*$ -representation, $\theta: C \rightarrow B$ be a unital completely positive map, and (K, π, V) be a Stinespring dilation for the composition $\pi_0\theta$. Then $S = V^*\pi(C)'V$ is a quantum graph for (B, π_0) , which is independent of the Stinespring dilation.*

Proof. To see that S is an operator system, notice that $\pi(C)'$ is self adjoint subspace of $\mathcal{B}(K)$, and contains the identity map on K . Then clearly $S = V^*\pi(C)'V$ is self adjoint, and contains the element $V^*\text{id}_K V = V^*V = \text{id}_H$. Thus, S is an operator system.

Next we want to show that S is a $\pi_0(B)'$ -bimodule. Recall that we have a representation $\rho: \pi_0\theta(C)' \rightarrow \mathcal{B}(\hat{K})$ characterized by (6.1), where $\hat{K}$ is the minimal model inside K . Moreover, the image of ρ lies in $\pi(C)'$ by the following computation:

$$\pi(x_1)\rho(y)(\pi(x_2)Vw) = \pi(x_1x_2)Vyw = \rho(y)\pi(x_1x_2)Vw = \rho(y)\pi(x_1)(\pi(x_2)Vw) \quad (x_1, x_2 \in C, w \in H).$$

Furthermore, by $\pi_0\theta(C) \subset \pi_0(B)$ we have $\pi_0(B)' \subset \pi_0\theta(C)'$. Then the above computation shows that $yVz = y\rho(z)V$ for $y \in \pi(C)'$ and $z \in \pi_0(B)'$. Thus $V^*yVz = V^*y\rho(z)V$ is an element of $V^*\pi(C)'V = S$, since $\rho(z) \in \pi(C)'$. This way we have obtained that S is closed under multiplication by $\pi_0(B)'$ from right. By a symmetric argument (or using the adjoint operation) S is also closed under multiplication by $\pi_0(B)'$ from left, hence it is a $\pi_0(B)'$ -bimodule.

The independence on Stinespring dilation follows from a comparison with the minimal model, which is unique up to unitary equivalence. $\square$

Conversely, we can ask whether a given quantum graph on (B, π_0) appears from the above construction. In the case where B is a matrix algebra and π_0 is the identity representation, we have the following construction by Duan [Dua09].

Theorem 6.9. *Let H be a finite dimensional Hilbert space and $S \subset \mathcal{B}(H)$ be an operator system, which we think of as a quantum graph for $\mathcal{B}(H)$ and its tautological representation on H . Then there exists a finite dimensional C^* -algebra C and a unital completely positive map $\theta: C \rightarrow \mathcal{B}(H)$ such that S is the quantum graph given by Theorem 6.8.*

Proof. We first show that S is spanned by its positive elements. Since S is self-adjoint, it is spanned by self-adjoint elements. Concretely, we can see this by writing any element $x \in S$ as

$$x = \frac{1}{2}(x + x^*) + i\frac{1}{2i}(x - x^*).$$

Furthermore, since S contains the identity id_H , for any self-adjoint element $x \in S$, the element $x + \lambda \text{id}_H$ is also in S for every $\lambda \in \mathbb{R}$. In particular we have that $x + \|x\| \text{id}_H \in S$, which is a positive operator on H . We may therefore write any self-adjoint element in S as

$$x = (x + \|x\| \text{id}_H) - \|x\| \text{id}_H$$

and conclude that S is spanned by its positive elements.

Now, let $(x_i)_{i=1}^{n-1}$ be positive elements of S that linearly spans S . By rescaling, we may assume that $\sum_{i=1}^{n-1} x_i \leq \text{id}_H$. By adding $x_n = \text{id}_H - \sum_{i=1}^{n-1} x_i$, we get a family of positive elements $(x_i)_{i=1}^n$ that spans S , with the extra property $\sum_{i=1}^n x_i = \text{id}_H$.

Next we want to construct a Hilbert space K and an isometry $V: H \rightarrow K$ to act as a concrete Stinespring dilation. With $(x_i)_{i=1}^n$ in S as above, choose operators $a_i \in \mathcal{B}(H)$ such that $a_i^* a_i = x_i$. We then set $K = H^{\oplus n}$, define the isometry V by

$$Vw = a_1 w \oplus \cdots \oplus a_n w \quad (w \in H).$$

This is indeed an isometry by

$$V^* V w = \sum_{i=1}^n a_i^* a_i w = \sum_{i=1}^n x_i w = w.$$

Now, we let the C^* -algebra C be the direct sum $\mathcal{B}(H)^{\oplus n}$, and $\pi: C \rightarrow \mathcal{B}(K)$ be the $*$ -representation given by letting $\mathcal{B}(H)$ act on H , block by block. Our unital completely positive map $\theta: C \rightarrow \mathcal{B}(H)$ is then given by $\theta(x) = V^* \pi(x) V$.

It remains to check $S = V^* \pi(C)' V$. Note that we may write $\pi(C)$ as the following collection of $\mathcal{B}(H)$ valued $n \times n$ matrices:

$$\begin{bmatrix} y_1 & 0 & \cdots & 0 \\ 0 & y_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & y_n \end{bmatrix} \quad (y_i \in \mathcal{B}(H)).$$

From this it we see that the commutant is given by $\pi(C)' = \mathbb{C} \text{id}_H \oplus \cdots \oplus \mathbb{C} \text{id}_H$. Then we get

$$V^* \pi(C)' V = \text{span}\{a_1^* a_1, \dots, a_n^* a_n\} = \text{span}\{x_1, \dots, x_n\} = S,$$

completing the proof. $\square$

7. CAPACITY OF CHANNELS

Our next goal is to understand the zero-error capacity of (quantum) channels, and relate it to (quantum) graphs.

7.1. Zero-error capacity in classical information theory. Let us first review the motivation from the classical information theory. We write Γ to denote an undirected graph. A communication channel can be formalized as follows: we have the input set I and the output set O , and the channel $F: I \rightarrow O$ is given by an independent collection of random variables F_x on O , parametrized by the elements $x \in I$. Then, the *confusability graph* of F is the graph Γ whose vertex set V_Γ is I , with the rule that two vertices $v, w \in V_\Gamma$ have an edge between them if and only if F_v and F_w can take the same value, i.e., the probability $\mathbb{P}[F_v \neq F_w]$ is non-zero. Then, an empty subgraph of Γ represents a collection of inputs that we can send through F without confusion. This motivates the following.

Definition 7.1. The *independence number* of Γ is the number

$$\alpha(\Gamma) = \max\{k \mid \text{there exists an empty subgraph of } \Gamma \text{ of size } k\}.$$

Note that an empty subgraph is sometimes called an *anticlique* or an *independent set*. Thus, the independence number is the size of maximal anticlique in Γ .

The above consideration have to do with *one letter* we send through the channel F . If we want to consider words of length n , we need to look at the n -fold product of the channel $F: I \rightarrow O$, that is, we should consider the channel $F^n: I^n \rightarrow O^n$ given by

$$F_{v_1, \dots, v_n}^n = (F_{v_1}, \dots, F_{v_n}).$$

The confusability graph of this channel is Γ^n , which has the vertex set I^n and we have an edge between two vertices $(v_1, \dots, v_n)$ and $(w_1, \dots, w_n)$ if and only if there is an edge between v_i and w_i in Γ for every $i = 1, \dots, n$.

This convention of graph product is sometimes called the *tensor product*, the *direct product*, or the *Kronecker product*. That is, the tensor product of two graphs Γ and Λ is the graph $\Gamma \times \Lambda$ with vertex set $V_\Gamma \times V_\Lambda$ and there is an edge between two vertices (v_1, w_1) and (v_2, w_2) if and only if there is an edge in Γ between v_1 and v_2 , and an edge in Λ between w_1 and w_2 .

Definition 7.2. The *zero-error capacity* of Γ is given by

$$c_0(\Gamma) = \lim_{n \rightarrow \infty} \frac{1}{n} \log \alpha(\Gamma^n).$$

As we have $\alpha(\Gamma^n) \geq \alpha(\Gamma)^n$, we have

$$c_0(\Gamma) = \sup_n \frac{1}{n} \log \alpha(\Gamma^n) \geq \log \alpha(\Gamma).$$

To get an estimate of $c_0(\Gamma)$ from the above, we need to find a quantity that bounds $\alpha(\Gamma)$ from above, and is multiplicative with respect to the graph (tensor) products.

Definition 7.3. The *Lovász number* of Γ is defined as

$$\vartheta(\Gamma) = \max\{\|A\| \mid \exists A \in M_{V_\Gamma}: A \geq 0, A_{vv} = 1, A_{vw} = 0 \text{ if there is an edge between } v \text{ and } w\}.$$

Proposition 7.4. We have $\alpha(\Gamma) \leq \vartheta(\Gamma)$.

Proof. Suppose the vertices $v_1, \dots, v_k \in V_\Gamma$ supports an empty graph of size $k = \alpha(\Gamma)$. We define a matrix A with entries

$$A_{vw} = \begin{cases} 1 & \text{if } v = w \text{ or } v, w \in \{v_1, \dots, v_k\}, \\ 0 & \text{otherwise,} \end{cases}$$

satisfies the criteria to compute Lovász estimate. We compute that $\|A\| = k$ and conclude that $\alpha(\Gamma) = \|A\| \leq \vartheta(\Gamma)$. $\square$

We have the following key identity for the tensor product of graphs.

Theorem 7.5 ([Lov06]). Suppose that Γ and Λ are two undirected graphs. We then have $\vartheta(\Gamma \times \Lambda) = \vartheta(\Gamma)\vartheta(\Lambda)$.

For now we will omit the proof of this statement. We will prove an analogue of this for quantum graphs based on semi-definite programming, and this can be proved in a similar way. Assuming this result, we get the following useful corollary.

Corollary 7.6. We have $c_0(\Gamma) \leq \log \vartheta(\Gamma)$.

Proof. From Proposition 7.4 and Theorem 7.5, we get

$$\frac{1}{n} \log \alpha(\Gamma^n) \leq \frac{1}{n} \log (\vartheta(\Gamma)^n) = \log \vartheta(\Gamma).$$

Taking the limit, we get the claim. $\square$

7.2. Zero-error capacity in quantum information theory. In the framework of quantum information theory, there are several different analogues of the independence number, as introduced in [DSW13]. Here we denote by H_I a finite dimensional Hilbert space, and by S an operator system in $\mathcal{B}(H_I)$.

A straightforward adaptation of the independence number in Definition 7.1 gives the following condition on the integer k .

Condition 7.7. There exists mutually orthogonal vectors $v_1, \dots, v_k \in H_I$ such that $\text{Tr}(xv_i v_j^*) = 0$, or equivalently, $v_j^* x v_i = 0$, holds for all $x \in S$ and $i \neq j$.

Indeed, if S corresponds to a classical graph Γ , and the vectors v_i are given as δ_{x_i} for some vertices $x_i \in V_\Gamma$, then the above orthogonality condition is equivalent to the k -tuple $(x_i)_i$ spanning an empty subgraph in Γ .

Definition 7.8. The *independence number* of S is the number given by

$$\alpha(S) = \max\{k \mid \text{Condition 7.7 holds}\}.$$

We can understand Condition 7.7 in terms of orthogonality of states we get by applying quantum channels, as follows.

Proposition 7.9. Let $N: \mathcal{B}(H_I) \rightarrow \mathcal{B}(H_O)$ be a quantum channel corresponding to S . Then $\text{Tr}(xv_i v_j^*) = 0$ holds for all $x \in S$ if and only if $N(v_i v_i^*)$ and $N(v_j v_j^*)$ are orthogonal.

Proof. Suppose we have a Kraus decomposition of N , given as $N(\rho) = \sum_a K_a \rho K_a^*$, so that S is the span of the operators $K_a^* K_b$. If we have $v_j^* K_a^* K_b v_i = 0$ for all indexes a and b , then we get $N(v_j v_j^*) N(v_i v_i^*) = 0$. Conversely, the vanishing of $N(v_j v_j^*) N(v_i v_i^*)$ is equivalent to the vanishing of its trace. Using the trace property, the latter is equivalent to

$$0 = \sum_{a,b} v_j^* K_a^* K_b v_i v_i^* K_b^* K_a v_j = \sum_{a,b} |v_j^* K_a^* K_b v_i|^2.$$

This forces $v_j^* K_a^* K_b v_i = 0$ for all a and b . □

If we ask for some sort of decoding scheme, it is more sensible to ask for the following condition on k .

Condition 7.10. There exists a projection $p \in \mathcal{B}(H_I)$ of rank k such that we have $\dim(pSp) = 1$, in other words, $pSp = \mathbb{C}p$.

Remark 7.11. Suppose that S is the quantum graph of a quantum channel N . Then the Knill–Laflamme error correction condition [KL97] says that Condition 7.10 corresponds to the existence of a quantum channel $D: \mathcal{B}(H_O) \rightarrow \mathcal{B}(H_I)$ such that $(DN)(vv^*) = vv^*$ for all $v \in pH_I$, which can be interpreted as a decoding channel for N .

Definition 7.12. The *quantum independence number* of S is the number given by

$$\alpha_q(S) = \max\{k \mid \text{Condition 7.10 holds}\}.$$

We can also ask for an encoding scheme with entangle assist. Suppose that S is the quantum graph of a quantum channel $N: \mathcal{B}(H_I) \rightarrow \mathcal{B}(H_O)$. We are then interested in the following condition on k .

Condition 7.13. There exist Hilbert spaces $H_{I'}$ and $H_{O'}$, a density matrix $\omega \in \mathcal{B}(H_{I'} \otimes H_{O'})$, quantum channels $E_i: \mathcal{B}(H_{I'}) \rightarrow \mathcal{B}(H_I)$ for $1 \leq i \leq k$, such that the density matrices $(NE_i \otimes \text{id})(\omega) \in \mathcal{B}(H_O \otimes H_{O'})$ are mutually orthogonal.

Remark 7.14. This condition is phrased in terms of the channel N , but Proposition 7.9 points to a way to formulate it directly in terms of S : the density matrices $\rho_i = (E_i \otimes \text{id})(\omega)$ should satisfy $\rho_i x \rho_j = 0$ for $x \in S \otimes \text{Cid}_{O'} \subset \mathcal{B}(H_I \otimes H_{O'})$ and $i \neq j$. See also Proposition 7.18 for a more concrete formulation.

Definition 7.15. The *entanglement independence number* of S is the number given by

$$\tilde{\alpha}(S) = \max\{k \mid \text{Condition 7.13 holds}\}.$$

Now we are ready to define the corresponding zero-error capacities.

$$C_0(S) = \lim_{n \rightarrow \infty} \frac{1}{n} \log \alpha(S^{\otimes n}), \quad Q_0(S) = \lim_{n \rightarrow \infty} \frac{1}{n} \log \alpha_q(S^{\otimes n}), \quad C_{0E}(S) = \lim_{n \rightarrow \infty} \frac{1}{n} \log \tilde{\alpha}(S^{\otimes n}).$$

Remark 7.16. Condition 7.10 is more restrictive than Condition 7.7, giving $\alpha_q(S) \leq \alpha(S)$. If we have such a projection p , then any choice of orthonormal basis $(v_i)_i$ in pH_I will satisfy Condition 7.7. Indeed, writing $p = \sum_i v_i v_i^*$, the requirement

$$p x p = \lambda p \quad (\lambda \in \mathbb{C})$$

for $x \in S$ will force $v_j^* x v_i = 0$ for $i \neq j$, which is equivalent to $\text{Tr}(x v_i v_j^*) = 0$. On the other hand, we have $\alpha(S) \leq \tilde{\alpha}(S)$, as the case of $\dim H_{I'} = \dim H_{O'} = 1$ in Condition 7.13 recovers the setting of Condition 7.7.

7.3. Quantum Lovász number. Now, it's a good time to head to Appendix A for quick overview on Semi-Definite Programming.

Once you are back, we are ready to continue with the estimate of entanglement independence number.

Definition 7.17. The *quantum Lovász number* of S is defined as

$$\tilde{\vartheta}(S) = \sup\{\|\text{id}_{H_I \otimes \mathbb{C}^n} + T\| \mid n \in \mathbb{N}, T \in (S \otimes M_n)^\perp, \text{id} + T \geq 0\}.$$

Proposition 7.18. Let $N: \mathcal{B}(H_I) \rightarrow \mathcal{B}(H_O)$ and $E_i: \mathcal{B}(H_{I'}) \rightarrow \mathcal{B}(H_I)$ be quantum channels, and $\omega \in \mathcal{B}(H_{I'} \otimes H_{O'})$ be a density matrix as in Condition 7.13. Take their Stinespring dilations

$$V: H_I \rightarrow H_O^n, \quad V^{(i)}: H_{I'} \rightarrow H_I^m,$$

so that we have $N(\rho) = \text{Tr}_{M_n}(V\rho V^*)$ with respect to the identification $\mathcal{B}(H_O^n) \simeq \mathcal{B}(H_O) \otimes M_n$, and similarly $E_i(\rho) = \text{Tr}_{M_m}(V^{(i)}\rho V^{(i)*})$. We then have

$$(V^{(i)} \otimes I_{O'})\omega(V^{(j)*} \otimes I_{O'}) \in (S \otimes M_m \otimes \mathbb{C}I_{O'})^\perp$$

for $i \neq j$.

Theorem 7.19. We have $\tilde{\vartheta}(S) \geq \tilde{\alpha}(S)$.

Proof. Let us take $(E_i)_{i=1}^k$ and ω as in Condition 7.13, and Stinespring dilations $V^{(i)}$ as in Proposition 7.18. Then the orthogonality of Proposition 7.18 can be rewritten as

$$V^{(i)}(\text{Tr}_{O'}(\omega))V^{(j)*} \in (S \otimes M_m)^\perp.$$

Set $\eta = \text{Tr}_{O'}(\omega)$. Since it is a positive matrix, by rescaling we may assume that its maximal eigenvalue $\lambda_{\max}(\eta)$ is equal to 1. Let v be a corresponding eigenvector.

Now, we consider the operator-valued matrix

$$T = [V^{(i)}\eta V^{(j)*}]_{i \neq j} \in M_k(\mathcal{B}(H_I^m)).$$

We identify T with

$$\sum_{i \neq j} V^{(i)}\eta V^{(j)*} \otimes e_{ij} \in \mathcal{B}(H_I^m) \otimes M_k,$$

and freely make identification of $M_k(\mathcal{B}(H_I^m))$ and $\mathcal{B}(H_I^m) \otimes M_k$ with $\mathcal{B}(H_I \otimes \mathbb{C}^{mk})$.

We first claim that T is orthogonal to $S \otimes M_{mk}$. Indeed, writing the components of V as $(K_a)_{a=1}^n$, so that S is the span of the $K_a^*K_b$, we compute

$$\text{Tr}(T(K_a^*K_b \otimes e_{cd} \otimes e_{ii})) = 0$$

by the fact that T does not have diagonal entries. For $i \neq j$, we have

$$\text{Tr}(T(K_a^*K_b \otimes e_{cd} \otimes e_{ji})) = \text{Tr}(V^{(i)} \text{Tr}_{O'}(\omega) V^{(j)*} (K_a^*K_b \otimes e_{cd})),$$

but this should vanish by $K_a^*K_b \otimes e_{cd} \in S \otimes M_m$.

We next claim that $\text{id} + T$ is positive. Consider

$$\tilde{T} = [V^{(i)}\eta V^{(j)*}]_{i,j} \in M_k(\mathcal{B}(H_I^m)).$$

This is positive, since we can write $\tilde{T} = xx^*$ with the operator-valued column vector

$$x = (V^{(i)}\eta^{1/2})_{i=1}^k \in \mathcal{B}(H_I^m)^k.$$

Now, it's enough to check the positivity of $\text{id} + T - \tilde{T}$. This is given by the diagonal operator-valued matrix with entries $\text{id} - V^{(i)}\eta V^{(i)*}$, which are positive because we arranged η to be a positive operator whose maximal eigenvalue is 1, and $V^{(i)}$ is an isometry.

It remains to check $\|\text{id} + T\| \geq k$. Consider the column vector

$$w = (V^{(i)}v)_{i=1}^k \in (H_I^m)^k.$$

By the above estimate, we have

$$\langle w, (\text{id} + T)w \rangle \geq \langle w, \tilde{T}w \rangle = \sum_{i,j=1}^k \langle v, \eta v \rangle = k^2.$$

On the other hand, we have $\langle w, w \rangle = \sum_{i=1}^k \langle v, v \rangle = k$, which implies the claim. $\square$

Proposition 7.20. *Let $(v_i)_i$ be an orthonormal basis of H_I , and consider the vector $\Phi = \sum_i v_i \otimes v_i^* \in H_I \otimes H_I^*$. We then have*

$$\tilde{\vartheta}(S) = \sup\{\langle \Phi, (\text{id}_{H_I} \otimes \rho + T')\Phi \rangle \mid \rho \in \mathcal{B}(H_I^*)_+, \text{Tr}(\rho) = 1, T' \in (S \otimes \mathcal{B}(H_I^*))^\perp, \text{id} \otimes \rho + T' \geq 0\}.$$

Proof. Let T be as in Definition 7.17. Take a unit eigenvector v for the maximal eigenvalue of $\text{id} + T$. Take an operator $x \in \mathcal{B}(H_I^*, \mathbb{C}^n)$ satisfying $v = (\text{id} \otimes x)\Phi$. Then the condition $\|v\| = 1$ is equivalent to $\text{Tr}(x^*x) = 1$. Taking $\rho = x^*x$ and $T' = (\text{id} \otimes x^*)T(\text{id} \otimes x)$, we see that T' satisfies the conditions in the claim, and we recover

$$\langle \Phi, (\text{id}_{H_I} \otimes \rho + T')\Phi \rangle = \|\text{id} + T\|.$$

This implies that $\tilde{\vartheta}(S)$ is majorized by the right hand side.

Conversely, suppose that ρ and T' satisfy the conditions in the claim. By a small perturbation, we may assume that ρ is invertible. As above, let us write $\rho = x^*x$ for some invertible linear map $x: H_I^* \rightarrow \mathbb{C}^n$. With $y = x^{-1}$, set $T = (\text{id}_I \otimes y^*)T'(\text{id}_I \otimes y)$, which is orthogonal to $S \otimes M_n$ by construction. We then have

$$\text{id}_{I^n} + T = (\text{id}_I \otimes y^*)(\text{id}_I \otimes \rho + T')(\text{id}_I \otimes y) \geq 0.$$

Moreover, the vector $v = (\text{id} \otimes x)\Phi$ is a unit vector in $H_I \otimes \mathbb{C}^n$, while we have

$$v^*(\text{id} + T)v = \Phi^*(\text{id} \otimes x^*)(\text{id} + T)(\text{id} \otimes x)\Phi = \Phi^*(\text{id} \otimes \rho + T')\Phi,$$

where we have used $T' = (\text{id}_I \otimes x^*)T'(\text{id}_I \otimes x)$. This means that $\|\text{id} + T\|$ can dominate the right hand side of the claim. $\square$

Theorem 7.21. *The formula from Proposition 7.20 is the (optimal) solution of the primal problem of an SDP scheme, whose dual problem is the following.*

Goal: minimize $\|(\text{Tr}_I \otimes \text{id})(Y)\|$.

Constraint: $Y \in (S \otimes \mathcal{B}(H_I^*))_{\text{sa}}$ satisfies $Y \geq \Phi\Phi^*$.

Moreover, the primal and the dual problems are in strong duality.

Proof. Let us start by setting up the relevant SDP scheme. Take $M_d = \mathcal{B}(H_I^* \oplus H_I \otimes H_I^*)$ together with its element

$$C = \begin{bmatrix} 0 & 0 \\ 0 & \Phi\Phi^* \end{bmatrix},$$

and a linear map $\ell: (M_d)_{\text{sa}} \rightarrow \mathbb{R} \oplus (S \otimes \mathcal{B}(H_I^*))_{\text{sa}}^*$ whose components ℓ_1 and ℓ_2 are given by

$$\ell_1(X) = \text{Tr}(X_{11}), \quad \ell_2(X)(x \otimes y) = \text{Tr}((X_{22} - \text{id} \otimes X_{11})(x \otimes y))$$

for $x \in S$ and $y \in \mathcal{B}(H_I^*)$, where we write

$$X = \begin{bmatrix} X_{11} & X_{12} \\ X_{21} & X_{22} \end{bmatrix} \quad (X_{11} \in \mathcal{B}(H_I^*), X_{22} \in \mathcal{B}(H_I \otimes H_I^*)).$$

We then take the target vector $b = 1 \oplus 0$ in $\mathbb{R} \oplus (S \otimes \mathcal{B}(H_I^*))_{\text{sa}}^*$.

Now, the corresponding primary problem is the following for X as above.

Goal: maximize $\text{Tr}(X_{22}\Phi\Phi^*) = \Phi^*X_{22}\Phi$.

Constraint: $X \geq 0$, $\text{Tr}(X_{11}) = 1$, and $X_{22} - \text{id} \otimes X_{11} \in (S \otimes \mathcal{B}(H_I^*))^\perp$.

By setting $\rho = X_{11}$ and $T' = X_{22} - \text{id} \otimes \rho$, the above is indeed equivalent to the quantity from Proposition 7.20.

Next, let us observe that the transpose of ℓ is given by

$$\ell_1^t(r) = r \text{id}_{I^*} \oplus 0, \quad \ell_2^t(x \otimes y) = \begin{bmatrix} -\text{Tr}(x)y & 0 \\ 0 & x \otimes y \end{bmatrix}.$$

Thus, the dual problem becomes the following.

Goal: minimize $r \in \mathbb{R}$.

Constraint: $r \text{id}_{I^*} - \sum_i \text{Tr}(x_i)y_i \geq 0$, $\sum_i x_i \otimes y_i \geq \Phi\Phi^*$.

That is, the dual problem asks to find the minimal value of $\|(\text{Tr}_I \otimes \text{id})(Y)\|$ for $Y \in (S \otimes \mathcal{B}(H_I^*))_{\text{sa}}$ satisfying $Y \geq \Phi\Phi^*$, as claimed.

Now, in view of Theorem A.6, it remains to check that the dual problem admits a strict solution, i.e., find v such that $\ell^t(v) > C$ holds. We can take any $Z \in (S \otimes \mathcal{B}(H_I^*))_{\text{sa}}$ satisfying $Z > C$, for example a big scalar, and any r satisfying $r > (\text{Tr}_I \otimes \text{id})(Z)$. Then $v = r \oplus Z$ will do. $\square$

Example 7.22. Consider the complete quantum graph $S = \mathcal{B}(H_I)$, which corresponds to $N = \text{Tr}$, allows $Y = \Phi\Phi^*$. Then $(\text{Tr} \otimes \text{id})(Y) = \text{id}_{I^*}$ has norm 1, which gives $\tilde{\vartheta}(S) = 1$.

Example 7.23. Next consider the empty quantum graph $S = \mathbb{C}\text{id}_I$, which corresponds to $N = \text{id}_{\mathcal{B}(H_I)}$. Then $(\text{Tr}_I \otimes \text{id})(Y)$ can be identified with Y for $Y \in S \otimes \mathcal{B}(H_I^*)$, hence we get $\tilde{\vartheta}(S) = \|\Phi\Phi^*\| = (\dim H_I)^2$.

Theorem 7.24. *For $i = 1, 2$, let $S_i \subset \mathcal{B}(H_i)$ be an operator system. We have $\tilde{\vartheta}(S_1 \otimes S_2) = \tilde{\vartheta}(S_1)\tilde{\vartheta}(S_2)$.*

Proof. Let us first check $\tilde{\vartheta}(S_1 \otimes S_2) \geq \tilde{\vartheta}(S_1)\tilde{\vartheta}(S_2)$. For $i = 1, 2$, take $T_i \in (S_i \otimes M_{n_i})^\perp$ satisfying $\text{id}_{H_i \otimes \mathbb{C}^{n_i}} + T_i \geq 0$ and $\|\text{id} + T_i\| \sim \tilde{\vartheta}(S_i)$. Then, consider

$$T = (\text{id} + T_1) \otimes (\text{id} + T_2) - \text{id} \otimes \text{id},$$

which is orthogonal to $S_1 \otimes M_{n_1} \otimes S_2 \otimes M_{n_2}$. By construction $\text{id} + T = (\text{id} + T_1) \otimes (\text{id} + T_2)$ is positive. We also have $\|\text{id} + T\| = \|(\text{id} + T_1)\| \|(\text{id} + T_2)\| \sim \tilde{\vartheta}(S_1)\tilde{\vartheta}(S_2)$, showing that $\tilde{\vartheta}(S_1 \otimes S_2)$ can be at least as large as $\tilde{\vartheta}(S_1)\tilde{\vartheta}(S_2)$.

Let us next check the converse inequality $\tilde{\vartheta}(S_1 \otimes S_2) \leq \tilde{\vartheta}(S_1)\tilde{\vartheta}(S_2)$. This time, for $i = 1, 2$, take $Y_i \in (S_i \otimes \mathcal{B}(H_i^*))_{\text{sa}}$ satisfying $Y_i \geq \Phi_i\Phi_i^*$ and $\|(\text{Tr} \otimes \text{id})(Y_i)\| \sim \tilde{\vartheta}(S_i)$. Observe that $\Phi_1\Phi_2\Phi_1^*\Phi_2^*$ is equal to $\Phi\Phi^*$ for $\Phi = \sum_j w_j \otimes w_j^*$, where $(w_j)_j$ is an orthonormal basis of $H_1 \otimes H_2$. On one hand, $Y = Y_1 \otimes Y_2$ dominates $\Phi_1\Phi_2\Phi_1^*\Phi_2^*$. On the other, we have

$$(\text{Tr}_{\mathcal{B}(H_1)} \otimes \text{Tr}_{\mathcal{B}(H_2)} \otimes \text{id})(Y) = (\text{Tr}_{\mathcal{B}(H_1)} \otimes \text{id})(Y_1) \otimes (\text{Tr}_{\mathcal{B}(H_2)} \otimes \text{id})(Y_2),$$

which has the norm $\|(\text{Tr}_{\mathcal{B}(H_1)} \otimes \text{id})(Y_1)\| \|(\text{Tr}_{\mathcal{B}(H_2)} \otimes \text{id})(Y_2)\|$. This means $\tilde{\vartheta}(S_1 \otimes S_2)$ is at least as small as $\tilde{\vartheta}(S_1)\tilde{\vartheta}(S_2)$. $\square$

Corollary 7.25. *Let S be a quantum graph. We then have $C_{0E}(S) \leq \log \tilde{\vartheta}(S)$.*

Example 7.26. With $H_I = \mathbb{C}^2 \otimes \mathbb{C}^d$, consider the operator system

$$S = \mathbb{C}I_{2d} + (\mathbb{C}I_2)^\perp \otimes M_d \subset M_{2d}.$$

Since S contains $M_2 \otimes \mathbb{C}I_d$, the dual formulation of the quantum Lovász number from Theorem 7.21 gives

$$\tilde{\vartheta}(S) \leq \tilde{\vartheta}(M_2 \otimes \mathbb{C}I_d) = \tilde{\vartheta}(M_2)\tilde{\vartheta}(\mathbb{C}I_d) = d^2,$$

where we used Examples 7.22 and 7.23 in the last part. The reverse inequality is explained in [Dua09]. Otherwise, we can observe $S^\perp = \mathbb{C}I_2 \otimes (\mathbb{C}I_d)^\perp$ and use the element

$$T = \sum_{ij} I_2 \otimes u_i^* u_j \otimes e_{ij} \in M_2 \otimes M_d \otimes M_{d^2}$$

for an orthonormal basis $(u_i)_{i=1}^{d^2}$ of M_d with respect to the trace inner product, which satisfies the conditions in Definition 7.17.

8. PUSHFORWARD AND PULLBACK OF QUANTUM GRAPHS

Theorem 8.1. *Let B, C be finite-dimensional C^* -algebras, $\pi_0: B \rightarrow \mathcal{B}(H_1), \sigma: C \rightarrow \mathcal{B}(H_2)$ be representations, $S \subset \mathcal{B}(H_2)$ be a quantum graph for (C, σ) , and $\theta: C \rightarrow B$ be a completely positive map. Moreover, let $(K, V: H_1 \rightarrow K, \pi: C \rightarrow \mathcal{B}(K))$ be a Stinespring dilation for $\pi_0\theta: C \rightarrow \mathcal{B}(H_1)$, and $S_\pi \subset \mathcal{B}(K)$ be the $\pi(C)'$ -bimodule operator system corresponding to S . Then $\theta_*S = V^*S_\pi V \subset \mathcal{B}(H_1)$ is a $\pi_0(B)'$ -bimodule.*

We can also write $\overrightarrow{S}$ to denote θ_*S (although it is denoted by $\overleftarrow{S}$ in [Daw22]).

Proposition 8.2. *Suppose that B and C have faithful tracial functionals ψ_B and ψ_C , and $\theta: C \rightarrow B$ is a completely positive map. Then the map $\hat{\theta}: B \rightarrow C$ characterized by*

$$\psi_B(b\theta(c)) = \psi_C(\hat{\theta}(b)c) \quad (b \in B, c \in C)$$

is completely positive.

Lemma 8.3. *Let $\theta: \mathcal{B}(H_2) \rightarrow \mathcal{B}(H_1)$ is a completely positive map with Kraus form $\theta(x) = \sum_i K_i^* x K_i$ for $K_i \in \mathcal{B}(H_1, H_2)$. Then $\hat{\theta}$ for Tr_{H_1} and Tr_{H_2} has the Kraus form $\hat{\theta}(y) = \sum_i K_i y K_i^*$.*

Definition 8.4. Let $B, C, \pi_0, \sigma, \theta$ be as in Theorem 8.1. Moreover, let $S \subset \mathcal{B}(H_1)$ be a quantum graph for (B, π_0) , and suppose that we are given faithful positive functionals ψ_B and ψ_C . Then $\theta^*S = \hat{\theta}_*S$, for $\hat{\theta}: B \rightarrow C$ as above, is a quantum graph for (C, σ) .

We can also write $\overleftarrow{S}$ to denote θ^*S (although it is denoted by $\overrightarrow{S}$ in [Daw22]).

Let $f: V \rightarrow W$ be a map of finite sets. We then get a trace preserving completely positive map

$$N_f: C(V) \rightarrow C(W), \quad \delta_v \mapsto \delta_{f(v)}.$$

On the other hand, given a graph Γ on V , we get the quantum graph

$$S_\Gamma = \{e_{v_1 v_2} \mid v_1 \sim_\Gamma v_2\} \subset M_V.$$

Proposition 8.5. *We have $(N_f)_* S_\Gamma = S_{f_* \Gamma}$.*

Definition 8.6 ([Wea21]). For $i = 1, 2$, let B_i be a finite dimensional C^* -algebra, $\pi_i: B_i \rightarrow \mathcal{B}(H_i)$ be a representation, $S_i \subset \mathcal{B}(H_i)$ be a quantum graph for (B_i, π_i) . A *CP-morphism* from S_1 to S_2 is a completely positive map $\theta: B_1 \rightarrow B_2$ such that $\theta_* S_1 \subset S_2$.

A special case of the above is the following situation for matrix algebras [Sta16]. Suppose we have operator systems $S_i \subset \mathcal{B}(H_i)$ for $i = 1, 2$. A *homomorphism* from $X_1 = (\mathcal{B}(H_1), S_1)$ to $X_2 = (\mathcal{B}(H_2), S_2)$ is given by a trace-preserving completely positive map $N: \mathcal{B}(H_1) \rightarrow \mathcal{B}(H_2)$ such that $N_*(S_1) \subset S_2$. If there is such a homomorphism, we have $\tilde{\vartheta}(S_1^c) \leq \tilde{\vartheta}(S_2^c)$, where S_i^c is the “complement” graph $\mathbb{C}I_i + S_i^\perp \subset \mathcal{B}(H_i)$.

9. BIMODULES FOR THE GNS MODEL

Throughout this section, we fix a finite-dimensional C^* -algebra B and faithful positive functional ψ on B . Let us consider the GNS representation $\pi_\psi: B \rightarrow \mathcal{B}(L^2(B, \psi))$.

Theorem 9.1. *Let A be a quantum adjacency matrix for (B, ψ) . Then the corresponding quantum graph on (B, π_ψ) is given by*

$$S_{A, \psi} = \{m(A \otimes T)m^* \mid T \in \mathcal{B}(L^2(B, \psi))\}.$$

For simplicity let us write π for π_ψ , and $L^2(B)$ instead of $L^2(B, \psi)$.

Proof. The claim is equivalent to the equality

$$S_\pi = \pi(B)' A \pi(B)'.$$

Indeed, $\pi(B)'$ is given by the right multiplication operators

$$\rho_a: L^2(B) \rightarrow L^2(B), \quad \Lambda(b) \mapsto \Lambda(ba).$$

Then we have

$$m(A \otimes \Lambda(a)\Lambda(b)^*)m^* = \rho_a A \rho_b^*,$$

which is indeed in $\pi(B)' A \pi(B)'$. Taking linear combinations of such operators, we obtain

$$S_{A, \psi} = \pi(B)' A \pi(B)'.$$

Now, recall the intermediate subspace $S_0 \subset \mathcal{B}(L^2(B))$ behind the construction of S_π in Section 5.4. We took the linear isomorphism

$$\Psi_{0,1/2}: \mathcal{B}(L^2(B, \psi)) \rightarrow B \otimes B^{\text{op}}, \quad \Lambda(b)\Lambda(a)^* \mapsto a^* \otimes \sigma_{i/2}(b)^{\text{op}},$$

which led to a projection $e = \Psi_{0,1/2}(A)$. Then the identification $H \otimes \bar{H} \simeq L^2(\mathcal{B}(H), \text{Tr})$ for $H = L^2(B)$ gives $S_0 \subset \mathcal{B}(L^2(B))$ corresponding to $V = (\pi \otimes \pi^{\text{op}})(e) \subset H \otimes \bar{H}$. This is a $\pi(B)'$ -bimodule satisfying $\pi(Q^{-1/2}) \in S_0$ and $\pi(Q^z)S_0\pi(Q^{-z}) = S_0$. From this, the operator system $S_{\pi, \psi, A}$ was given as $\pi(Q^{1/2})S_0 = \pi(Q)^{1/4}S_0\pi(Q)^{1/4}$.

A standard bookkeeping gives the following.

Lemma 9.2. *For the GNS representation π , the subspace $V \subset L^2(B) \otimes \overline{L^2(B)}$ as above agrees with*

$$(\pi(B)' \otimes \pi(B)^{\text{op}'}) (\Lambda \otimes \Lambda)(e) \subset L^2(B) \otimes L^2(B^{\text{op}}),$$

up to the identification $\overline{L^2(B)} \simeq L^2(B^{\text{op}}, \psi^{\text{op}})$ given by $\Lambda(b)^ \mapsto \Lambda((b^*)^{\text{op}})$. (This is a unitary isomorphism of B^{op} -modules, with the convention $a^{\text{op}}\Lambda(b)^* = \Lambda(a^*b)^*$.)*

Now, consider the “modular operators” $\nabla^z \in \mathcal{B}(L^2(B))$ for $z \in \mathbb{C}$ given by

$$\nabla^z \Lambda(a) = \Lambda(\sigma_{-iz}(a)) = \Lambda(Q^z a Q^{-z}).$$

When $z = 1$, we recover the operator $\Lambda(a) \mapsto \Lambda(\sigma(a))$, which is self adjoint by the properties $\sigma(a)^* = \sigma^{-1}(a^*)$ and $\psi \circ \sigma = \psi$.

Lemma 9.3. *Up to the identification*

$L^2(\mathcal{B}(L^2(B)), \text{Tr}) \simeq L^2(B) \otimes \overline{L^2(B)} \simeq L^2(B) \otimes L^2(B^{\text{op}})$, $\Lambda(b)\Lambda(a)^* \mapsto \Lambda(b) \otimes \Lambda((a^*)^{\text{op}})$,
the vector $\Lambda_{\text{Tr}}(\nabla^{-1/2}A)$ corresponds to $(\Lambda_\psi \otimes \Lambda_{\psi^{\text{op}}})(e)$.

Proof. Writing $A = \sum_j \Lambda(b_j)\Lambda(a_j)^*$, we see that the above map sends $\Lambda(\nabla^{-1/2}A)$ to the vector

$$\sum_j \Lambda(\sigma_{i/2}(b_j)) \otimes \Lambda((a_j^*)^{\text{op}}).$$

We also have

$$(\Lambda \otimes \Lambda)(e) = \sum_j \Lambda(a_j^*) \otimes \Lambda(\sigma_{-i/2}(b)^{\text{op}}).$$

We get the claim by using

$$e = \Sigma(e) = (\sigma_z \otimes \sigma_z^{\text{op}})(e),$$

see Theorem 5.10. □

Proof of Theorem 9.1, continued. We now have $S_0 = \pi(B)' \nabla^{-1/2} A \pi(B)'$, which is the span of the operators

$$\Lambda(a) \mapsto \Lambda(Q^{-1/2} A (ab) Q^{-1/2} c)$$

for $b, c \in B$. Then $S_{\pi, \psi, A} = \pi(Q)^{1/2} S_0$ is the span of operators

$$\Lambda(a) \mapsto \Lambda(A(ab)c')$$

for $b, c' \in B$, which agrees with $\pi(B)' A \pi(B)'$, as claimed. □

Let us record the key observation as a separate corollary.

Corollary 9.4. *Consider $\mathcal{B}(L^2(B))$ as a B -bimodule by $a \cdot T \cdot b = \rho(a)T\rho(b)$, where $\rho(a)$ is the right multiplication operator given by $\rho(a)\Lambda(b) = \Lambda(ba)$. The subspace $S_{A, \psi}$ is the bimodule generated by A .*

Theorem 5.13 states that $S_{A, \psi}$ should be invariant under conjugation by $\pi(Q)$. Let us provide an alternative proof of this fact. One key is to consider the inner product

$$(9.1) \quad \langle T_1, T_2 \rangle = \eta^* m(\text{id} \otimes T_1^* T_2) m^* \eta$$

on $\mathcal{B}(L^2(B))$, and the antilinear involution

$$j: T \mapsto \nabla^{1/2} T^* \nabla^{-1/2}$$

on the space $\mathcal{B}(L^2(B))$.

Lemma 9.5. *The transform j is isometric for the above inner product.*

Proof. We first claim that

$$\eta^* m(\text{id} \otimes \nabla T) m^* \eta = \eta^* m(\text{id} \otimes T \nabla) m^* \eta$$

holds for all $T \in \mathcal{B}(L^2(B))$. Indeed, consider the case $T = \Lambda(a)\Lambda(b)^*$. Using Proposition 4.7, we compute

$$\eta^* m(\text{id} \otimes \nabla T) m^* \eta = \eta^* m\left(\text{id} \otimes ((\text{id} \otimes \eta^* m)(\text{id} \otimes \Lambda(a) \otimes \text{id}) m^* \eta \Lambda(b)^*)\right) m^* \eta,$$

which can be simplified to $\Lambda(b)^* \Lambda(a)$. Similarly, using $\Lambda(b)^* \nabla = (\nabla \Lambda(b))^*$ and a similar manipulation, the composition $\eta^* m(\text{id} \otimes T \nabla) m^* \eta$ also agrees with $\Lambda(b)^* \Lambda(a)$.

We then have

$$\eta^* m(\text{id} \otimes \nabla^z T) m^* \eta = \eta^* m(\text{id} \otimes T \nabla^z) m^* \eta$$

for all nonnegative integer z , then by interpolation the same claim for all $z \in \mathbb{C}$.

Now, using the above for $z = 1/2$, we have

$$\langle j(T_1), j(T_2) \rangle = \eta^* m(\text{id} \otimes \nabla^{-1/2} T_1 \nabla T_2^* \nabla^{-1/2}) m^* \eta = \eta^* m(\text{id} \otimes T_1 \nabla T_2^* \nabla^{-1}) m^* \eta.$$

Again assuming $T_i = \Lambda(a_i)\Lambda(b_i)^*$, we see that the right hand side is equal to

$$\Lambda(a_1)^* \Lambda(a_2) \eta^* m(\text{id} \otimes \Lambda(b_1)\Lambda(b_2)^*) m^* \eta,$$

but this is equal to $\eta^* m(\text{id} \otimes T_2^* T_1) m^* \eta = \overline{\langle T_2, T_1 \rangle}$. Taking the linear combination of this case, we obtain the assertion. □

Lemma 9.6. *The subspace $S_{A, \psi}$ is preserved under the conjugation map $T \mapsto \nabla T \nabla^{-1}$.*

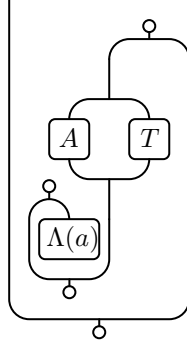


FIGURE 13. Diagrammatic presentation of $\nabla m(A \otimes T) m^* \nabla^{-1} \Lambda(a)$

Proof. In view of Proposition 4.7, $\nabla m(A \otimes T) m^* \nabla^{-1} \Lambda(a)$ can be represented as Figure 13. Our task is to show that this can be written as $m(A \otimes T') m^* \Lambda(a)$ for some T' .

In general, given an operator $T \in \mathcal{B}(L^2(B))$, define another operator $T^\vee$ by Figure 14. This can be

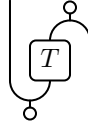


FIGURE 14. The operator $T^\vee$

characterized by $\eta^* m(\text{id} \otimes T^\vee) = \eta^* m(T \otimes \text{id})$. We claim that

$$\eta^* m(m(T_1 \otimes T_2) m^* \otimes \text{id}) = \eta^* m(\text{id} \otimes m(T_2^\vee \otimes T_1^\vee) m^*)$$

holds for $T_1, T_2 \in \mathcal{B}(L^2(B))$. This can be checked as in Figure 15. Using this and $A^\vee = A$, we can move

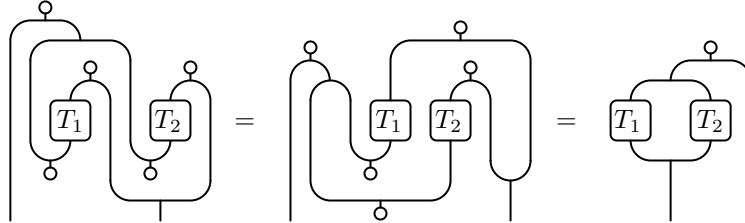


FIGURE 15. Convolution product and $\eta^* m$

the convolution product of A and T in Figure 13 to the right-most strand by changing T to $T^\vee$. An analogous argument moves them to the left-most strand, by changing $T^\vee$ to a suitably defined operator $T' = {}^\vee(T^\vee)$. We then use the conjugate equation to clean up the “snake”, and get the claim. $\square$

Proposition 9.7. *The subspace $S_{A,\psi}$ is preserved under the isometry j .*

Proof. By $A = A^*$, we have the invariance of $S_{A,\psi}$ under $T \mapsto T^*$. It remains to show the invariance of $S_{A,\psi}$ under $T \mapsto \nabla^{1/2} T \nabla^{-1/2}$.

Since σ is implemented as conjugation by positive definite matrices (see Section 4.2), it is diagonalizable with positive eigenvalues. The same holds for ∇ , then also for the conjugation map $T \mapsto \nabla T \nabla^{-1}$. By Lemma 9.6, $S_{A,\psi}$ is spanned by some eigenvectors of this map. Consequently, it is invariant under the maps of the form $T \mapsto \nabla^z T \nabla^{-z}$. $\square$

Proposition 9.8. *Let E denote the orthogonal projection $\mathcal{B}(L^2(B)) \rightarrow S_{A,\psi}$ for the inner product (9.1). We then have $E(T) = m(A \otimes T) m$.*

Proof. Since the claimed formula has the right range, it is enough to check $E(T) = 0$ when T is orthogonal to $S_{A,\psi}$ for the above inner product. We then have

$$\langle T, m(A \otimes T') m^* \rangle = \langle m(A \otimes T) m^*, T' \rangle$$

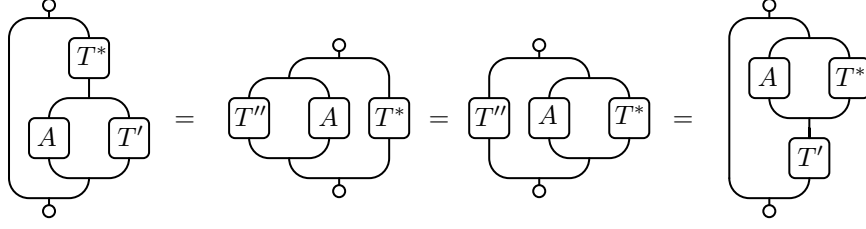


FIGURE 16. Convolution product and inner product

using the argument in the proof of Lemma 9.6, see Figure 16. (Note also $A = A^*$.) If this is 0 for all T' , we must have $m(A \otimes T)m^* = 0$, hence the claim. $\square$

Corollary 9.9. *The element A is invariant under the isometry j .*

Proof. By Proposition 9.8, we have $A = E(\eta\eta^*)$. We have $\nabla\eta = \eta$ from $\sigma(1) = 1$. This implies $\nabla^z\eta = \eta$ for all integer z , then for all complex number z . In particular we get $j(\eta\eta^*) = \eta\eta^*$. Proposition 9.7 implies that E and j commute, hence we obtain the assertion. $\square$

Proposition 9.10. *The map E is a homomorphism $\pi(B)'$ -bimodules.*

Proof. Recall that $\pi(B)'$ is given by right multiplication operators $\Lambda(a) \mapsto \Lambda(ab)$. The assertion follows from Proposition 9.8 and the associativity of m . $\square$

Corollary 9.11. *The subspace $S_{A,\psi}$ is invariant under $T \mapsto \pi(Q)T\pi(Q)^{-1}$.*

Proof. By Lemma 9.6, $S_{A,\psi}$ is invariant under conjugation by ∇ . Note that ∇ is the composition of $\pi(Q)$ and the right multiplication by Q^{-1} , and a similar relation holds for ∇^{-1} . By Proposition 9.10, $S_{A,\psi}$ is closed under composition with right multiplication operators, hence we obtain the assertion. $\square$

10. QUANTUM HOMOMORPHISMS AND ISOMORPHISMS

Our next goal is to make sense of “quantum homomorphisms” between quantum graphs. We will see that the concept of Hopf algebras (“quantum groups”) naturally appear from the universal algebra governing quantum homomorphisms.

10.1. Basic setup. For $i = 1, 2$, let B_i be a finite dimensional C^* -algebra, ψ_i be a faithful positive functional on B_i , and $A_i \in \mathcal{B}(L^2(B_i, \psi_i))$ be a quantum adjacency matrix operator. We denote the corresponding quantum graph by G_i .

Definition 10.1. A *quantum homomorphism* from G_1 to G_2 is given by:

- a C^* -algebra C (which can be infinite-dimensional); and
- a $*$ -homomorphism $\theta: B_2 \rightarrow B_1 \otimes C$; such that

the element $\tilde{\theta} \in \mathcal{B}(L^2(B_2, \psi_2), L^2(B_1, \psi_1)) \otimes C$ corresponding to θ satisfies

$$(10.1) \quad \tilde{\theta}^*(S_{A_1, \psi_1} \otimes 1_C)\tilde{\theta} \subset S_{A_2, \psi_2} \otimes C.$$

The element $\tilde{\theta}$ is defined as follows: Let $(b_i)_i$ be a basis of B_2 , and write

$$\theta(b_i) = \sum_j b'_{ij} \otimes c_{ij} \quad (b'_{ij} \in B_1, c_{ij} \in C).$$

Moreover, take the basis $(b^i)_i$ in B_2 satisfying $\Lambda(b^i)^*\Lambda(b_j) = \delta_{ij}$. Then we set

$$\tilde{\theta} = \sum_{ij} \Lambda(b'_{ij})\Lambda(b^i)^* \otimes c_{ij}.$$

More conceptually, $\tilde{\theta}$ represents a homomorphism of Hilbert C -modules

$$L^2(B_2) \otimes C \rightarrow L^2(B_1) \otimes C, \quad \Lambda(b) \otimes c \mapsto (\Lambda \otimes \text{id})(\theta(b)(1 \otimes c)).$$

Definition 10.2. A *quantum isomorphism* from G_1 to G_2 is given by a C^* -algebra C and $*$ -homomorphism $\theta: B_2 \rightarrow B_1 \otimes C$ satisfying the following conditions:

- (1) (C, θ) defines a quantum homomorphism from G_1 to G_2 ;
- (2) $(\psi_1 \otimes \text{id})\theta(b) = \psi_2(b) \otimes 1$;

- (3) $(m^* \otimes \text{id})\tilde{\theta} = (\tilde{\theta}_{13}\tilde{\theta}_{23})m^*$;
(4) $\tilde{\theta}^*(S_{A_1, \psi_1} \otimes C)\tilde{\theta} = S_{A_2, \psi_2} \otimes C$.

If G_1 and G_2 are the same, we call this a *quantum automorphism* of G_1 .

As a special case, we often consider quantum isomorphism of quantum sets $X = (B, \psi)$, which can be modelled by the above for the empty quantum graphs $A = \eta\eta^*$.

The classical case corresponds to $B_i = C(V_i)$ for some finite sets V_i , and $C = \mathbb{C}$. Then a $*$ -homomorphism $\theta: C(V_2) \rightarrow C(V_1)$ corresponds to a map $g: V_1 \rightarrow V_2$, by the correspondence

$$\theta(f)(v) = f(g(v)).$$

Then, if S_i corresponds to the graph Γ_i , the conditions $\tilde{\theta}^*S_1\tilde{\theta} \subset S_2$ is equivalent to the condition

$$v_1 \sim_{\Gamma_1} v_2 \Rightarrow g(v_1) \sim_{\Gamma_2} g(v_2).$$

Remark 10.3. The above map θ is different from the trace-preserving completely positive map N_g we introduced in Section 8.

Proposition 10.4. *Let $\theta: B_2 \rightarrow B_1$ be a $*$ -homomorphism giving a quantum isomorphism from G_1 to G_2 with $C = \mathbb{C}$. Then θ is an isomorphism of C^* -algebras, and it satisfies $\tilde{\theta}^*A_1\tilde{\theta} = A_2$.*

Proof. Let us first check the injectivity of θ . Condition (2) of Definition 10.2 becomes $\psi_2 = \psi_1 \circ \theta$. If $a \in B_2$ is in the kernel of θ , we would have $\psi_2(a^*a) = 0$, hence $a = 0$ by the faithfulness of ψ_2 .

To check the surjectivity, observe that $\tilde{\theta}^*$, regarded as a map $B_1 \rightarrow B_2$, is an algebra homomorphism by Condition (3) of Definition 10.2. Then taking the adjoint of $\eta_1 = \theta \circ \eta_2$ for the unit maps $\mathbb{C} \rightarrow B_i$, we obtain $\psi_1 = \psi_2 \circ \tilde{\theta}^*$, and we can repeat the argument above to obtain the surjectivity of θ .

Recall that A_i is the image of $\eta_i\eta_i^*$ under the orthogonal projection $\mathcal{B}(L^2(B_i, \psi_i)) \rightarrow S_{A_i, \psi_i}$ as in Section 9. Since the map $\mathcal{B}(L^2(B_1)) \rightarrow \mathcal{B}(L^2(B_2))$ given by $T \mapsto \tilde{\theta}^*T\tilde{\theta}$ preserves the inner product, we obtain $\tilde{\theta}^*A_1\tilde{\theta} = A_2$. $\square$

10.2. Quantum isomorphism of classical structures. Let us look at quantum automorphisms of classical structures. Consider the commutative algebras $\mathbb{C}^n$ and the standard functional $\psi_{\text{std}}(\delta_i) = 1$ ($i = 1, \dots, n$) on them.

Proposition 10.5. *A quantum automorphism of $(\mathbb{C}^n, \psi_{\text{std}})$ is given by a C^* -algebra C , together with its elements p_{ij} such that:*

- each p_{ij} satisfies $p_{ij} = p_{ij}^2 = p_{ij}^*$ (a projection in C); and
- $\sum_i p_{ij} = 1_C = \sum_j p_{ij}$ (the magic square condition) holds.

Proof. The homomorphism $\theta: \mathbb{C}^n \rightarrow \mathbb{C}^n \otimes C$ can be expressed as $\theta(\delta_j) = \sum_i \delta_i \otimes p_{ij}$, with uniquely defined elements $p_{ij} \in C$.

First, $\delta_j^2 = \delta_j = \delta_j^*$ and $\delta_i\delta_j = 0$ for $i \neq j$ imply $p_{ij}^2 = p_{ij} = p_{ij}^*$. Next, $\sum_j \delta_j = 1_{\mathbb{C}^n}$ implies $\sum_j p_{ij} = 1_C$ for each i . Then,

$$(\psi_{\text{std}} \otimes \text{id})\theta(\delta_j) = \psi(\delta_j)1_C = 1_C$$

implies $\sum_i p_{ij} = 1_C$ for each j . $\square$

This motivates the following algebra of *free permutation group* S_n^+ , which controls the quantum automorphisms of $(\mathbb{C}^n, \psi_{\text{std}})$.

Definition 10.6. We define $\mathcal{O}(S_n^+)$ as the universal $*$ -algebra with generators $(p_{ij})_{i,j=1}^n$ and the following relations:

- the p_{ij} are projections;
- $\sum_i p_{ij} = 1 = \sum_j p_{ij}$; and
- relations that are valid in *all* unitary representations, i.e., kill the joint kernel of the $*$ -homomorphisms $\mathcal{O}(S_n^+) \rightarrow \mathcal{B}(H)$.

The last condition implies that, among others, $p_{ij}p_{ik} = 0$ for $j \neq k$.

The *coproduct* on $\mathcal{O}(S_n^+)$ is the $*$ -homomorphism

$$\mathcal{O}(S_n^+) \rightarrow \mathcal{O}(S_n^+) \otimes \mathcal{O}(S_n^+), \quad p_{ij} \mapsto \sum_{k=1}^n p_{ik} \otimes p_{kj}.$$

When we manipulate formulas involving Δ , we often use *Sweedler's notation*

$$\Delta(a) = a_{(1)} \otimes a_{(2)}.$$

Of course, $\Delta(a)$ is in general a linear combination of simple tensors, so what we really have is

$$\Delta(a) = \sum_i a'_i \otimes a''_i, \quad (a'_i, a''_i \in \mathcal{O}(S_n^+)).$$

However, as we will soon see, in most cases we can safely use Sweedler's notation in the intermediate steps and check the consistency later.

The coproduct map describes the composition of quantum automorphisms. Namely, suppose we have representations $\pi_i: \mathcal{O}(S_n^+) \rightarrow \mathcal{B}(H_i)$ for $i = 1, 2$. They give rise to quantum automorphisms

$$\mathbb{C}^n \rightarrow \mathbb{C}^n \otimes \mathcal{B}(H_i).$$

The representation

$$(\pi_1 \otimes \pi_2)\Delta: \mathcal{O}(S_n^+) \rightarrow \mathcal{B}(H_1 \otimes H_2)$$

corresponds to the composition

$$\mathbb{C}^n \rightarrow \mathbb{C}^n \otimes \mathcal{B}(H_2) \rightarrow \mathbb{C}^n \otimes \mathcal{B}(H_1) \otimes \mathcal{B}(H_2).$$

The *antipode* on $\mathcal{O}(S_n^+)$ is the linear transform on $\mathcal{O}(S_n^+)$ characterized by

$$S(p_{ij}) = p_{ji}, \quad S(ab) = S(b)S(a).$$

Proposition 10.7. *We have the following properties for S and Δ .*

- $S^2 = \text{id}$.
- The linear map $m(\text{id} \otimes S)\Delta: \mathcal{O}(S_n^+) \rightarrow \mathbb{C}$ agrees with the homomorphism

$$\epsilon: \mathcal{O}(S_n^+) \rightarrow \mathbb{C}, \quad p_{ij} \mapsto \delta_{ij}.$$

The same holds for $m(S \otimes \text{id})\Delta$.

- $(\epsilon \otimes \text{id})\Delta = \text{id} = (\text{id} \otimes \epsilon)\Delta$ (ϵ is the counit for Δ).

Proof. The property $S^2 = \text{id}$ follows from the fact that S^2 is an algebra automorphism of $\mathcal{O}(S_n^+)$ that fixes each generator p_{ij} , by $S^2(p_{ij}) = S(p_{ji}) = p_{ij}$.

Next, let us check how $m(\text{id} \otimes S)\Delta$ acts on the generators. Unpacking the definitions, we get

$$p_{ij} \mapsto \sum_k p_{ik} \otimes p_{kj} \mapsto \sum_k p_{ik} \otimes p_{jk} \mapsto \sum_k p_{ik} p_{jk}.$$

As remarked above, we have the orthogonality $p_{ik} p_{jk} = 0$ for $i \neq j$, hence the result is $\delta_{ij} \sum_k p_{ik} = \delta_{ij}$. We then argue by induction on the degree of polynomials in p_{ij} . Suppose that we have two elements $a, b \in \mathcal{O}(S_n^+)$ on which we have verified the equality $m(\text{id} \otimes S)\Delta = \epsilon$. We then claim that the equality holds on the element ab . Indeed, writing $\Delta(a) = a_{(1)} \otimes a_{(2)}$, etc., we see that $m(\text{id} \otimes S)\Delta$ acts by

$$ab \mapsto a_{(1)} b_{(1)} \otimes a_{(2)} b_{(2)} \mapsto a_{(1)} b_{(1)} \otimes S(b_{(2)}) S(a_{(2)}) \mapsto a_{(1)} b_{(1)} S(b_{(2)}) S(a_{(2)}).$$

Now, using the assumption on b , we have $b_{(1)} S(b_{(2)}) = \epsilon(b)$. Since this is a scalar, we can bring it to the right of $S(a_{(2)})$ and we are left with

$$a_{(1)} S(a_{(2)}) \epsilon(b) = \epsilon(a) \epsilon(b) = \epsilon(ab),$$

hence the claim.

Finally, we can check the equality $(\epsilon \otimes \text{id})\Delta = \text{id}$ by first testing it on generators, and then build it up on polynomials by a similar argument as above. $\square$

Proposition 10.8. *Consider $B = \mathbb{C}^n$ together with the standard functional ψ , and let A_1, A_2 be adjacency matrix operators of some graphs Γ_1, Γ_2 with n vertices. Then $\theta: B \rightarrow B \otimes C$ is a quantum isomorphism from Γ_1 to Γ_2 if and only if it satisfies*

$$(A_1 \otimes \text{id})\tilde{\theta} = \tilde{\theta}(A_2 \otimes \text{id}).$$

In terms of the elements p_{ij} , the above condition can be expressed as

$$A_2 P = P A_1,$$

where $P \in M_n(C)$ is the matrix with entries p_{ij} .

Proof. We first claim that $\tilde{\theta}$ is unitary, in the sense that

$$\tilde{\theta}^* \tilde{\theta} = \text{id}_{B \otimes C} = \tilde{\theta} \tilde{\theta}^*$$

holds. For example, $\tilde{\theta}^* \tilde{\theta}$ corresponds to the matrix product $P^t P$, where $P = [p_{ij}]_{i,j=1}^n \in M_n(C)$ as above. Then $P^t P$ has entries $\sum_k p_{ki} p_{kj} = \delta_{ij}$, hence the claim.

Now, the assertion is equivalent to $\tilde{\theta}^*(A_1 \otimes \text{id}) \tilde{\theta} = (A_2 \otimes \text{id})$.

The space $\mathcal{B}(L^2(B)) \otimes C$ has a C -valued inner product given by

$$\langle T_1 \otimes c_1, T_2 \otimes c_2 \rangle_C = \langle T_1, T_2 \rangle_{\mathcal{B}(L^2(B))} c_1^* c_2 \quad (T_i \in \mathcal{B}(L^2(B)), c_i \in C)$$

where $\langle T_1, T_2 \rangle$ is the inner product on $\mathcal{B}(L^2(B))$ given by (9.1).

On one hand, $\tilde{\theta}$ preserves this inner product, and it conjugates $S_{A_1} \otimes 1_C$ into $S_{A_2} \otimes C$, as in (10.1). On the other, $A_i \otimes 1_C$ is the image of $\Lambda(1_B) \Lambda(1_B)^* \otimes 1_C$ under $E \otimes \text{id}: \mathcal{B}(L^2(B)) \otimes C \rightarrow S_{A_i} \otimes C$, where E is the orthogonal projection for the above inner product. We also have the invariance of $\Lambda(1_B) \Lambda(1_B)^* \otimes 1_C$ under conjugation by $\tilde{\theta}$, hence we obtain the claim. $\square$

Definition 10.9. Consider two graphs Γ and Λ with $|V_\Gamma| = |V_\Lambda| = n$. We define $\mathcal{O}(\text{Iso}^+(\Gamma, \Lambda))$ to be the quotient algebra of $\mathcal{O}(S_n^+)$ by the extra relation

$$A_\Lambda U = U A_\Gamma$$

in $M_n(\mathcal{O}(S_n^+))$, where U is the matrix $[p_{ij}]_{i,j}$.

Proposition 10.8 says that a quantum isomorphism from Γ to Λ given by $C \subset \mathcal{B}(H)$ corresponds to a representation $\mathcal{O}(\text{Iso}^+(\Gamma, \Lambda)) \rightarrow \mathcal{B}(H)$.

The algebra $\mathcal{O}(\text{Aut}^+(\Gamma)) = \mathcal{O}(\text{Iso}^+(\Gamma, \Gamma))$ is a Hopf $*$ -algebra quotient of $\mathcal{O}(S_n^+)$, that is, the coproduct Δ , antipode S , and the counit ϵ on $\mathcal{O}(S_n^+)$ induce maps

$$\Delta: \mathcal{O}(\text{Aut}^+(\Gamma)) \rightarrow \mathcal{O}(\text{Aut}^+(\Gamma))^{\otimes 2}, \quad S: \mathcal{O}(\text{Aut}^+(\Gamma)) \rightarrow \mathcal{O}(\text{Aut}^+(\Gamma)), \quad \epsilon: \mathcal{O}(\text{Aut}^+(\Gamma)) \rightarrow \mathbb{C}$$

satisfying the properties in Proposition 10.7. Other notations are: $\mathcal{O}(\text{Qut}(\Gamma))$, $\mathcal{O}(\text{QAut}(\Gamma))$, $\dots$

Remark 10.10. When $\mathcal{O}(\text{Iso}^+(\Gamma, \Lambda))$ is nontrivial, this gives a *Hopf-Galois object* between the Hopf $*$ -algebras $\mathcal{O}(\text{Aut}^+(\Gamma))$ and $\mathcal{O}(\text{Aut}^+(\Lambda))$.

Remark 10.11. The tensor category of finite dimensional corepresentations of $\mathcal{O}(\text{Aut}^+(\Gamma))$ can be described by the “spin model” of Γ [Jae92, Ban05]. This leads to the following combinatorial criterion: the algebra $\mathcal{O}(\text{Iso}^+(\Gamma, \Lambda))$ is nontrivial if and only if, for any planar graph Δ , the number of graph homomorphisms from Δ to Γ is the same as those to Λ [MR20].

10.3. Quantum isomorphism of quantum sets. We want to understand Hopf algebraic structures behind quantum isomorphisms of quantized structures. Let us first stick to quantum isomorphism of quantum sets, i.e., when the quantum adjacency matrix is trivial (for example, we can take the complete graphs).

Proposition 10.12. *Let $\theta: B_2 \rightarrow B_1 \otimes C$ be a quantum isomorphism. Then $\tilde{\theta}$ is a unitary morphism of Hilbert C -modules.*

Proof. We check the conditions in Remark B.4.

Let us first check that $\tilde{\theta}$ preserves the C -valued inner product, that is,

$$\langle \tilde{\theta}(\Lambda(b_1) \otimes c_1), \tilde{\theta}(\Lambda(b_2) \otimes c_2) \rangle_C = \langle \Lambda(b_1) \otimes c_1, \Lambda(b_2) \otimes c_2 \rangle_C$$

holds. The right hand side is $\psi_2(b_1^* b_2) c_1^* c_2$. Using the C -linearity of the inner product, the left hand side can be written as

$$c_1^* \langle \tilde{\theta}(\Lambda(b_1) \otimes 1), \tilde{\theta}(\Lambda(b_2) \otimes 1) \rangle_C c_2.$$

Now, the middle inner product is

$$(\psi_1 \otimes \text{id})(\theta(b_1)^* \theta(b_2) \otimes 1) = (\psi_1 \otimes \text{id})(\theta(b_1^* b_2) \otimes 1) = \psi_1(b_1^* b_2),$$

hence we obtain the equality.

Next, let us check that $\tilde{\theta}$ is surjective. By C -linearity, it is enough to check that $L^2(B_1, \psi_1) \otimes 1_C$ is contained in $\text{ran } \tilde{\theta}$. Let us take a basis $(x_i)_i$ in B_1 , and let $(x^i)_i$ be the dual basis for pairing via ψ_1 , that is, we ask for $\psi_1(x_i x^j) = \delta_{ij}$. We then have $\sum_i x^i \psi_1(x_i b) = b$. Recall that this can be written as $m^*(\Lambda(1)) = \sum_i \Lambda(x^i) \otimes \Lambda(x_i)$.

Now, let us take the operators on both sides of the equality $(m_1^* \otimes \text{id})\tilde{\theta} = \tilde{\theta}_{13}\tilde{\theta}_{23}(m_2^* \otimes \text{id})$, apply them on $\Lambda(1) \otimes 1$, then apply the transform

$$b' \otimes b'' \otimes c \mapsto \psi(b''b)b' \otimes c \quad (b', b'' \in B_1, c \in C).$$

Then the left hand side gives $\sum_i \Lambda(x^i)\psi(x_i b)1_C = \Lambda(b) \otimes 1_C$, while the right hand side gives an element of $\theta(B_2)(1 \otimes C)$. This proves the assertion. $\square$

Definition 10.13. For $i = 1, 2$, let $X_i = (B_i, \psi_i)$ denote the pair of finite-dimensional C^* -algebra B_i and a faithful positive functional ψ_i , i.e., a “quantum finite set”. We define $\mathcal{O}(\text{Iso}^+(X_1, X_2))$ to be the universal $*$ -algebra such that:

- there is a $*$ -homomorphism $\theta: B_2 \rightarrow B_1 \otimes \mathcal{O}(\text{Iso}^+(X_1, X_2))$ satisfying
- $$(10.2) \quad (\psi_1 \otimes \text{id})\theta(b) = \theta_2(b)1, \quad (m^* \otimes \text{id})\theta = \theta_{13}\theta_{23}m^*.$$
- relations that are valid in all unitary representations should hold, i.e., kill the joint kernel of the $*$ -homomorphisms $\mathcal{O}(\text{Iso}^+(X_1, X_2)) \rightarrow \mathcal{B}(H)$.

Thus, a representation $\pi: \mathcal{O}(\text{Iso}^+(X_1, X_2)) \rightarrow \mathcal{B}(H)$ is the same thing as a quantum isomorphism from X_1 to X_2 given by $C \subset \mathcal{B}(H)$.

Suppose we have three quantum sets $X_i = (B_i, \psi_i)$, for $i = 1, 2, 3$. The composition of quantum isomorphisms

$$B_3 \rightarrow B_2 \otimes \mathcal{O}(\text{Iso}^+(X_2, X_3)), \quad B_2 \rightarrow B_1 \otimes \mathcal{O}(\text{Iso}^+(X_1, X_2))$$

gives a quantum isomorphism of the form

$$B_3 \rightarrow B_1 \otimes \mathcal{O}(\text{Iso}^+(X_1, X_2)) \otimes \mathcal{O}(\text{Iso}^+(X_2, X_3)).$$

By universality, we get a homomorphism

$$\Delta: \mathcal{O}(\text{Iso}^+(X_1, X_3)) \rightarrow \mathcal{O}(\text{Iso}^+(X_1, X_2)) \otimes \mathcal{O}(\text{Iso}^+(X_2, X_3)).$$

When the two quantum sets are the same, let us write $\mathcal{O}(\text{Aut}^+(X))$ to represent $\mathcal{O}(\text{Iso}^+(X, X))$. By considering the identity map of B as a quantum isomorphism with coefficient $C = \mathbb{C}$, we get a homomorphism

$$\epsilon: \mathcal{O}(\text{Aut}^+(X)) \rightarrow \mathbb{C}.$$

Next, we want to relate the quantum isomorphisms

$$\theta_{12}: B_2 \rightarrow B_1 \otimes \mathcal{O}(\text{Iso}^+(X_1, X_2)), \quad \theta_{21}: B_1 \rightarrow B_2 \otimes \mathcal{O}(\text{Iso}^+(X_2, X_1)).$$

Roughly speaking, θ_{21} should correspond to θ_{12} . More generally, suppose that $\theta: B_2 \rightarrow B_1 \otimes C$ is a quantum isomorphism. Taking the adjoint of the second equality in (10.2), we get

$$\tilde{\theta}^* m_{B_1} = m_{B_2} \tilde{\theta}_{23}^* \tilde{\theta}_{13}^*.$$

Thus, $\tilde{\theta}^*$ gives a homomorphism $B_1 \rightarrow B_2 \otimes C$. The problem is whether this is a $*$ -homomorphism.

Proposition 10.14. *If ψ_1 and ψ_2 are traces, then $\tilde{\theta}^*$ is a $*$ -homomorphism.*

Proof. Let us write

$$\theta(x) = \sum_i \psi_2(b_i^* x) b_i'' \otimes c_i \quad (x \in B_2)$$

with $b_i' \in B_2$, $B_i'' \in B_1$, and $c_i \in C$. We then have

$$\tilde{\theta}^*(b^*) = \sum_i \psi_1(b_i''^* b^*) b_i' \otimes c_i^*, \quad \tilde{\theta}^*(b^*)^* = \left(\sum_i \psi_1(b_i''^* b) b_i' \otimes c_i^* \right)^* = \sum_i \psi_1(b^* b_i'') b_i'^* \otimes c_i$$

using $\psi_1(y^*) = \overline{\psi_1(y_1)}$. By the trace property of ψ_1 , we can write $\psi_1(b^* b_i'')$ as

$$\psi_1(b_i''^* b^*) = \psi_1((b_i''^*)^* b^*) = \Lambda_{\psi_1}(b_i''^*)^* \Lambda_{\psi_1}(b^*).$$

Thus, the assertion is equivalent to

$$\sum_i \Lambda_{\psi_2}(b_i') \Lambda_{\psi_1}(b_i'')^* \otimes c_i^* = \sum_i \Lambda_{\psi_2}(b_i^*) \Lambda_{\psi_1}(b_i''^*)^* \otimes c_i.$$

Since θ is a $*$ -homomorphism, we have $\theta(x^*) = \theta(x)^*$, which is equivalent to

$$\sum_i \psi_2(b_i^* x^*) b_i'' \otimes c_i = \sum_i \psi_2(x^* b_i') b_i''^* \otimes c_i^*$$

Again using the trace property of ψ_2 on the right hand side, this can be written as

$$\sum_i \Lambda_{\psi_1}(b_i'') \Lambda_{\psi_2}(b_i')^* \otimes c_i = \sum_i \Lambda_{\psi_1}(b_i'') \Lambda_{\psi_2}(b_i'^*)^* \otimes c_i^*.$$

By taking the adjoint of both sides, we obtain the desired equality. $\square$

We then get a map

$$S: \mathcal{O}(\text{Iso}^+(X_1, X_2)) \rightarrow \mathcal{O}(\text{Iso}^+(X_2, X_1))$$

relating θ and $\tilde{\theta}^*$. This satisfies the antimultiplicativity $S(ab) = S(b)S(a)$, and the additional properties $S^2 = \text{id}$ and $S(a^*) = S(a)^*$.

Theorem 10.15. *Let X be a quantum set represented by a finite dimensional C^* -algebra B and a tracial faithful positive functional ψ . We then have the antipode property for S on $\mathcal{O}(\text{Aut}^+(X))$, i.e., it satisfies*

$$m(\text{id} \otimes S)\Delta(x) = \epsilon(x)1 = m(S \otimes \text{id})\Delta(x).$$

Proof. Morally speaking, the claim corresponds to the unitarity property $\tilde{\theta}\tilde{\theta}^* = \text{id} = \tilde{\theta}^*\tilde{\theta}$. Let us elaborate on the details.

We first check the claim for elements of the form

$$x_{b_1, b_2} = (\Lambda(b_1)^* \otimes \text{id})\tilde{\theta}(\Lambda(b_2)) \in \mathcal{O}(\text{Aut}^+(X)), \quad (b_1, b_2 \in B).$$

Expanding the definitions, we have

$$\epsilon(x_{b_1, b_2}) = \Lambda(b_1)^* \text{id}(\Lambda(b_2)) = \psi(b_1^* b_2), \quad S(x_{b_1, b_2}) = (\Lambda(b_1)^* \otimes \text{id})\tilde{\theta}^*(\Lambda(b_2)),$$

and

$$\Delta(x_{b_1, b_2}) = \sum_i x_{b_1, b_i'} \otimes x_{b_i', b_2}.$$

where $(\Lambda(b_i'))_i$ is any choice of an orthonormal basis in $L^2(B, \psi)$. Then $m(\text{id} \otimes S)\Delta(x_{b_1, b_2})$ is computing

$$\sum_i (\Lambda(b_1)^* \otimes \text{id})\tilde{\theta}(\Lambda(b_i')\Lambda(b_i'^*) \otimes \text{id})\tilde{\theta}^*(\Lambda(b_1) \otimes 1).$$

By assumption on b_i' , we have $\sum_i \Lambda(b_i')\Lambda(b_i'^*) = \text{id}$, hence this represents

$$\Lambda(b_1)^* \tilde{\theta}\tilde{\theta}^* \Lambda(b_2) = \Lambda(b_1)^* \Lambda(b_2) = \psi(b_1^* b_2) = \epsilon(x_{b_1, b_2}),$$

as claimed.

Now, the general claim follows by induction on degree as in the proof of Proposition 10.7. The equality with $m(S \otimes \text{id})\Delta$ can be proved in a similar way. $\square$

When the functional ψ is not tracial, we still get an analogous structure through the theory of compact quantum groups. A *compact quantum group* is given by a unital C^* -algebra A and a $*$ -homomorphism $\Delta: A \rightarrow A \otimes A$ satisfying the coassociativity condition

$$(\Delta \otimes \text{id})\Delta = (\text{id} \otimes \Delta)\Delta$$

and the *cancellativity condition*

$$A \otimes A = [\Delta(A)(A \otimes \mathbb{C})] = [\Delta(A)(\mathbb{C} \otimes A)],$$

where $[\dots]$ represents the (norm) closure of linear span.

Theorem 10.16. *Let X be a quantum set. The bialgebra $\mathcal{O}(\text{Aut}^+(X))$ satisfies the cancellativity condition (without norm closure).*

Proof. Let us sketch the strategy. To check the equality

$$[\Delta(\mathcal{O}(\text{Aut}^+(X)))(\mathbb{C} \otimes \mathcal{O}(\text{Aut}^+(X)))] = \mathcal{O}(\text{Aut}^+(X)),$$

it is enough to show that the left hand side contains elements of the form $x_{b_1, b_2} \otimes 1$. Indeed, if we can have $x_{b_1, b_2} \otimes 1$ and $x_{b_1', b_2'} \otimes 1$ in $[\Delta(\mathcal{O}(\text{Aut}^+(X)))(\mathbb{C} \otimes \mathcal{O}(\text{Aut}^+(X)))]$, then their is also in this space, since we have

$$\Delta(x)(1 \otimes y)(x_{b_1', b_2'} \otimes 1) = \Delta(x)(x_{b_1', b_2'} \otimes 1)(1 \otimes y) \in [\Delta(\mathcal{O}(\text{Aut}^+(X)))(\mathbb{C} \otimes \mathcal{O}(\text{Aut}^+(X)))].$$

Then, it will be enough to check that the coaction map $\alpha: B \rightarrow B \otimes \mathcal{O}(\text{Aut}^+(X))$ satisfies

$$\alpha(B) \otimes \mathbb{C} \subset (\alpha \otimes \text{id})(\alpha(B))(B \otimes \mathbb{C} \otimes \mathcal{O}(\text{Aut}^+(X))).$$

This follows from the last part of the proof for Proposition 10.12.

Next, to check the equality

$$[\Delta(\mathcal{O}(\text{Aut}^+(X)))(\mathcal{O}(\text{Aut}^+(X)) \otimes \mathbb{C})] = \mathcal{O}(\text{Aut}^+(X)),$$

it is enough to have $1 \otimes x_{b_1, b_2}$ in the left hand side. This time, we want an inclusion of the form

$$\alpha(B)_{13} \subset (\alpha \otimes \text{id})(\alpha(B))(B \otimes \mathcal{O}(\text{Aut}^+(X)) \otimes \mathbb{C}).$$

We can use the last part of the proof for Proposition 10.12 again, to find $\alpha(B)_{13}$ in $(\alpha \otimes \text{id})(\alpha(B))(1 \otimes \mathcal{O}(\text{Aut}^+(X)) \otimes 1)$. $\square$

Then a C^* -algebraic closure of $\mathcal{O}(\text{Aut}^+(X))$ becomes gives a compact quantum group in the above sense. In turn, this implies that $\mathcal{O}(\text{Aut}^+(X))$ is a Hopf algebra, that is, we can find an antipode S . However, we do not have $S^2 = \text{id}$ and $S(a^*) = S(a)^*$ unless ψ is tracial, and S is not bounded with respect to sensible norms on $\mathcal{O}(\text{Aut}^+(X))$.

10.4. Quantum isomorphisms of quantum graphs. Suppose that we have two quantum graphs G_1 and G_2 as in Section 10.1. Let us denote the underlying quantum sets by X_i (that is, just the pair (B_i, ψ_i)). Proposition 10.8 motivates the following alternative definition of quantum isomorphisms: a quantum isomorphism from G_1 to G_2 is given by a quantum isomorphism $f: B_2 \rightarrow B_1 \otimes C$ representing a quantum isomorphism from X_1 to X_2 , which satisfies

$$(10.3) \quad (A_1 \otimes \text{id})\tilde{f} = \tilde{f}(A_2 \otimes \text{id})$$

for the induced homomorphism of Hilbert C -modules $\tilde{f}: L^2(B_2) \otimes C \rightarrow L^2(B_1) \otimes C$.

Proposition 10.17. *A quantum isomorphism in the above sense satisfies (10.1), and*

$$\tilde{f}(S'_2 \otimes \mathbb{C}1_C)\tilde{f}^* \subset S'_1 \otimes C,$$

where $S'_i \subset \mathcal{B}(L^2(B_i))$ is the operator system defined by

$$S'_i = \{m(T \otimes A_i)m^* \mid T \in \mathcal{B}(L^2(B_i))\}.$$

Proof. Let us first check (10.1). We use the equality $(m^* \otimes \text{id})\tilde{f} = \tilde{f}_{13}\tilde{f}_{23}(m^* \otimes \text{id})$ to get

$$\tilde{f}^*m(A_1 \otimes T \otimes \text{id}_C)m^*\tilde{f} = m\tilde{f}_{23}^*\tilde{f}_{13}^*(A_1 \otimes T \otimes \text{id}_C)\tilde{f}_{13}\tilde{f}_{23}m^* \quad (T \in \mathcal{B}(L^2(B_1))).$$

Using the commutation of T with $\tilde{f}_{13}$ and $\tilde{f}_{13}^*A_1\tilde{f}_{13} = A_2$, we see that the above agrees with

$$m(A_2 \otimes T_1)m^* \otimes T_2 \in S_{A_2, \psi_2} \otimes C$$

for $T_1 \otimes T_2 = \tilde{f}^*(T \otimes \text{id}_C)\tilde{f}$.

The relation between $\tilde{f}$ and operator systems S'_i can be proved in a similar way from $\tilde{f}m = m\tilde{f}_{13}\tilde{f}_{23}$. $\square$

Remark 10.18. Now, we have several candidates for the formulation of quantum isomorphisms of quantum graphs. First is Definition 10.2, which builds on the comparison of operator systems $S_{A, \psi} \otimes C$. The second is (besides being a quantum isomorphism of underlying quantum sets) to ask for quantum homomorphism property as in Definition 10.1, and a similar property for the ‘opposite’ operator systems S'_i , as in the conclusion of the above proposition. The third is (again besides the quantum isomorphism property) the compatibility with quantum adjacency matrix, as in (10.3). When $G_1 = G_2$ and C is a C^* -algebra of a compact quantum group, these are indeed equivalent by [Daw22, Theorem 9.18].

Definition 10.19. We define $\mathcal{O}(\text{Iso}^+(G_1, G_2))$ to be universal $*$ -algebra such that

- there is a $*$ -homomorphism $\theta: B_2 \rightarrow B_1 \otimes \mathcal{O}(\text{Iso}^+(G_1, G_2))$;
- θ implements a quantum isomorphism from X_1 to X_2 ;
- θ satisfies (10.3).

Again we obtain the coproduct $*$ -homomorphism

$$\Delta: \mathcal{O}(\text{Iso}^+(G_1, G_3)) \rightarrow \mathcal{O}(\text{Iso}^+(G_1, G_2)) \otimes \mathcal{O}(\text{Iso}^+(G_2, G_3))$$

representing the composition of quantum isomorphisms. In particular, for a single quantum graph G with underlying quantum set X , the algebra $\mathcal{O}(\text{Aut}^+(G)) = \mathcal{O}(\text{Iso}^+(G, G))$ becomes a Hopf algebra quotient of $\mathcal{O}(\text{Aut}^+(X))$.

Example 10.20. Consider the operator system

$$S_{\text{sym}} = \{X \in M_d \mid X^t = X\} \subset M_d,$$

and let G_{sym} be the corresponding quantum graph on M_d (for the tautological representation on $\mathbb{C}^d$). Then $\mathcal{O}(\text{Aut}^+(G_{\text{sym}}))$ is the algebra of regular functions on the projective orthogonal group $\text{PO}(d)$. Analogously, consider the operator system

$$S_{\text{sp}} = \{X \in M_{2d} \mid JX^t J^t = X\} \subset M_{2d}$$

defined by the symplectic matrix $J \in M_{2d}$, and the corresponding quantum graph G_{sp} . Then the algebra $\mathcal{O}(\text{Aut}^+(G_{\text{sp}}))$ is that of regular functions on the compact projective symplectic group $\text{PSp}(d)$ (which is the adjoint group of the compact symplectic group $\text{Sp}(d)$).

Example 10.21. More generally, the algebras of q -deformed compact quantum groups $\text{PO}_q(d)$ and $\text{PSp}_q(d)$ for $q > 0$ appear as $\mathcal{O}(\text{Aut}^+(G))$ for suitable quantum graphs deforming the above examples. Here is a sketch: the space $B = M_n$, for $n = d$ or $2d$ depending on the orthogonal or symplectic case, is in the corepresentation category of $\mathcal{O}(\text{Aut}^+(G))$, and is an algebra object in this tensor category. We get a 2-category by looking at module objects and bimodule objects over this algebra, and we have a control on the dimensions of morphisms spaces for the objects $B^{\otimes m}$, interpreted as various module objects, for small m . By a classification of 2-categories with such dimension restrictions, we get the claimed correspondence with $\text{PO}_q(d)$ and $\text{PSp}_q(d)$.

10.5. Recognizing quantum isomorphisms. Suppose we have a quantum graph $X = (B_X, \psi_X, A_X)$, and a quantum automorphism of X given by $C = \mathcal{B}(H^* \otimes H)$ for some finite-dimensional Hilbert space H , and a $*$ -homomorphism $\theta: B_X \rightarrow B_X \otimes C$. We consider the following additional ‘matrix structure’ on quantum automorphism [MRV19]. Consider the map

$$\mu: H^* \otimes H \otimes H^* \otimes H \rightarrow H^* \otimes H, \quad \xi_1^* \otimes \eta_1 \otimes \xi_2^* \otimes \eta_2 \mapsto (\xi_2, \eta_1) \xi_1^* \otimes \eta_2$$

and its ‘adjoint’

$$\mu^*: H^* \otimes H \rightarrow H^* \otimes H \otimes H^* \otimes H, \quad \xi^* \otimes \eta \mapsto \sum_{i=1}^d \xi^* \otimes e_i \otimes e_i^* \otimes \eta$$

for $d = \dim H$ and an orthonormal basis $(e_i)_i$. We then assume that θ and $\theta^{(2)}: B_X \rightarrow B_X \otimes C^{\otimes 2}$ are compatible with these maps, in the sense that we have

$$(10.4) \quad \theta(b)(\text{id}_{B_X} \otimes \mu) = (\text{id}_{B_X} \otimes \mu)\theta^{(2)}(b), \quad (\text{id}_{B_X} \otimes \mu^*)\theta(b) = \theta^{(2)}(b)(\text{id}_{B_X} \otimes \mu^*).$$

Let us consider

$$E: B_X \otimes \mathcal{B}(H^*) \rightarrow B_X \otimes \mathcal{B}(H^*), \quad a \otimes T \mapsto \frac{1}{\dim H} (\text{id} \otimes \bar{R}^*) \theta(a) (\text{id} \otimes \bar{R}),$$

where $\bar{R}: \mathbb{C} \rightarrow H \otimes H^*$ is the map sending 1 to $\sum_i e_i \otimes e_i^*$, and $\bar{R}^*$ is its adjoint $H \otimes H^* \rightarrow \mathbb{C}$ given by $\xi \otimes \eta^* \mapsto \langle \eta, \xi \rangle$.

Proposition 10.22. *We have $E^2 = E$, and E is a ucp map.*

Proof. The ucp conditions follows from the definition.

To check $E^2 = E$, we observe that $(\dim H)^2 E^2(a \otimes T)$ is given by $\theta^{(2)}$, μ , and μ^* as

$$(\text{id}_{B_X} \otimes \bar{R}^*)(\text{id}_{B_X} \otimes \mu \otimes \text{id}_{H^*})(\theta^{(2)}(a) \otimes T)(\text{id}_{B_X} \otimes \mu^* \otimes \text{id}_{H^*})(\text{id}_{B_X} \otimes \bar{R}).$$

Using the compatibility between θ and μ as above, this is equal to

$$\dim H (\text{id} \otimes \bar{R}^*) \theta(a) (\text{id} \otimes \bar{R}) = (\dim H)^2 E(a \otimes T),$$

hence the claim. $\square$

Proposition 10.23. *The subspace $\text{ran } E \subset B_X \otimes \mathcal{B}(H^*)$ is closed under product.*

Proof. We need to check

$$E(E(a \otimes T)E(b \otimes S)) = E(a \otimes T)E(b \otimes S) \quad (a, b \in B_X, T, S \in \mathcal{B}(H^*)).$$

Let us write $\theta(a) = a_{(1)} \otimes a_{(2)} \otimes a_{(3)}$ with $a_{(1)} \in B_X$, $a_{(2)} \in \mathcal{B}(H^*)$, and $a_{(3)} \in \mathcal{B}(H)$. We thus have

$$E(a \otimes T) = \frac{1}{\dim H} a_{(1)} \otimes a_{(2)} \otimes \bar{R}^*(a_{(3)} \otimes T) \bar{R}.$$

Then $E(E(a \otimes T)E(b \otimes S))$ becomes

$$\frac{1}{(\dim H)^3} (\text{id}_{B_X \otimes H^*} \otimes \bar{R}^*) (\theta(a_{(1)} b_{(1)}) \otimes a_{(2)} b_{(2)}) (\text{id}_{B_X \otimes H^*} \otimes \bar{R}) \bar{R}^* (a_{(3)} \otimes T) \bar{R} \bar{R}^* (b_{(3)} \otimes S) \bar{R}.$$

Since θ is a homomorphism, we have $\theta(a_{(1)} b_{(1)}) = \theta(a_{(1)}) \theta(b_{(1)})$, and we get the product of $\theta^{(2)}(a)$ and $\theta^{(2)}(b)$. To be precise, writing

$$\theta^{(2)}(a) = a_{(1)} \otimes a_{(2)} \otimes a_{(3)} \otimes a_{(4)} \otimes a_{(5)}$$

for $a_{(2)}, a_{(4)} \in \mathcal{B}(H^*)$ and $a_{(3)}, a_{(5)} \in \mathcal{B}(H)$, the above is

$$\frac{1}{(\dim H)^3} a_{(1)} b_{(1)} \otimes a_{(2)} b_{(2)} \bar{R}^* (a_{(3)} b_{(3)} \otimes a_{(4)} b_{(4)}) \bar{R} \bar{R}^* (a_{(5)} \otimes T) \bar{R} \bar{R}^* (b_{(5)} \otimes S) \bar{R}.$$

We then use (10.4) and $\bar{R}^* \bar{R} = \dim H$ to get

$$\frac{1}{(\dim H)^2} a_{(1)} b_{(1)} \otimes a_{(2)} b_{(2)} \bar{R}^* (a_{(3)} \otimes T) \bar{R} \bar{R}^* (b_{(3)} \otimes S) \bar{R},$$

which is $E(a \otimes T)E(b \otimes S)$. $\square$

Thus, $B_Y = \text{ran } E$ is a C^* -subalgebra of $B_X \otimes \mathcal{B}(H^*)$.

Proposition 10.24. *We have*

$$(\psi_X \otimes \text{id})(x) = (\psi_X \otimes \text{tr}_{\mathcal{B}(H^*)})(x) \text{id}_{H^*} \quad (x \in B_Y),$$

where $\text{tr}_{\mathcal{B}(H^*)} = \frac{1}{\dim H} \text{Tr}_{\mathcal{B}(H^*)}$ is the normalized trace functional on $\mathcal{B}(H^*)$.

Proof. Let us compute $(\psi_X \otimes \text{id})E(a \otimes T)$ for $a \in B_X$ and $T \in \mathcal{B}(H^*)$. We have $(\psi_X \otimes \text{id})\theta(a) = \psi_X(a) \text{id}_{H^* \otimes H}$ by the quantum isomorphism assumption on θ . We thus have

$$(\psi_X \otimes \text{id})E(a \otimes T) = \frac{1}{\dim H} \psi_X(a) \text{id}_{H^*} \bar{R}^* (\text{id}_H \otimes T) \bar{R} = \psi_X(a) \text{tr}(T) \text{id}_{H^*},$$

proving the claim. $\square$

Corollary 10.25. *The embedding $\rho: B_Y \rightarrow B_X \otimes \mathcal{B}(H^*)$ induces an isometric embedding*

$$L^2(B_Y, \psi_Y) \rightarrow L^2(B_X \otimes \mathcal{B}(H^*), \psi_X \otimes \text{tr})$$

for the functional ψ_Y on B_Y given by the restriction of $\psi_X \otimes \text{id}$.

Proposition 10.26. *The $*$ -homomorphism $\rho: B_Y \rightarrow B_X \otimes \mathcal{B}(H^*)$ defines a quantum isomorphism of quantum sets.*

Proof. We need to check the consistency condition with m^* . Corollary 10.25 implies that m_Y^* is the restriction of $(E \otimes E)m_X^* m_{\mathcal{B}(H^*)}^*$ (we make sense it by appropriate shuffle of tensor factors). We thus get

$$(10.5) \quad \rho_{13} \rho_{23} m_Y^* = m_{\mathcal{B}(H^*)}^* (E \otimes E) m_X^* m_{\mathcal{B}(H^*)}^* \rho,$$

up to appropriate shuffle.

Let us write $m_X^*(a) = a_{(1)} \otimes a_{(2)}$ and $m_{\mathcal{B}(H^*)}^*(T) = T_{(1)} \otimes T_{(2)}$. Then the right hand side of (10.5) acts by

$$\frac{1}{(\dim H)^2} \theta(a_{(1)})_1 \otimes \theta(a_{(2)})_1 \otimes (\text{id} \otimes \bar{R}^*) (\theta(a_{(1)})_2 \otimes T_{(1)}) (\text{id} \otimes \bar{R} \bar{R}^*) (\theta(a_{(2)})_2 \otimes T_{(2)}) (\text{id} \otimes \bar{R}),$$

which becomes

$$\frac{1}{\dim H} \theta(a_{(1)})_1 \otimes \theta(a_{(2)})_1 \otimes (\text{id} \otimes \bar{R}^*) (\theta(a_{(1)})_2 \otimes T_{(1)}) (\text{id} \otimes \bar{R})$$

by the defining property of $m_{\mathcal{B}(H^*)}^*$, which can be further simplified to

$$\frac{1}{\dim H} m_X^* (\theta(a)_1) \otimes (\text{id} \otimes \bar{R}^*) (\theta(a)_2 \otimes T) (\text{id} \otimes \bar{R}) = m_X^* E(a \otimes T).$$

This proves the claim. $\square$

Moreover, we have a quantum graph structure on (B_Y, ψ_Y) , as follows. The condition $\theta A_X = (A_X \otimes \text{id})\theta$ implies that $A_X \otimes \text{id}_{\mathcal{B}(H^*)}$ preserves B_Y . Let A_Y denote its restriction on B_Y .

Proposition 10.27. *The map A_Y , as a linear transform on $L^2(B_Y, \psi_Y)$, is a quantum adjacency matrix operator for (B_Y, ψ_Y) .*

Proof. The self-adjointness $A_Y^* = A_Y$ follows from the construction.

Let us check $m_Y(A_Y \otimes A_Y)m_Y^* = A_Y$. Using $m_Y^* = (E \otimes E)m_X^*m_{\mathcal{B}(H^*)}^*$, the action of convolution square of A_Y on $E(a \otimes T)$ can be written as

$$\frac{1}{(\dim H)^2} (A_X \theta(a_{(1)})_1) (A_X \theta(a_{(2)})_1) \otimes (\text{id} \otimes \bar{R}^*) (\theta(a_{(1)})_2 \otimes T_{(1)}) (\text{id} \otimes \bar{R} \bar{R}^*) (\theta(a_{(2)})_2 \otimes T_{(2)}) (\text{id} \otimes \bar{R}),$$

which can be transformed as before to

$$\frac{1}{\dim H} m_X (A_X \otimes A_X) m_X^* (\theta(a)_1) \bar{R}^* (\theta(a)_2 \otimes T) \bar{R}.$$

Using $m_X(A_X \otimes A_X)m_X^* = A_X$, we see that this is equal to $A_X E(a \otimes T)$, proving the claim.

The equality $m(A_Y \otimes \text{id})m^* = \text{id}$ can be proved in a similar way. $\square$

Thus, we obtain a quantum graph $Y = (B_Y, \psi_Y, A_Y)$. Moreover, ρ is a quantum isomorphism of quantum graphs.

11. QUANTUM ISOMORPHISM GAME FOR GRAPHS

11.1. Non-local games and their algebras. Suppose we have a collection of self adjoint operators $(A_x)_x$ and $(B_y)_y$ on a Hilbert space H , satisfying $A_x B_y = B_y A_x$. Then, what can we say about the numbers

$$(11.1) \quad \langle \xi, A_x^k B_y^l \xi \rangle \quad (\xi \in H),$$

and what happens when we ask for some algebraic consistency?

The first reduction is to assume that each A_x and B_y have finite spectra, so that we can write

$$A_x = \sum_a \alpha_{xa} P_{xa}, \quad B_y = \sum_b \beta_{yb} Q_{yb},$$

where P_{xa} and Q_{yb} are projections on H satisfying

$$P_{xa} Q_{yb} = P_{xa} Q_{yb}, \quad \sum_a P_{xa} = \text{id}_H = \sum_b Q_{yb}.$$

Then we can recover (11.1) from the numbers $\langle \xi, P_{xa} Q_{yb} \xi \rangle$ by

$$\langle \xi, A_x^k B_y^l \xi \rangle = \sum_{a,b} \alpha_{xa}^k \beta_{yb}^l \langle \xi, P_{xa} Q_{yb} \xi \rangle.$$

The theory of *nonlocal games* gives a powerful paradigm to give algebraic consistency conditions on the projections P_{xa} and Q_{yb} and the vector ξ . Consider a function $\lambda(x, y, a, b)$ that takes value 0 or 1. We then impose the condition

$$(11.2) \quad \lambda(x, y, a, b) = 0 \Rightarrow \langle \xi, P_{xa} Q_{yb} \xi \rangle = 0.$$

We interpret this as λ giving the rule of a game for two players, Alice and Bob, in the following way.

- Alice receives input x , and gives output a ;
- Bob receives input y , and gives output b ;
- $\lambda(x, y, a, b) = 0$ means they “lose” the game;
- $\lambda(x, y, a, b) = 1$ means they “win”.

Then, P_{xa} , Q_{yb} , and ξ satisfying (11.2) gives a quantum mechanical winning strategy for Alice and Bob, in the sense that given inputs x and y , they select observables A_x and B_y whose possible values (α_{xa}) and (β_{yb}) are labeled by a and b , and measure them. They get the outputs a and b with probability $\langle \xi, P_{xa} Q_{yb} \xi \rangle$, which is guaranteed to be consistent with the rule of the game. This way, as long as they start by sharing the factors of the state vector ξ , they can win the game without communication after receiving the inputs x and y .

The second reduction is to go to a universal algebraic setting. We look at the universal $*$ -algebra $\mathcal{A}$ with generators p_{xa} and q_{yb} for indexes x, y, a, b , subject to the following relations.

- p_{xa} and q_{yb} are projections;
- $p_{xa} q_{yb} = q_{yb} p_{xa}$;
- $\sum_a p_{xa} = 1_{\mathcal{A}} = \sum_b q_{yb}$ for each x and y ;
- if $\lambda(x, y, a, b) = 0$, then $p_{xa} q_{yb} = 0$.

Then, a state functional on $\mathcal{A}$ gives a quantum winning strategy $(P_{xa})_{x,a}$, $(Q_{yb})_{y,b}$, and ξ by the GNS construction.

11.2. Non-local games from graph isomorphism problems. Now, let us present a class of non-local games motivated by graph isomorphism problems [AMR⁺19].

For $i = 1, 2$, let Γ_i be a graph with vertex set V_i . (We assume that V_1 and V_2 are disjoint, and Γ_1 and Γ_2 do not have loops around vertices.) We set

$$I = O = V_1 \cup V_2$$

for the input and output sets, both for Alice and Bob. As for the rule function $\lambda(x, y, a, b)$, we have $\lambda(x, y, a, b) = 0$ when either of the following holds:

- (1) $x, a \in V_i$ or $y, b \in V_i$ for some i ; given input $x \in V_i$, Alice should answer with $a \in V_j$ for $j \neq i$, and the same for Bob.
- (2) given the consistency as above, suppose $\{v_1, w_1\} = \{x, y, a, b\} \cap V_1$ (resp. $\{v_2, w_2\} = \{x, y, a, b\} \cap V_2$). Then the incidence relation between v_1 and w_1 should be the same as that between v_2 and w_2 .

Othwise we have $\lambda(x, y, a, b) = 1$. Here, the incidence relation between v_1 and w_1 is either $v_1 = w_1$, $v_1 \sim_{\Gamma_1} w_1$, or “neither of these”.

Let us derive some properties of quantum winning strategies given by $(P_{x,a})_{x,a}$, $(Q_{y,b})_{y,b}$, and ξ for this game. Let us set

$$p(a, b \mid x, y) = \langle \xi, P_{x,a} Q_{y,b} \xi \rangle.$$

Proposition 11.1. *We have $p(a, b \mid x, x) = 0$ for $a \neq b$.*

Proof. By condition (2) above, we have $\lambda(x, x, a, b) = 0$ for $a \neq b$. This forces $p(a, b \mid x, x) = 0$ by (11.2). $\square$

A non-local game that forces the above condition for its quantum winning strategies is called a *synchronous game*. For now, consider a synchronous game with input set I and output set O .

Consider the universal $*$ -algebra $\mathcal{A}_1$ generated by projections $(p_{x,a})_{x \in I, a \in O}$, subject to the relations that are always valid for $(P_{x,a})_{x,a}$ that appear as part of a quantum winning strategy for the game we are considering. For example, we have $\sum_a p_{x,a} = 1$.

Let us also fix a concrete quantum winning strategy given by $(P_{x,a})_{x,a}$, $(Q_{y,b})_{y,b}$, and ξ on H .

Lemma 11.2. *We have $P_{x,a} \xi = Q_{x,a} \xi$.*

Proof. From $\sum_a P_{x,a} = \text{id}_H = \sum_b Q_{y,b}$, we get

$$\sum_{a,b} p(a, b \mid x, x) = \sum_{a,b} \langle \xi, P_{x,a} Q_{y,b} \xi \rangle = \langle \xi, \text{id}_H \text{id}_H \xi \rangle = 1.$$

We get 0 from the terms with $a \neq b$, hence $\sum_a p(a, a \mid x, x) = 1$, that is, $\sum_a \langle \xi, P_{x,a} Q_{y,a} \xi \rangle = 1$. We also have

$$\sum_a \|P_{x,a} \xi\|^2 = \sum_a \langle \xi, P_{x,a} \xi \rangle = 1.$$

Now observe that the Cauchy–Schwartz inequality gives

$$\left| \sum_a \langle \xi, P_{x,a} Q_{x,a} \xi \rangle \right| \leq \left(\sum_a \|P_{x,a} \xi\| \right)^{1/2} \left(\sum_a \|Q_{x,a} \xi\| \right)^{1/2},$$

and the equality happens if and only if $P_{x,a} \xi = Q_{x,a} \xi$ holds for all a . $\square$

Theorem 11.3 ([PSS⁺16]). *Let $\mathcal{A}_1 \rightarrow \mathcal{B}(H)$ denote the representation defined by $p_{x,a} \mapsto P_{x,a}$.*

- (1) *The functional τ on $\mathcal{A}_1$ defined by $\tau(r) = \langle \xi, \pi(r) \xi \rangle$ is a tracial state on $\mathcal{A}_1$ (we have $\tau(sr) = \tau(rs)$);*
- (2) *We have $\langle \xi, P_{x,a} Q_{y,b} \xi \rangle = \tau(p_{x,a} p_{y,b})$.*

Proof. Condition 2 is a direct consequence of Lemma 11.2.

Let us check condition 1. By induction, we may reduce the claim to the case $s = p_{x,a}$. Using Lemma 11.2, we get

$$\langle \xi, \pi(r) \pi(p_{x,a}) \xi \rangle = \langle \xi, \pi(r) P_{x,a} \xi \rangle = \langle \xi, \pi(r) Q_{x,a} \xi \rangle.$$

Since $\pi(r)$ is a polynomial of the operators $P_{x',a'}$, it commutes with $Q_{x,a}$. Then the above is equal to

$$\langle \xi, Q_{x,a} \pi(r) \xi \rangle = \langle Q_{x,a} \xi, \pi(r) \xi \rangle = \langle P_{x,a} \xi, \pi(r) \xi \rangle,$$

the second equality again by Lemma 11.2. Then we get

$$\langle P_{x,a} \xi, \pi(r) \xi \rangle = \langle \xi, P_{x,a} \pi(r) \xi \rangle = \langle \xi, \pi(r) \pi(p_{x,a}) \xi \rangle,$$

hence the trace condition for τ . $\square$

Note that a tracial state τ on $\mathcal{A}_1$ leads to a quantum winning strategy by setting H to be GNS Hilbert space, ξ to be the GNS vector, P_{xa} to be the standard action of p_{xa} (coming from the left multiplication), and Q_{yb} to be the right multiplication action of p_{yb} . Thus, for a synchronous game, we can reduce the problem of finding quantum winning strategies to the one for tracial states on the algebra $\mathcal{A}_1$.

Now, let us get back to the case of graph isomorphisms game for Γ_1 and Γ_2 .

Proposition 11.4. *We have a $*$ -homomorphism $\mathcal{A}_1 \rightarrow \mathcal{O}(\text{Iso}^+(\Gamma_1, \Gamma_2))$ characterized by*

$$p_{vw} \mapsto e_{vw}, \quad p_{wv} \mapsto e_{vw} \quad (v \in V_1, w \in V_2).$$

Proof. We need to check that $e_{v_1 w_1} e_{v_2 w_2} = 0$ holds whenever the incidence relation between v_1, v_2 is different from that between w_1, w_2 . Let us note that $\sum_a p_{xa} = 1$ corresponds to $\sum_w e_{vw} = 1$ and $\sum_v e_{vw} = 1$.

First let us check that $v_1 = v_2 = v$ and $w_1 \neq w_2$ implies $e_{v w_1} e_{v w_2} = 0$. This is a cosequence of the mutual orthogonality of projections $(e_{vw})_w$, which follows from $\sum_w e_{vw} = 1$.

Next let us check that $v_1 \sim_{\Gamma_1} v_2$ and $w_1 \not\sim_{\Gamma_2} w_2$ implies $e_{v_1 w_1} e_{v_2 w_2} = 0$. If $w_1 = w_2$, this is a consequence of mutual orthogonality of $(e_{vw_1})_v$ as above. If $w_1 \neq w_2$ (and $w_1 \not\sim w_2$), consider the map $\theta: L^2(V_2) \rightarrow L^2(V_1) \otimes \mathcal{O}(\text{Iso}^+(\Gamma_1, \Gamma_2))$, where we write $L^2(C(V_{\Gamma_1}), \psi_{\text{std}}) = L^2(V_1)$, etc. Then $\theta_{13}\theta_{23}$ is the map

$$L^2(V_2) \otimes L^2(V_2) \rightarrow L^2(V_1) \otimes L^2(V_1) \otimes \mathcal{O}(\text{Iso}^+(\Gamma_1, \Gamma_2)), \quad \Lambda(\delta_w) \otimes \Lambda(\delta_{w'}) \mapsto \sum_{v, v'} \Lambda(\delta_v) \otimes \Lambda(\delta_{v'}) \otimes e_{vw} e_{v'w'}.$$

We also consider $m(\text{id} \otimes A_2)$, which is the map

$$L^2(V_2) \otimes L^2(V_2) \rightarrow L^2(V_2), \quad \Lambda(\delta_{w_1}) \otimes \Lambda(\delta_{w_2}) \mapsto \sum_{w' \sim w_2} \Lambda(\delta_w \delta_{w_2}).$$

If the input satisfies $w_1 \not\sim w_2$, then the output must be 0.

Now, observe that $\theta m = m\theta_{13}\theta_{23}$ (homomorphism property of θ) and $(A_1 \otimes \text{id})\theta = \theta A_2$ implies

$$\theta m(\text{id} \otimes A_2) = m(\text{id} \otimes A_1)\theta_{13}\theta_{23}.$$

The left hand side on $\Lambda(\delta_{w_1}) \otimes \Lambda(\delta_{w_2})$ is 0 by the above consideration. The right hand side gives

$$\sum_{v, v', v'' \sim v'} \Lambda(\delta_v \delta_{v''}) \otimes e_{vw_1} e_{v'w_2}.$$

The terms from $v = v_1$ and $v' = v_2$ give $\Lambda(\delta_{v_1})$ in the first factor, hence $e_{v_1 w_1} e_{v_2 w_2}$ must be 0.

The remaining case is to check $v_1 \not\sim v_2$ (and $v_1 \neq v_2$) and $w_1 \sim w_2$ implies $e_{v_1 w_1} e_{v_2 w_2} = 0$. This can be proved by a similar argument as above. $\square$

Proposition 11.5. *We have $p_{vw} = p_{wv}$ in $\mathcal{A}_1$.*

Proof. The first step is to check $p_{vw} p_{w'v} = 0$ for $w \neq w'$. We have $p(w, v \mid v, w') = 0$ from the incompatible “incidence relation” $v_1 = v_2 = v$ and $w_1 = w \neq w_2 = w'$. Observe that this is

$$\tau(p_{vw} p_{w'v}) = \langle \xi, P_{vw} Q_{w'v} \xi \rangle \langle \xi, Q_{w'v} P_{vw}^2 Q_{w'v} \xi \rangle = \|P_{vw} Q_{w'v} \xi\|^2.$$

Thus, we have $P_{vw} Q_{w'v} \xi = 0$, and by Lemma 11.2 we get $P_{vw} P_{w'v} \xi = 0$.

Then, for any $x, y \in \mathcal{A}_1$ we have

$$\tau(x p_{vw} p_{w'v} y) = \tau(y x p_{vw} p_{w'v}) = \langle \xi, \pi(yx) P_{vw} P_{w'v} \xi \rangle = 0.$$

But $\tau(x p_{vw} p_{w'v} y)$ represents $\langle \pi(x^*) \xi, P_{vw} P_{w'v} \pi(y) \xi \rangle$. Since the vectors $\pi(x^*) \xi$ for $x \in \mathcal{A}_1$ span H , and same for the $\pi(y) \xi$, we see that the operator $P_{vw} P_{w'v}$ is 0 as an operator. Since (π, H) is an arbitrary choice of quantum winning strategy, we have $p_{vw} p_{w'v} = 0$ in $\mathcal{A}_1$. $\square$

Corollary 11.6. *We have $\sum_v p_{vw} = 1$.*

Proof. This follows from $\sum_v p_{wv} = 1$ and the above proposition. $\square$

Theorem 11.7 ([AMR⁺19]). *The $*$ -homomorphism from Proposition 11.4 is an isomorphism.*

Proof. The goal is to check that the matrix $U = [p_{vw}]_{v \in V_1, w \in V_2} \in M_{V_1 \times V_2}(\mathcal{A}_1)$ satisfies $A_1 U = U A_2$. Combined with the properties we have established already, we will get a well-defined homomorphism $\mathcal{O}(\text{Iso}^+(\Gamma_1, \Gamma_2)) \rightarrow \mathcal{A}_1$ that sends e_{vw} to p_{vw} . In other words, we want to establish

$$\sum_{v' \sim v} p_{v'w} = \sum_{w' \sim w} p_{vw'}$$

for all v, w . Using $\sum_{w'} p_{vw'} = 1$, we have $\sum_{v' \sim v} p_{v'w} = \sum_{v' \sim v} p_{v'w} \sum_{w'} p_{vw'}$. By the consistency with incidence relation, the latter is $\sum_{v' \sim v} p_{v'w} \sum_{w' \sim w} p_{vw'} p_{vw'}$. Going back by a similar argument for v' , we arrive at $\sum_{w' \sim w} p_{vw'}$, hence the claim. $\square$

To get a nontrivial example of quantum isomorphisms between graphs, we use the idea of 2-cocycle deformation.

Theorem 11.8 ([MRV19]). *Suppose that a finite group G acts faithfully on a graph Γ . Moreover, let $\sigma: G \times G \rightarrow \mathbb{T}$ be a 2-cocycle on G such that $\mathbb{C}_\sigma[G]$ is isomorphic to the matrix algebra M_d for some d . Then we get a quantum automorphism of Γ with matrix structure as in Section 10.5.*

Let Y be the resulting quantum graph. It is a classical graph (that is, B_Y is commutative) if and only if the stabilizer subgroup

$$\text{Stab}(v) = \{g \in G \mid gv = v\}$$

is coisotropic ($\sigma|_{\text{Stab}(v)^2} = 1$) for each $v \in V_\Gamma$.

As a concrete example, we can consider the graph Γ encoding the 3×3 Binary Magic Square problem. A BMS is a matrix $[a_{ij}]_{i,j=1}^3 \in M_3(\mathbb{Z}/2)$ satisfying $\sum_i a_{ij} = 0$ and $\sum_j a_{ij} = 0$. The vertices of Γ are given by a row or a column (including its location) in a BMS. Two vertices are connected if they have mismatching entries. Since there are 3 rows, 3 columns, and each has 4 possible configurations, Γ has $(3+3) \times 4 = 24$ vertices. There is an action of $G = \mathbb{Z}_2^4$, whose generators flip entries in a 2×2 -square. The stabilizer of each vertex is isomorphic to $\mathbb{Z}_2^2$. There is a nondegenerate 2-cocycle σ for which the stabilizers are always coisotropic, hence we get a graph Λ with 24 vertices which is quantum isomorphic to Γ . As it happens, Λ is the graph of another BMS scheme, this time with the modified condition $\sum_i a_{3i} = 1$ (but otherwise the same as the original conditions).

APPENDIX A. SEMI-DEFINITE PROGRAMMING

We review basics on Semi-Definite Programming (SDP) following [Gup11].

A.1. Primary and dual problems. Consider the collection of $d \times d$ self-adjoint complex matrices, $(M_d)_{\text{sa}}$, as an Euclidean space whose inner product given by the trace inner product. Suppose we are given a matrix $C \in (M_d)_{\text{sa}}$, a real linear map $\ell: (M_d)_{\text{sa}} \rightarrow \mathbb{R}^n$, and a vector $b \in \mathbb{R}^n$. We want to solve the following problem, called the *primal problem*.

Goal: maximize the quantity $\text{Tr}(CX)$ for $X \in (M_d)_{\text{sa}}$.

Constraint: $X \in (M_d)_{\text{sa}}$ is positive semi-definite, and satisfies the equation $\ell(X) = b$.

Definition A.1. In the setting of a primal problem, we say that a matrix $X \in (M_d)_{\text{sa}}$ is a *feasible solution* if X is positive semi-definite and satisfies the equation $\ell(X) = b$ (but we do not require X to maximize $\text{Tr}(CX)$ at this point). If we additionally have that X is invertible we say that X is a *strict solution*.

Given a primal problem as above, we can also consider the *dual problem*, as follows.

Goal: minimize the quantity $b^t v = \langle b, v \rangle$ for $v \in \mathbb{R}^n$.

Constraint: $v \in \mathbb{R}^n$ satisfies $\ell^t(v) \geq C$.

Here $\ell^t: \mathbb{R}^n \rightarrow (M_d)_{\text{sa}}$ is the transpose of ℓ , characterized by $v^t \ell(X) = \text{Tr}(\ell^t(v)X)$.

Definition A.2. In the setting of a dual problem, we say that a vector $v \in \mathbb{R}^n$ is a *feasible solution* if v satisfies $\ell^t(v) \geq C$. If we additionally have that $\ell^t(v) - C$ is invertible, we say that v is a *strict solution*.

Remark A.3. There are other conventions, where the primal problem and the dual problem are switched, or we want to minimize the quantity $\text{Tr}(CX)$ and maximize $b^t v$, and so on.

Observe that if $X \in (M_d)_{\text{sa}}$ and $v \in \mathbb{R}^n$ are feasible solutions, we then have

$$(A.1) \quad b^t v = \ell(X)^t v = \text{Tr}(\ell^t(v)X) \geq \text{Tr}(CX),$$

where the last inequality follows by positivity of X and the fact that $\ell^t(v) \geq C$.

Definition A.4. Given the primal and the dual problems as above, we say that a pair of feasible solutions $X \in (M_d)_{\text{sa}}$ and $v \in \mathbb{R}^n$ are *optimal solutions* if the equality $b^t v = \text{Tr}(CX)$ holds.

By the above estimate, optimal solutions achieve the goals of primal and dual problems.

Example A.5. Let us cast the problem of finding the largest eigenvalue of a self-adjoint matrix into semi-definite programming. Let us fix a matrix $C \in (M_d)_{\text{sa}}$. The maximum eigenvalue $\lambda_{\max}(C)$ is found by solving the following primal problem: maximize $\text{Tr}(CX)$ where $X \in (M_d)_{\text{sa}}$ is positive semi-definite, and satisfies $\text{Tr}(X) = 1$. Or dually, by solving the following dual problem: minimize $r \in \mathbb{R}$ such that $\text{rid} \geq C$.

Here, our linear map ℓ is Tr , and we take $1 \in \mathbb{R}$ as b . Thus, our goal is to exhibit a pair of optimal solutions (X, r) such that $\lambda_{\max}(C) = r \cdot 1 = \text{Tr}(CX)$ holds. From this requirement we clearly have only one option for our choice of r , namely $\lambda_{\max}(C)$. As the matrix $\lambda_{\max}(C)\text{id} - C$ is positive semi-definite, $\lambda_{\max}(C)$ is a feasible solution to the dual problem.

Consider now the eigendecomposition $UDU^* = C$, with a diagonal matrix D and a unitary matrix U . We may assume that $D_{11} = \lambda_{\max}(C)$. Let $Y \in (M_d)_{\text{sa}}$ be the matrix where $Y_{11} = 1$, and all other entries are zero. Then $X = UYU^*$ is positive semi-definite and satisfies $\text{Tr}(X) = \text{Tr}(Y) = 1$, hence X is a feasible solution to the primal problem. We then compute that

$$\text{Tr}(CX) = \text{Tr}(UDU^*UYU^*) = \text{Tr}(DY) = D_{11} = \lambda_{\max}(C).$$

Thus, the pair X and $\lambda_{\max}(C)$ are optimal solutions.

A.2. Strong duality. One goal is to characterize a situation where we can guarantee the existence of optimal solutions to a problem. We prove a version of the very useful paradigm, called the *strong duality*, as follows.

Theorem A.6. Suppose that we are given $C \in (M_d)_{\text{sa}}$, $\ell: (M_d)_{\text{sa}} \rightarrow \mathbb{R}^n$, and $b \in \mathbb{R}^n$, such that we have a feasible solution to the corresponding primal problem. Moreover, suppose that there is a strict solution to the dual problem. Then there exists a pair of optimal solutions.

The key step is a following variation of the Farkas lemma due to Lovász.

Lemma A.7. There exists a nonzero positive semi-definite matrix $X \in (M_d)_{\text{sa}}$ satisfying $\ell(X) = 0$ and $\text{Tr}(CX) \geq 0$ if and only if the dual problem has no strict solutions, i.e., there is no $v \in \mathbb{R}^n$ such that $\ell^t(v) - C$ is positive definite.

Proof. As a first step of the proof let us establish the following special case corresponding to $C = 0$: there exists a nonzero positive semi-definite matrix $X \in (M_d)_{\text{sa}}$ with $\ell(X) = 0$ if and only if there is no vector $v \in \mathbb{R}^n$ such that $\ell^t(v)$ is positive definite.

For the “only if” direction, we argue by contradiction, so suppose that we have a nonzero positive semi-definite X with $\ell(X) = 0$, while there is $v \in \mathbb{R}^n$ such that $\ell^t(v)$ is positive definite.

We claim that $\text{Tr}(\ell^t(v)X) > 0$ holds. Indeed, by assumption on v , there is some $\epsilon > 0$ such that $\ell^t(v) \geq \epsilon I_d$ holds. By the positivity of X , we have

$$\text{Tr}(\ell^t(v)X) = \text{Tr}(X^{1/2}\ell^t(v)X^{1/2}) \geq \text{Tr}(X^{1/2}\epsilon I_d X^{1/2}) = \epsilon \text{Tr}(X) > 0.$$

Combining this the defining property of ℓ^t , we get

$$0 < \text{Tr}(\ell^t(v)X) = \langle v, \ell(X) \rangle = 0,$$

which a contradiction.

For the “if” direction, let us look at the following subsets of $(M_d)_{\text{sa}}$:

$$F = \{\ell^t(v) \mid v \in \mathbb{R}^n\}, \quad C = \{X \in (M_d)_{\text{sa}} \mid X \text{ is positive definite}\}.$$

Note that F is a subspace of $(M_d)_{\text{sa}}$ by the linearity of ℓ^t , and that C is open and its closure is a cone at 0. By assumption, their intersection is empty.

By a standard separation argument (cf. the Hahn–Banach separation theorem), we get a linear functional $\phi: (M_d)_{\text{sa}} \rightarrow \mathbb{R}$ such that $\phi(F) = 0$ and $\phi(C) \subset (0, \infty)$. By the non-degeneracy of trace pairing, there is a unique $Y \in (M_d)_{\text{sa}}$ such that $\phi(X) = \text{Tr}(YX)$ holds. Note that Y is positive semi-definite, since for every positive semi-definite $X \in (M_d)_{\text{sa}}$ we get $\text{Tr}(YX) = \phi(X) \geq 0$ by the continuity of ϕ (every positive semi-definite matrix is in the closure of C). We also have that $Y \neq 0$ by $\phi \neq 0$. Finally, we compute that $\ell(Y) = 0$ by

$$\|\ell(Y)\|^2 = \langle \ell(Y), \ell(Y) \rangle = \text{Tr}(Y\ell^t(\ell(Y))) = \phi(\ell^t(\ell(Y))) = 0,$$

which completes the proof of first step.

Now we are ready to prove the general claim. Let us prove the “only if” direction by contradiction. Suppose we have an X as in the claim, and that $v \in \mathbb{R}^n$ is a strict solution to the dual problem. Then we compute

$$0 \leq \text{Tr}(CX) < \text{Tr}(\ell^t(v)X) = \langle v, \ell(X) \rangle = 0,$$

which is a contradiction.

Next let us prove the “if” direction. Assume that there is no $v \in \mathbb{R}^n$ such that $\ell^t(v) - C$ is positive definite. Define $\tilde{C} \in (M_{d+1})_{\text{sa}}$ to be the matrix written in block form as

$$\tilde{C} = \begin{bmatrix} -C & 0 \\ 0 & 1 \end{bmatrix},$$

and a linear map $\tilde{\ell}: (M_{d+1})_{\text{sa}} \rightarrow \mathbb{R}^{n+1}$ by

$$\tilde{\ell}(Y) = \begin{bmatrix} \ell(X) \\ z - \text{Tr}(CX) \end{bmatrix}, \quad \left(Y = \begin{bmatrix} X & w \\ w^* & z \end{bmatrix} \right).$$

Then the transpose of $\tilde{\ell}$ is given by

$$\tilde{\ell}^t \left(\begin{bmatrix} v \\ r \end{bmatrix} \right) = \begin{bmatrix} \ell^t(v) - rC & 0 \\ 0 & r \end{bmatrix}.$$

Now, since we assume that there is no $v \in \mathbb{R}^n$ such that $\ell^t(v) - C$ is positive definite, there is not $w \in \mathbb{R}^{n+1}$ such that $\tilde{\ell}(w)$ is positive definite. Hence, by the first step of the proof, we get that there is a positive semi-definite $Y \in (M_{d+1})_{\text{sa}}$ such that $\tilde{\ell}(Y) = 0$.

Writing Y in the block matrix form as above, we get $\ell(X) = 0$ and $z - \text{Tr}(CX) = 0$, in other words, that $\text{Tr}(CX) = z \geq 0$. (The last inequality follows from the positivity of Y .) Positivity of Y also imply that X is positive semi-definite. Finally, X cannot be zero: if it is, we also have $z = \text{Tr}(CX) = 0$, which forces the positive semi-definite Y to be zero as well, which is a contradiction. $\square$

Proof of Theorem A.6. Put

$$\text{Opt}_D = \min\{b^t v \mid \ell^t(v) \geq C\}.$$

We want to show that there exists $X \in (M_d)_{\text{sa}}$ such that $\text{Tr}(CX) = \text{Opt}_D$ holds. Define $\tilde{C} \in (M_{d+1})_{\text{sa}}$ to be the matrix written in block form as

$$\tilde{C} = \begin{bmatrix} C & 0 \\ 0 & -\text{Opt}_D \end{bmatrix},$$

and a linear map $\tilde{\ell}: (M_{d+1})_{\text{sa}} \rightarrow \mathbb{R}^n$ by $\tilde{\ell}(Y) = \ell(Z) - zb$, where we write Y as a block matrix in the following way

$$Y = \begin{bmatrix} Z & w \\ w^* & z \end{bmatrix}.$$

Then the transpose of $\tilde{\ell}$ is given by

$$\tilde{\ell}^t(v) = \begin{bmatrix} \ell^t(v) & 0 \\ 0 & -b^t v \end{bmatrix}.$$

Let us look at the primal and the dual problems given by the triple $(\tilde{C}, \tilde{\ell}, b)$. Feasible solutions to the dual problem are given by vectors $v \in \mathbb{R}^n$ such that the matrix

$$\begin{bmatrix} \ell^t(v) - C & 0 \\ 0 & \text{Opt}_D - b^t v \end{bmatrix}$$

is positive semi-definite. Note that by definition of the number Opt_D , this dual problem has no strict solutions.

By Lemma A.7, there is a nonzero positive semi-definite $Y \in (M_{d+1})_{\text{sa}}$ such that $\tilde{\ell}(Y) = 0$ and $\text{Tr}(\tilde{C}Y) \geq 0$ holds. If we write Y in the above form, we see that $\tilde{\ell}(Y) = 0$ implies that $\ell(Z) = zb$, and the positivity of $\text{Tr}(\tilde{C}Y)$ implies $\text{Tr}(CZ) \geq z\text{Opt}_D$.

Note that z must be non-negative by the positivity of Y , and nonzero by the following argument: If $z = 0$ then we get $\ell(Z) = zb = 0$ and $\text{Tr}(CZ) \geq z\text{Opt}_D = 0$. On the other hand Z is positive semi-definite by the positivity of Y . Then Lemma A.7 implies that the original dual problem has no strict solutions, contradicting our overall assumptions.

Now that we know $z > 0$, we define $X = z^{-1}Z$, which is positive semi-definite and satisfies $\ell(X) = b$, hence X is a feasible solution to the primal problem. Moreover, we have the following inequalities:

$$\text{Tr}(CX) \geq \text{Opt}_D \geq \text{Tr}(CX),$$

where the first inequality follows by the fact that $\text{Tr}(CZ) \geq z\text{Opt}_D$, and the second inequality follows from the general estimate (A.1). This completes the proof. $\square$

APPENDIX B. HILBERT C^* -MODULES

Definition B.1. Let A be a C^* -algebra. A *pre-Hilbert A -module* is given by the following:

- a right A -module E ;
- a map $E \times E \rightarrow A$, denoted by $\langle x, y \rangle_A$ for $x, y \in E$;

such that

- $\langle x, y \rangle_A$ is linear in y and conjugate linear in x ;
- $\langle x, ya \rangle_A = \langle x, y \rangle_A a$ for $a \in A$;
- $\langle y, x \rangle_A = \langle x, y \rangle_A^*$;
- $\langle x, x \rangle_A = a^*a$ for some $a \in A$.

A *Hilbert A -module* is a pre-Hilbert A -module such that $\|x\| = \|\langle x, x \rangle_A\|^{1/2}$ is a Banach norm on E , that is, E is complete for this norm.

Let B be a finite-dimensional C^* -algebra and ψ be a positive functional on B . When C is a C^* -algebra, we make $L^2(B, \psi) \otimes C$ a Hilbert C -module by setting

$$\langle \Lambda(b_1) \otimes c_1, \Lambda(b_2) \otimes c_2 \rangle_A = \langle \Lambda(b_1), \Lambda(b_2) \rangle_{c_1^* c_2}.$$

Given a $*$ -homomorphism $B_2 \rightarrow B_1 \otimes C$, we set

$$\tilde{\theta}: L^2(B_2, \psi_2) \otimes C \rightarrow L^2(B_1, \psi_1) \otimes C, \quad \Lambda(b) \otimes c \mapsto (\Lambda \otimes \text{id})(\theta(b)(1 \otimes c)).$$

Proposition B.2. Suppose θ is given by

$$\theta(b) = \sum_i \psi(b_i'^* b) b_i'' \otimes c_i$$

for some elements $b_i' \in B_2$, $b_i'' \in B_1$, and $c_i \in C$. Then the right C -module homomorphism

$$\tilde{\theta}^* = \sum_i \Lambda(b_i') \Lambda(b_i'')^* \otimes c_i^*: L^2(B_1, \psi_1) \otimes C \rightarrow L^2(B_2, \psi_2) \otimes C$$

satisfies

$$\langle \tilde{\theta}(\Lambda(b_1) \otimes c_1), \Lambda(b_2) \otimes c_2 \rangle_C = \langle \Lambda(b_1) \otimes c_1, \tilde{\theta}^*(\Lambda(b_2) \otimes c_2) \rangle_C.$$

Definition B.3. Let E_1, E_2 be Hilbert A -modules, and $T: E_1 \rightarrow E_2$ be a homomorphism of right A -modules. We say that T is *adjointable* if there is a map $T^*: E_2 \rightarrow E_1$ satisfying

$$\langle Tx, y \rangle_A = \langle x, T^*y \rangle_A \quad (x \in E_1, y \in E_2).$$

We say that T is *unitary* if it is adjointable and the equalities $TT^* = \text{id}_{E_2}$, $T^*T = \text{id}_{E_1}$ hold.

Remark B.4. An adjointable map T is unitary if and only if the following conditions hold:

- $\langle Tx, Ty \rangle_A = \langle x, y \rangle_A$ (T is an isometry);
- $\text{ran } T = E_2$ (T is surjective).

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