

Classification of Quantum Graphs on  $M_2$   
and algebraic characterization of  
properties of quantum graphs

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## Abstract

Motivated by the string diagrammatic approach to undirected tracial quantum graphs by [B. Musto, D. Reutter, D. Verdon, *Journal of Mathematical Physics*, 59(8), 081706, (2018)], this thesis diagrammatically formulates directed nontracial quantum graphs. To understand quantum graphs by example, we supply a concrete classification of undirected reflexive quantum graphs on  $M_2$  and their quantum automorphism groups in both tracial and nontracial settings. We also obtain quantum isomorphisms between tracial quantum graphs on  $M_2$  and certain classical graphs, which reproves the monoidal equivalences between  $SO(3)$  and  $S_4^+$ , and  $O(2)$  and  $H_2^+$ .

The latter part of this thesis investigates the connectedness and bipartiteness of quantum graphs. We introduce the notion of connectedness and bipartiteness of quantum graphs in terms of graph homomorphisms. We show that regular tracial quantum graphs have the same algebraic characterization of connectedness and bipartiteness as classical graphs. We also prove the equivalence between bipartiteness and two-colorability of quantum graphs by comparing two notions of graph homomorphisms respecting adjacency matrices or edge spaces. In particular, all kinds of quantum two-colorability are shown to be mutually equivalent for regular connected tracial quantum graphs.

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## 0 Introduction

### 0.1 Presentation of results

This thesis is organized as follows.

Section 0 is the introduction including the summary of the results and the outline of this thesis.

Section 1 is dedicated to reviewing the historical background of quantum graph theory and explaining the important perspectives that connect classical and quantum graph theory.

In section 2, we review the basic properties of quantum graphs and generalize the string diagrammatic formulation in [30] to nontracial cases. An important difference is that the tracial cases allow topological deformation of diagrams while the nontracial cases do not allow deformation through a cusp. We also introduce the regularity of quantum graphs, which helps the classification in the following sections. We compare several properties of directed quantum graphs, in particular, an equivalence between realness and complete positivity of quantum graphs is proved.

In section 3, we review the notion of quantum isomorphisms [30] and extend it to nontracial settings. We also explain what is a quantum automorphism group of a quantum graph. As a straightforward generalization of [30, Proposition 5.19], we show that the category of quantum automorphisms of a quantum graph is isomorphic to the finite-dimensional representation category of the quantum automorphism group algebra of the quantum graph.

In section 4, we directly compute the reflexive undirected quantum graphs on  $M_2$  and classify them up to quantum and classical isomorphisms. In the tracial case, they are regular and classified by their degree  $d \in \{1, 2, 3, 4\}$ . In the nontracial case, they are not always regular but still have a similar form.

In section 5, we identify the quantum automorphism groups of the quantum graphs on  $M_2$  classified in section 3. In the tracial case,  $SO(3)$  and  $O(2)$  appear as quantum automorphism groups. In the nontracial case, the quantum special orthogonal groups  $SO_q(3)$  and the unitary torus  $\mathbb{T} = U(1)$  appear. Observing the spectra, the regular tracial quantum graphs on  $M_2$  are isospectral to regular classical graphs on four vertices, which implies the possibility of quantum isomorphisms between them. Therefore we compute the bigalois extension, the universal coefficient algebra of quantum isomorphisms between quantum graphs introduced by [8, Definition 4.1], to find that they are indeed quantum isomorphic. Since a quantum isomorphism of quantum graphs induces a monoidal equivalence of their quantum automorphism groups by [8, Theorem 4.7], it follows that  $SO(3)$  and  $S_4^+$ ,  $O(2)$  and  $H_2^+$  are monoidally equivalent respectively. Although this is already known in quantum group theory [3, 6], it exhibits a new approach to monoidal equivalence using quantum graph theory.

Gromada [23, Proposition 8.1] also obtains the same quantum isomorphisms and monoidal equivalence differently using a cocycle twist of classical Cayley graphs.

In section 6, we introduce the graph gradient to show the positivity of graph Laplacian. From the positivity, we deduce the spectral bound by the degree of regular real quantum graphs. On the way, we show that quantum graphs do not admit an orientation in general.

Similarly to the classical case, the degree of a regular quantum graph is shown to be the spectral radius of the adjacency matrix. Thus it makes sense to consider the behavior of the spectrum in  $[-d, d]$  for  $d$ -regular undirected quantum graphs.

**Theorem** (Proposition 6.10). *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular real quantum graph. The spectral radius  $r(A)$  of the adjacency matrix satisfies  $r(A) = d$ .*

**Theorem** (Theorem 6.11). *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular quantum graph. Then the identity of the operator norm on  $B(L^2(\mathcal{G}))$  and the degree*

$$\|A\|_{\text{op}} = d$$

*holds if either of the following is satisfied:*

- (1)  $\mathcal{G}$  is undirected, whence  $\text{spec}(A) \subset [-d, d]$ ;
- (2) both  $A$  and  $A^\dagger$  are real;
- (3)  $\mathcal{G}$  is real and tracial.

In section 7, we introduce our notion of graph homomorphism and define connectedness and bipartiteness in terms of graph homomorphisms. And then, we prove their algebraic characterizations by the spectrum of the adjacency matrix. In the proof, Lemma 7.3 plays an essential role in controlling the decomposition of a self-adjoint operator into a subtraction of positive elements.

**Theorem** (Theorem 7.7, Theorem 7.8, Theorem 7.9). *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular undirected tracial quantum graph.*

- $\mathcal{G}$  is connected if and only if  $d \in \text{spec}(A)$  is a simple root.
- $\mathcal{G}$  has a bipartite component if and only if  $-d \in \text{spec}(A)$ . If  $d = 0$ , we require  $\dim B \geq 2$ .

*If moreover  $\mathcal{G}$  is connected, then*

- $\mathcal{G}$  is bipartite if and only if  $-d \in \text{spec}(A)$ . If  $d = 0$ , we require  $\dim B \geq 2$ .

In section 8, we give a modified generalization of  $t$ -homomorphisms ( $t \in \{loc, q, qa, qc, C^*, alg\}$ ) introduced in the quantum-to-classical cases by [10]. Regarding the notion of graph homomorphisms, we compare two notions of graph homomorphisms, one is the graph homomorphisms defined in this thesis and compatible with adjacency matrices, and the other is the  $t$ -homomorphisms defined in [10] and compatible with edge spaces. We prove that these two notions are equivalent particularly in the case of quantum-to-classical graph homomorphisms, that is, any edge is mapped to the edges if the adjacency matrix is mapped to edges. In the proof, string diagrams (c.f. [40, 30, 28]) play a significant role to deduce positivity from the symmetry of the diagram.

Then we prove that our graph homomorphisms and *loc*-homomorphisms coincide under some assumptions.

**Theorem** (Theorem 8.9). *Let  $\mathcal{G}_j$  for  $j = 0, 1$  be real tracial quantum graphs such that  $\mathcal{G}_1$  is Schur central. Then  $f^{op} : \mathcal{G}_0 \rightarrow \mathcal{G}_1$  is a graph homomorphism if and only if  $(f, \mathbb{C}) : \mathcal{G}_0 \rightarrow \mathcal{G}_1$  is a *loc*-homomorphism.*

As its corollary, we obtained that the local two-colorability is equivalent to bipartiteness for tracial real quantum graphs.

**Theorem** (Theorem 8.13). *Let  $\mathcal{G}$  be a real tracial quantum graph. Then  $\mathcal{G}$  is bipartite if and only if it is *loc*-2 colorable.*

Moreover, combining the results in this thesis, it follows that all kinds of quantum two-colorability are mutually equivalent for connected regular undirected tracial quantum graphs.

**Theorem** (Corollary 8.14). *Let  $\mathcal{G} = (B, \psi, A)$  be a connected  $d$ -regular undirected tracial quantum graph. The following are equivalent:*

- (1)  $\mathcal{G}$  is *loc*-2 colorable;
- (2)  $\mathcal{G}$  is *alg*-2 colorable;
- (3)  $\mathcal{G}$  has a symmetric spectrum;
- (4)  $-d \in \text{spec}(A)$ . If  $d = 0$ , we require  $\dim B \geq 2$ ;
- (5)  $\mathcal{G}$  is bipartite.

Our main results are restricted to regular tracial quantum graphs. So the nontracial versions and the equivalence of the spectral gap of the graph Laplacian and the connectedness of irregular quantum graphs are left open. The relation between our connectedness and the operator space theoretic connectedness [13] of quantum graphs is also left open.

## 0.2 Notation

Throughout this thesis, we consider everything over the complex number field  $\mathbb{C}$ , hence  $M_n$  stands for the  $n \times n$  complex matrix algebra. We often identify  $\mathbb{C}^n$  with the diagonal  $n \times n$  complex matrix algebra. Given Banach spaces  $\mathcal{X}, \mathcal{Y}$ , we denote the space of bounded operators between them by  $B(\mathcal{X}, \mathcal{Y})$ , and we set  $B(\mathcal{X}) = B(\mathcal{X}, \mathcal{X})$ . The dual space of  $\mathcal{X}$  is denoted by  $\mathcal{X}^* = B(\mathcal{X}, \mathbb{C})$ .

**Definition 0.1** (cf. Davidson [16], Folland [20, Chapter 1], Pedersen [34, Chapter 4]). A *\*-algebra*  $B$  is an algebra over  $\mathbb{C}$  equipped with an antilinear involution  $(\cdot)^* : B \rightarrow B$  satisfying  $(xy)^* = y^*x^*$ ,  $(x^*)^* = x$  for all  $x, y \in B$ . A *normed algebra*  $B$  is an algebra over  $\mathbb{C}$  equipped with a norm  $\|\cdot\| : B \rightarrow [0, \infty)$  satisfying submultiplicativity  $\|xy\| \leq \|x\|\|y\|$  for all  $x, y \in B$ . A *Banach algebra* is a normed algebra equipped with a complete norm.

A *C\*-algebra* is a Banach \*-algebra  $B$  satisfying the *C\*-condition*

$$\|x^*x\| = \|x\|^2 \quad \forall x \in B.$$

An algebra is said to be *unital* if there exists a multiplicative unit. A *homomorphism* between unital algebras is a unital multiplicative linear operator. A \*-preserving homomorphism between \*-algebras is called a *\*-homomorphism*. A *\*-representation* of a C\*-algebra  $B$  is a \*-homomorphism from  $B$  to the C\*-algebra  $B(H)$  for a Hilbert space  $H$  satisfying nondegeneracy, i.e.,  $BH = \text{span}\{xv \mid x \in B, v \in H\}$  is dense in  $H$ .

A *state*  $\psi$  on a unital C\*-algebra  $B$  is a linear functional  $\psi \in B^*$  satisfying  $\psi(1) = 1$  and positivity  $\psi(x^*x) \geq 0$  for all  $x \in B$ . A *state*  $\psi$  on  $B$  is *tracial* if  $\psi(xy) = \psi(yx)$  for all  $x, y \in B$ .

In order to avoid confusion, we denote Hilbert space adjoint by  $(\cdot)^\dagger$  and C\*-algebra involution by  $(\cdot)^*$ .

C\*-algebras form a category with \*-homomorphisms. For its subcategories, we have important duality theorems so-called *Gelfand duality*:

**Theorem 0.2** (Gelfand Naimark [22, Lemma 1], Negrepointis [32, Theorem 2.4]). *The category of unital commutative C\*-algebras with unital \*-homomorphisms is equivalent to the opposite of the category of compact Hausdorff spaces with continuous functions. The correspondence is explicitly given as follows:*

$$\begin{array}{ccc}
 \text{C}^*\text{-algebras} & & \text{compact spaces} \\
 C(X) & & X \\
 \uparrow \circ f & \longleftrightarrow & f \downarrow \\
 B & & \text{spec}(B)
 \end{array}$$



where  $\text{spec}(B) = \{\text{unital } *- \text{homomorphisms: } B \rightarrow \mathbb{C}\} \subseteq B^*$  is the spectrum of  $B$  equipped with the weak\* topology and  $C(X)$  is the complex continuous function algebra on  $X$  equipped with the uniform norm.

Via Gelfand duality, non-commutative  $C^*$ -algebras are regarded as virtual function spaces over quantum (non-commutative) spaces.

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# 1 History and backgrounds

The word ‘quantum’ indicates a certain non-commutative analogue of classical objects in the context of operator algebra. Motivated by quantum information theory, The notion of quantum graphs was introduced in the early 2010s and has developed in the interactions between theories of operator algebra, quantum group, tensor category, non-commutative geometry, and quantum information.

Quantum graphs were first defined as operator systems on matrix algebras [18], and this viewpoint was refined as quantum relations on von Neumann algebras [43, 45]. Applications of this approach include the quantum Ramsey theory [44, 25], nonlocal games in quantum information theory [1], and the connectivity for quantum graphs [13]. Musto, Reutter, Verdon [30] introduced quantum graphs as adjacency matrices, which is the main approach in this thesis. The definition by adjacency matrices enabled us to develop various approaches to quantum graphs, for instance, the quantum automorphism groups and bigalois extensions of quantum graphs [30, 8] related to quantum group theory and tensor category theory [33], and graph isomorphism game in quantum information theory; quantum isomorphic deformation of quantum graphs [31, 23] related to the monoidal Morita equivalence in tensor category theory; quantum Cuntz-Krieger algebras of quantum graphs [9] related to  $C^*$ -algebra and  $K$ -theory; quantum Cayley graphs [42]; spectral properties of quantum graphs [21, 29] related to quantum chromatic numbers.

## 1.1 Classical graph theory

Before stepping into the quantum graph world, we review classical graph theory.

A classical (directed multiple) graph is a diagram consisting of directed edges between discrete vertices, combinatorially defined as a tuple  $\mathcal{G} = (V, E, s, t)$  of vertex set  $V$ , edge set  $E$ , and source and target maps  $s, t : E \rightarrow V$  that indicate the source vertex and the target vertex of each edge. A graph is called finite if both  $V$  and  $E$  are finite. An edge  $e$  is called a (self-)loop if its source and target coincide  $s(e) = t(e)$ . Two (or more) edges  $e, e'$  are called multiple if they have the same source and target  $s(e) = s(e'), t(e) = t(e')$ , and a graph is called multiplicity-free if it has no multiple edges. Throughout this thesis, we assume that a graph is finite and multiplicity-free. We identify  $E$  with the relation  $\{(s(e), t(e)) | e \in E\} \subset V \times V$  and just write  $\mathcal{G} = (V, E)$ . A graph is called undirected if every edge has its opposite  $(i, j) \in E \implies (j, i) \in E$ . It is commonly assumed that a graph is simple, i.e., an undirected multiplicity-free graph with no loops.

An operator algebraic description of classical graphs is given by the adjacency matrix  $A = (A_{ij})_{i, j \in V}$  defined as  $A_{ij} = 1$  if there is an edge

$(j, i) \in E$  from  $j$  to  $i$ ;  $A_{ij} = 0$  otherwise. This acts on the function algebra  $C(V) = \{(\text{continuous}) f : V \rightarrow \mathbb{C}\}$  over the vertices by  $Af(i) = \sum_{j \in V} A_{ij}f(j) = \sum_{e \in E; t(e)=i, s(e)=j} f(j)$  for  $f \in C(V)$ , i.e., each edge sends the value from the source to the target, and the adjacency matrix sums up the sent values. An important point is that the  $\{0, 1\}$ -valued adjacency matrix is idempotent  $A \bullet A = A$  with respect to the entrywise product  $(\cdot) \bullet (\cdot)$ , which is also known as the Schur product or Hadamard product.

Another operator algebraic description is given by the operator space  $\mathcal{S} = \{T \in M_V(\mathbb{C}) \mid T_{ij} = 0 \text{ if } A_{ij} = 0\} \subset M_V(\mathbb{C})$ , which is the linear span of the nonzero entries of the adjacency matrix. Such an operator space  $\mathcal{S}$  is characterized as a  $C(V)$ - $C(V)$ -bimodule in  $M_V(\mathbb{C}) = B(\ell^2(V))$ , where  $C(V)$  is identified with the diagonal subalgebra of  $M_V(\mathbb{C})$  via pointwise multiplication with  $\ell^2(V)$ .

There is a one-to-one correspondence between multiplicity-free graphs on  $V$ , Schur idempotent adjacency matrices, and  $C(V)$ - $C(V)$ -bimodules in  $M_V(\mathbb{C}) = B(\ell^2(V))$ . We will later explain that similar correspondence holds for quantum graphs.

### 1.1.1 Basic properties

Let  $\mathcal{G} = (V, E, s, t)$  be a directed graph and  $v \in V$ . The indegree of  $v$  is the number  $|t^{-1}(v)|$  of edges to  $v$  and the outdegree of  $v$  is the number  $|s^{-1}(v)|$  of edges from  $v$ . If  $\mathcal{G}$  is undirected, then the indegree and outdegree coincide, which we call the degree of  $v$ .

A graph  $\mathcal{G}$  is called  $d$ -regular if the indegree and outdegree of every vertex of  $\mathcal{G}$  are all  $d$ . Note that  $\mathcal{G}$  is  $d$ -regular if and only if the constant function  $1_V$  on  $V$  is an eigenvector for eigenvalue  $d$  of the adjacency matrix  $A$  and its adjoint  $A^\dagger$ . This characterization enables us to define regular quantum graphs.

A subgraph of  $\mathcal{G} = (V, E, s, t)$  is a graph  $(V', E')$  of subsets  $V' \subset V, E' \subset E$  satisfying  $s(E'), t(E') \subset V'$ . Each vertex subset  $V' \subset V$  defines an induced subgraph  $(V', E' = s^{-1}(V') \cap t^{-1}(V'))$ , that is the maximal subgraph on  $V'$ .

An undirected graph  $\mathcal{G}$  is connected if there exists no nontrivial partition of vertices  $V = V_0 \sqcup V_1$  with no edges between  $V_0$  and  $V_1$ ; otherwise, it is called disconnected. Each maximal connected subgraph is called a (connected) component of the graph. By considering each component, we may often assume that a graph is connected in classical graph theory.

An undirected graph  $\mathcal{G}$  is bipartite if there exists a nontrivial partition of vertices  $V = V_0 \sqcup V_1$  with edges only between  $V_0$  and  $V_1$ .

An undirected graph  $\mathcal{G}$  is  $c$ -colorable for  $c \in \mathbb{Z}_{>0}$  if it has a  $c$ -coloring, i.e., a partition  $V = V_1 \sqcup \dots \sqcup V_c$  with edges only between different cosets. The chromatic number of  $\mathcal{G}$  is the infimum of the integer  $c$  where  $\mathcal{G}$  is  $c$ -colorable.

### 1.1.2 Spectral properties

It is classically known that the spectrum of the adjacency matrix can characterize some properties of a (regular) classical graph. Hoffman [24] showed that a connected  $d$ -regular graph is bipartite if and only if  $-d$  is an eigenvalue of the adjacency matrix. It was already known in Fiedler [19] that the connectedness of an undirected graph is equivalent to the nonzero spectral gap (the gap between the smallest eigenvalue 0 and the second smallest eigenvalue) of the normalized graph Laplacian (cf. [14]). In particular, a  $d$ -regular graph is connected if and only if the adjacency matrix has a nonzero spectral gap (the gap between the largest eigenvalue  $d$  and the second largest eigenvalue).

The latter half of this thesis argues the generalization of such a spectral characterization of connectedness and bipartiteness.

The notion of expander graphs is also defined by the spectrum. Expander graphs are ‘sparse (with low degree) but highly connected’ graphs, which have a large spectral gap, large Cheeger constant, and rapid mixing of random walks. Let  $\mathcal{G}$  be a  $d$ -regular undirected graph on  $N$  vertices with  $\text{spec}(A) = \{\lambda_N \leq \dots \leq \lambda_2 \leq \lambda_1 = d\}$  and  $\varepsilon > 0$ .  $\mathcal{G}$  is called a one-sided  $\varepsilon$ -expander if the normalized spectral gap  $\varepsilon(\mathcal{G}) := (\lambda_1 - \lambda_2)/d$  is at least  $\varepsilon$ , i.e.,  $\lambda_2 \leq (1 - \varepsilon)d$ .

$\mathcal{G}$  is called a two-sided  $\varepsilon$ -expander if  $\lambda_2, |\lambda_N| \leq (1 - \varepsilon)d$

A one-sided (resp. two-sided)  $\varepsilon$ -expander family  $(\mathcal{G}_n)_{n \in \mathbb{N}}$  is a sequence of one-sided (resp. two-sided)  $\varepsilon$ -expander graphs with the number of vertices  $N_n \rightarrow \infty$ .

Expander graphs are also characterized by the Cheeger constant (isoperimetric constant) or the rapid mixing of random walks (cf. [38]). The generalization and its equivalence of these characterizations of expander graphs to quantum graphs are left open.

The Alon-Boppana bound shows that the best possible  $\varepsilon$ -expander family is with  $\varepsilon = 1 - 2\sqrt{d-1}/d$ . Such an expander family is called Ramanujan graphs.

The construction of an expander family or Ramanujan graphs is itself very nontrivial. Lubotzky, Phillips, Sarnak [26] constructed the first concrete Ramanujan graphs as Cayley graphs on projective linear groups over finite fields. There are various constructions using residually finite groups with property (T), random graphs, quasi-random groups, etc. (cf. [38])

### 1.1.3 Cayley graphs

An important source of regular graphs is the Cayley graphs. Given a discrete group  $G$  and a finite subset  $S \subset G$ , the (right-invariant) Cayley graph generated by  $S$  on  $G$  is  $\text{Cay}(G, S) = (G, \{(x, sx) | x \in G, s \in S\})$ , which is  $|S|$ -regular. We assume  $S = S^{-1}$  (if and only if  $\text{Cay}(G, S)$  is undirected)

and  $e \notin S$  (if and only if  $\text{Cay}(G, S)$  has no loops).

The group structure of  $G$  defines the convolution  $f * g$  of  $f, g \in c_c(G)$  by  $f * g(x) = \sum_{y \in G} f(y)g(y^{-1}x)$ , which is extended to  $\ell^p(G) \times \ell^q(G) \ni (f, g) \mapsto f * g \in \ell^r(G)$  for  $1/p + 1/q = 1/r + 1$ . The adjacency matrix  $A$  of  $\text{Cay}(G, S)$  is described by the convolution on  $c_c(G)$  by  $Af(x) = \sum_{s \in S} f(s^{-1}x) = \sum_{s \in G} \chi_S(s)f(s^{-1}x) = \chi_S * f(x)$ , where  $\chi_S \in c_c(G)$  is the indicator function of  $S$ .

From this viewpoint, Wasilewski [42, Definition 5.1] introduced quantum Cayley graphs on a discrete quantum group  $G$  by the convolution with a projection  $P \in c_c(G)$ . On the other hand, Vergnioux [39] introduced quantum Cayley graphs from another perspective, with the edges described as the pairs  $(g, s) \in G \times S$  of source vertices  $g$  and the directions  $s$ . The precise relationship between these notions of quantum Cayley graphs is left open.

#### 1.1.4 Properties via homomorphisms and minors

When we define certain properties of quantum graphs, the characterization by graph homomorphisms behaves well.

A graph homomorphism  $f : \mathcal{G}_0 \rightarrow \mathcal{G}_1$  between finite graphs  $\mathcal{G}_k = (V_k, E_k)$  is a map  $f : V_0 \rightarrow V_1$  that sends edges to edges  $E_0 \ni (i, j) \mapsto (f(i), f(j)) \in E_1$ . In terms of the adjacency matrix,  $f$  is a homomorphism if and only if the precomposition map  $\hat{f} := \cdot \circ f : \ell^2(V_1) \rightarrow \ell^2(V_0)$  satisfies  $A_1 \bullet \hat{f}^\dagger A_0 \hat{f} = \hat{f}^\dagger A_0 \hat{f}$ , i.e., the pushforward  $\hat{f}^\dagger A_0 \hat{f}$  of  $A_0$  by  $f$ , whose  $(i, j)$ -entry is the number of edges from  $f^{-1}(j)$  to  $f^{-1}(i)$ , has nonzero  $(i, j)$ -entry only if  $[A_1]_{ij} = 1$ .

The following are the characterizations of graph properties used in this thesis.

- A graph  $\mathcal{G}$  is connected if and only if there is no vertex-surjective graph homomorphism from  $\mathcal{G}$  to  $T_2$ .
- A graph  $\mathcal{G}$  is bipartite if and only if there is a vertex-surjective graph homomorphism from  $\mathcal{G}$  to  $K_2$ .
- A graph  $\mathcal{G}$  has a bipartite component if and only if there is a graph homomorphism from  $\mathcal{G}$  to  $K_2 \sqcup T_1$  that is vertex-surjective to  $K_2$ .
- A graph  $\mathcal{G}$  is  $c$ -colorable if and only if there is a graph homomorphism from  $\mathcal{G}$  to  $K_c$ .

The graph minors are another notion to characterize some geometric properties of graphs. Given an undirected graph  $\mathcal{G}$  without loops, its graph minors are the graphs obtained from  $\mathcal{G}$  by the recursive operations of either of the following: deleting an edge; deleting a vertex and its adjacent edges; contract an edge and merge the two end vertices and multiple edges (identifying two adjacent vertices and eliminating the resulting loop and multiple edges).

A graph is called planar if it is embedded into the 2-dimensional plane  $\mathbb{R}^2$  with no crossing of edges. An undirected graph  $\mathcal{G}$  is planar if and only if neither  $K_5$  nor  $K_{3,3}$  is a graph minor of  $\mathcal{G}$ .

The notion of graph minors has not been generalized for quantum graphs yet. The difficulty is the contraction of an edge.

### 1.1.5 Quantum symmetry and graph isomorphism game

Symmetry of a finite graph or an isomorphism between finite graphs  $\mathcal{G}_0, \mathcal{G}_1$  on vertex set  $V$  can be described by a permutation matrix  $P : C(V) \rightarrow C(V)$  satisfying  $PA_1 = A_0P$ . Analogously, quantum symmetry (quantum automorphism) or a quantum isomorphism of finite graphs is described by a quantum permutation matrix, also known as a magic unitary, which is an operator-valued unitary matrix  $P = (p_{ij})$  with entries of projections  $p_{ij}$  whose rows and columns sum up to 1. A permutation matrix is nothing but a  $\mathbb{C}$ -valued magic unitary. More precisely, a quantum isomorphism is a matrix  $M_N$ -valued magic unitary for some natural number  $N$ , a quantum commuting isomorphism is such a tracial  $C^*$ -algebra-valued magic unitary, and there are similar notions depending on what kind of algebras are allowed in the coefficients.

The  $C^*$ -algebra generated by mutually commuting universal coefficients of the magic unitary  $P$  satisfying  $PA_{\mathcal{G}} = A_{\mathcal{G}}P$  is the continuous function algebra  $C(\text{Aut}(\mathcal{G}))$  of the automorphism group  $\text{Aut}(\mathcal{G})$ , and the  $p_{ij}$  is the matrix elements  $\pi_{ij} : \text{Aut}(\mathcal{G}) \ni x \mapsto \pi(x)_{ij} \in \mathbb{C}$  of the fundamental representation  $\pi : \text{Aut}(\mathcal{G}) \rightarrow U_N$ . By dropping the commuting assumption, we get the function algebra  $C(\text{Qut}(\mathcal{G}))$  of the quantum automorphism group  $\text{Qut}(\mathcal{G})$  as the  $C^*$ -algebra generated by universal coefficients of the magic unitary  $P$  satisfying  $PA_{\mathcal{G}} = A_{\mathcal{G}}P$ .

A graph is said to have no quantum symmetry if  $\text{Qut}(\mathcal{G}) = \text{Aut}(\mathcal{G})$ , i.e., the entries of a magic unitary compatible with adjacency matrices commute each other automatically.

The Petersen graph is one of the simplest examples of regular graphs with no quantum symmetry [36]. The smallest example of non-isomorphic but quantum isomorphic graphs is given as 9-regular Cayley graphs on 24 vertices in [1].

Classical and quantum isomorphisms are related to the graph isomorphism game [1] in quantum information theory. It is a kind of nonlocal game, where players share a strategy beforehand and are not allowed to communicate during the game, i.e., they do not know the others' inputs and outputs. In a graph isomorphism game, players are Alice and Bob trying to win cooperatively, and two graphs  $\mathcal{G}_0 = (V_0, E_0)$  and  $\mathcal{G}_1 = (V_1, E_1)$  are given. Among the vertex set  $V = V_0 \sqcup V_1$ , the referee sends vertices  $x_A$  to Alice and  $x_B$  to Bob, and receives vertices  $y_A$  from Alice and  $y_B$  from Bob. Alice and Bob win if the input  $x_A$  and output  $y_A$  ( $x_B$  and  $y_B$  as well) belong

to different graphs and the relationship between  $x_A$  and  $x_B$  is equal to the relationship between  $y_A$  and  $y_B$ , i.e., either:  $y_A = y_B$  if  $x_A = x_B$ ;  $y_A, y_B$  are adjacent if  $x_A, x_B$  are adjacent;  $y_A, y_B$  are neither equal nor adjacent if  $x_A, x_B$  are neither equal nor adjacent. Alice and Bob share a strategy before the game to decide the outputs  $y_A$  and  $y_B$  respectively from the inputs  $x_A$  and  $x_B$ , and the strategy is said to be perfect if they can win with probability 1. A classical deterministic strategy of the graph isomorphism game is a map  $f : V \rightarrow V$  to define  $y_A = f(x_A), y_B = f(x_B)$ . A probabilistic strategy is (a way to give) a collection of conditional probabilities  $(p(y_A, y_B | x_A, x_B))_{y_A, y_B, x_A, x_B \in V}$  of the outputs  $y_A, y_B$  and the inputs  $x_A, x_B$  satisfying  $\sum_{y_A, y_B} p(y_A, y_B | x_A, x_B) = 1$  for each  $x_A, x_B$ , and this is perfect if  $p(y_A, y_B | x_A, x_B) = 0$  for all losing tuples  $(y_A, y_B, x_A, x_B)$ .

The quantum strategy consists of the following procedure. Alice and Bob prepare a normal vector  $\psi \in \ell^2(V) \otimes \ell^2(V)$  (the so-called shared entanglement state, where Alice has access to the first  $\ell^2(V)$  and Bob the other), and positive operator-valued measures in  $B(\ell^2(V))$ :  $\mathcal{E}_x = (E_{xy})_{y \in V}$  for Alice and  $\mathcal{F}_x = (F_{xy})_{y \in V}$  for Bob for every input  $x \in V$ , i.e.,  $E_{xy}, F_{xy}$  are positive operators and  $\sum_y E_{xy} = \text{id}_{\ell^2(V)} = \sum_y F_{xy}$  holds. Given inputs  $x_A$  and  $x_B$ , Alice and Bob performs the quantum measurements  $\mathcal{E}_{x_A}$  and  $\mathcal{F}_{x_B}$  on the shared entanglement state  $\psi$ , and obtain outputs  $y_A$  and  $y_B$  with probability  $p(y_A, y_B | x_A, x_B) = \psi^\dagger (E_{x_A y_A} \otimes F_{x_B y_B}) \psi$ .

It is known [1] that the graph isomorphism game has a perfect classical deterministic strategy if and only if the graphs are isomorphic, and the game has a perfect quantum strategy if the graphs are quantum isomorphic. [1] showed that we may assume  $E_{ij}$ 's are projections without loss of generality, and then  $(E_{ij})_{i \in V_1, j \in V_0}$  is a magic unitary that yields a quantum isomorphism between  $\mathcal{G}_0$  and  $\mathcal{G}_1$ .

## 1.2 Quantum graphs as operator systems

The notion of quantum graphs (called non-commutative graphs in [18]) was first introduced by Duan, Severini, Winter [18] in terms of operator systems as the confusability graph of a quantum channel in quantum information theory.

An operator space is a weak\*-closed subspace  $\mathcal{S}$  of  $B(H) = TC(H)^*$ , and an operator system is a unital ( $\text{id}_H \in \mathcal{S}$ ) and self-adjoint ( $\mathcal{S}^\dagger = \mathcal{S}$ ) operator space  $\mathcal{S}$ .

A quantum channel  $\Phi$  is a completely positive trace-preserving (CPTP) map between operator systems, i.e.,  $\Phi : \mathcal{S}_1 \rightarrow \mathcal{S}_2$  where  $\mathcal{S}_j \subset B(H_j)$ ,  $\text{Tr}_2 \circ \Phi = \text{Tr}_1$ , and  $\Phi^{(n)}(M_n(\mathcal{S}_1)_+) \subset M_n(\mathcal{S}_2)_+$  for all positive integer  $n$ . Here,  $\Phi^{(n)}$  is the amplified map  $\Phi \otimes \text{id}_{M_n} : \mathcal{S}_1 \otimes M_n \rightarrow \mathcal{S}_2 \otimes M_n$  and  $M_n(\mathcal{S}_j)_+ = \mathcal{S}_j \otimes M_n \cap B(H_j \otimes \mathbb{C}^n)_+$ .

For any quantum channel  $\Phi$ , there are the so-called Kraus operators  $(K_i)_{i=1}^n \subset B(H_1, H_2)$  such that  $\Phi = \sum_i K_i(\cdot)K_i^\dagger$ . A non-commutative con-

fusability graph of  $\Phi$  is an operator system  $\mathcal{S} = \text{span}\{\text{id}_{H_1}, K_i^\dagger K_j | i, j = 1, \dots, n\} \subset B(H_1)$ . This is an analogue of the confusability graph of a classical channel. Classical channels send binary words to binary words probabilistically, e.g.,  $\{00, 01, 10, 11\}$  to  $\{00, 101, 1\}$ , and the confusability graph is the graph on the source words  $\{00, 01, 10, 11\}$  with edges  $(v, w)$  if  $v$  and  $w$  can be sent to the same word, i.e., confusable for the receiver. In this sense, operator systems are called quantum graphs.

As an analogue of the fact that simple undirected classical graphs are irreflexive symmetric relations, Weaver [45] formulated quantum graphs as reflexive symmetric quantum relations (weak\*-closed  $B'-B'$ -bimodules in  $B(H)$ ) [43] on a von Neumann algebra  $B \subset B(H)$ , which includes the operator systems as  $\mathbb{C} = B(H)'$ -bimodules [18].

(Quantum) information theory is interested in how much information can be sent by a (quantum) channel with zero error, and it can be measured by the size of a maximal anticlique (induced subgraph with no edges) in the confusability graph. Thus it is natural that the quantum Ramsey theory [44, 25] appears, as the classical Ramsey theory states the existence of a certain size of clique or anticlique in sufficiently large graphs.

### 1.3 Quantum graphs as adjacency matrices

Musto, Reutter, Verdon [30] formulated finite quantum graphs as adjacency operators on tracial finite quantum sets, and Brannan et al. [8] generalized them for nontracial settings.

The key tool of [30] are string diagrams formulated by Vicary [40], but it should be treated with care if applied to nontracial quantum graphs in [8]. So in the former part of this thesis, we discuss the diagrammatic formulation of nontracial quantum graphs.

Brannan et al. [8] also introduced the quantum automorphism groups and bigalois extensions of quantum graphs in order to refine the notion of quantum isomorphisms between quantum graphs. The quantum automorphism group of classical graphs was first introduced by Bichon [7, Definition 3.1] in a slightly different way from [8]. The origin of the formulation in [8] is due to Banica [5, Definition 3.2], following the quantum symmetry group of finite spaces introduced by Wang [41, Definition 2.3].

Although some abstract constructions of a quantum graph from others are given categorically by Musto, Reutter, Verdon [31] and algebraically by Brannan, Eifler, Voigt, Weber [9], few nontrivial concrete examples of them were known. This motivated the author to compute and classify undirected reflexive quantum graphs and their quantum automorphism groups on the most basic noncommutative algebra  $M_2$  as a first step.

Gromada [23] independently studied partially the same topic. This thesis classifies undirected reflexive quantum graphs on  $M_2$ , while Gromada classified undirected tracial quantum graphs on  $M_2$  [23, section 3.3] in an



insightful way using Lie algebras and the correspondence between the adjacency operators on tracial  $M_2$  and projections in  $M_2 \otimes M_2^{op}$ .

Since quantum graphs as adjacency matrices were introduced by [30], there has been substantial activity towards clarifying the relation between the property of a quantum graph and the spectrum of the adjacency matrix.

It is natural to expect that quantum graphs have similar spectral characterizations of properties, and indeed Ganesan [21] showed that such a spectral approach is valid for the Hoffman bound of the chromatic numbers of quantum graphs.

## 2 Foundations in quantum graph theory

Let  $B$  be a finite dimensional unital  $C^*$ -algebra.  $B$  is equipped with the bilinear multiplication map  $B \times B \ni (a, b) \mapsto ab \in B$ , which induces a linear multiplication operator  $m : B \otimes B \ni a \otimes b \mapsto ab \in B$  by the universality of tensor product. We identify  $x \in B$  with a linear map  $\mathbb{C} \ni 1 \mapsto x \in B$ , in particular  $1_B$  denotes the multiplicative unit in  $B$  and the unital  $*$ -homomorphism  $\mathbb{C} \hookrightarrow B$ .

For a state  $\psi$  on a  $C^*$ -algebra  $B$ , we denote the GNS space by  $L^2(B, \psi)$ , which is the Hausdorff completion of  $B$  with respect to the sesquilinear form  $\langle x|y \rangle = \langle x|y \rangle_\psi = \psi(x^*y)$  for  $x, y \in B$ . The subscript  $\psi$  of the inner product is often abbreviated if there is no concern of confusion. If  $\dim B$  is finite and  $\psi$  is faithful, we identify  $B \ni x = |x \rangle \in L^2(B, \psi)$ . Via the Hilbert adjoint with respect to  $\langle \cdot | \cdot \rangle_\psi$ ,  $x \in B$  induces  $x^\dagger = \langle x | = \psi(x^* \cdot) : B \rightarrow \mathbb{C}$ . The algebra  $(B, m, 1)$ , a vector space  $B$  equipped with the multiplication  $m$  and the unit  $1$  satisfying

$$\begin{array}{ll} \text{associativity} & \text{existence of a unit} \\ (x y) z = x (y z) \quad \forall x, y, z \in B & 1_B x = x = x 1_B \quad \forall x \in B \\ m(m \otimes \text{id}) = m(\text{id} \otimes m) & m(1 \otimes \text{id}) = \text{id} = m(\text{id} \otimes 1) \end{array}$$

induces a coalgebra  $(B, m^\dagger, \psi)$ , a vector space  $B$  equipped with the comultiplication  $m^\dagger$  and the counit  $\psi = 1^\dagger$  satisfying

$$\begin{array}{ll} \text{coassociativity} & \text{existence of a counit} \\ (m^\dagger \otimes \text{id})m^\dagger = (\text{id} \otimes m^\dagger)m^\dagger & (\psi \otimes \text{id})m^\dagger = \text{id} = (\text{id} \otimes \psi)m^\dagger \end{array}$$

### 2.1 String diagrams

Following Vicary [40], we adopt the string diagram notation of operators, which encodes the compositions of operators from the bottom to the top and enables our visual understanding and topological calculation. For operators  $f : H_0 \rightarrow H_1$  and  $g : H_1 \rightarrow H_2$  between Hilbert spaces, we associate Hilbert spaces with strings, operators with nodes, and read diagrams from bottom to top:

$$f = \begin{array}{c} H_1 \\ | \\ \textcircled{f} \\ | \\ H_0 \end{array}, \quad g = \begin{array}{c} H_2 \\ | \\ \textcircled{g} \\ | \\ H_1 \end{array}.$$

The composition  $gf = g \circ f : H_0 \rightarrow H_2$  and the tensor product  $f \otimes g : H_0 \otimes H_1 \rightarrow H_1 \otimes H_2$  are denoted by the vertical and horizontal composition of the diagrams respectively, and the Hilbert adjoint  $f^\dagger : H_1 \rightarrow H_0$  by the

vertical mirroring of the diagram:

$$g \circ f = \begin{array}{c} H_1 \\ \circlearrowleft g \\ \circlearrowleft f \\ H_0 \end{array}, \quad f \otimes g = \begin{array}{cc} H_1 & H_2 \\ \circlearrowleft f & \circlearrowleft g \\ H_0 & H_1 \end{array}, \quad f^\dagger = \begin{array}{c} H_0 \\ \circlearrowleft f^\dagger \\ H_1 \end{array}.$$

When a Hilbert space  $H$  and its dual  $H^*$  or a  $C^*$ -algebra  $B$  appear in a string diagram, we draw  $H$  as an oriented string from bottom to top,  $H^*$  as an oriented string from top to bottom, and  $B$  as an unoriented string:

$$\text{id}_H = \begin{array}{c} \downarrow \\ H \end{array}, \quad \text{id}_{H^*} = \begin{array}{c} \downarrow \\ H^* \end{array}, \quad \text{id}_B = \begin{array}{c} \downarrow \\ B \end{array}$$

We denote the coupling operators of  $H$  and  $H^*$  and their adjoints by

$$\begin{array}{c} \mathbb{C} \\ \curvearrowright \\ H \end{array} \begin{array}{c} f(v) \\ \uparrow \\ H^*v \otimes f \end{array}, \quad \begin{array}{c} \mathbb{C} \\ \curvearrowleft \\ H^* \end{array} \begin{array}{c} f(v) \\ \uparrow \\ Hf \otimes v \end{array}, \quad \begin{array}{c} H \\ \curvearrowright \\ \mathbb{C} \end{array} \begin{array}{c} H^* \sum v_i \otimes v_i^\dagger \\ \uparrow \\ 1 \end{array}, \quad \begin{array}{c} H^* \\ \curvearrowleft \\ \mathbb{C} \end{array} \begin{array}{c} H \sum v_i^\dagger \otimes v_i \\ \uparrow \\ 1 \end{array} \quad (2.1)$$

where  $\{v_i\}_i$  is an orthonormal basis (ONB) for  $H$ , and  $v^\dagger = \langle v | = \langle v | \cdot \rangle \in H^*$  for  $v = |v\rangle \in H$ . Note that we can naturally identify  $H \otimes H^*$  with  $B(H)$  by  $H \otimes H^* \ni |v\rangle \otimes \langle w| \mapsto |v\rangle \langle w| \in B(H)$ . Then (2.1) is identified with the unit map  $\mathbb{C} \ni 1 \rightarrow \text{id}_H \in B(H)$  and the canonical trace  $\text{Tr} : B(H) \rightarrow \mathbb{C}$ .

The operators (2.1) satisfy the following equalities, the so-called snake equation in [30, section 2.2, (5)]:

$$\begin{array}{c} \curvearrowright \\ \downarrow \end{array} = \begin{array}{c} \downarrow \\ \downarrow \end{array} = \begin{array}{c} \downarrow \\ \curvearrowleft \end{array}, \quad \begin{array}{c} \curvearrowleft \\ \downarrow \end{array} = \begin{array}{c} \downarrow \\ \downarrow \end{array} = \begin{array}{c} \downarrow \\ \curvearrowright \end{array}. \quad (2.2)$$

The canonical operators associated with  $(B, \psi)$  are denoted by

$$1 = \begin{array}{c} B \\ \circlearrowleft \\ \mathbb{C} \end{array}, \quad m = \begin{array}{c} B \\ \curvearrowright \\ B \quad B \end{array}, \quad \psi = 1^\dagger = \begin{array}{c} \mathbb{C} \\ \circlearrowleft \\ B \end{array}, \quad m^\dagger = \begin{array}{c} B \quad B \\ \curvearrowleft \\ B \end{array}.$$

For simplicity we denote  $\psi m$  and  $m^\dagger 1$  without the vertical segment and node as follows:

$$\psi m = \begin{array}{c} \mathbb{C} \\ \circ \\ \text{---} \\ B \quad B \end{array} = \begin{array}{c} \mathbb{C} \\ \text{---} \\ B \quad B \end{array}, \quad m^\dagger 1 = \begin{array}{c} B \quad B \\ \text{---} \\ \circ \\ \mathbb{C} \end{array} = \begin{array}{c} B \quad B \\ \text{---} \\ \mathbb{C} \end{array}.$$

The linear extension of the flip map  $\sigma : x \otimes y \mapsto y \otimes x$  is denoted by a crossing of the strings  $\times$ .

The algebra and coalgebra structure of  $(B, m, 1, m^\dagger, \psi)$  is depicted as follows:

$$\begin{array}{cc} \text{associative} & \text{unital} \\ \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ m(m \otimes \text{id}) = m(\text{id} \otimes m) \end{array} & \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ m(1 \otimes \text{id}) = \text{id} = m(\text{id} \otimes 1) \end{array} \\ \text{coassociative} & \text{counital} \\ \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ (m^\dagger \otimes \text{id})m^\dagger = (\text{id} \otimes m^\dagger)m^\dagger \end{array} & \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ (\psi \otimes \text{id})m^\dagger = \text{id} = (\text{id} \otimes \psi)m^\dagger \end{array} \end{array}$$

The quintuple  $(B, m, 1, m^\dagger, \psi)$  forms a Frobenius algebra:

**Definition 2.1** (cf. Vicary [40, Definition 3.2]). An algebra with coalgebra structure is called a Frobenius algebra if the multiplication and comultiplication satisfy the *Frobenius equation*:

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ (m \otimes \text{id})(\text{id} \otimes m^\dagger) = m^\dagger m = (\text{id} \otimes m)(m^\dagger \otimes \text{id}) \end{array}. \quad (2.3)$$

By composing the unit and the counit, we also have the following snake equation:

$$\begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ (\psi m \otimes \text{id})(\text{id} \otimes m^\dagger 1) = \text{id} = (\text{id} \otimes \psi m)(m^\dagger 1 \otimes \text{id}) \end{array}. \quad (2.4)$$

Note that we may compute string diagrams by topological deformation via Frobenius equality, snake equality, associativity, and coassociativity.

**Definition 2.2** (Banica [4, section 1], Musto, Reutter, Verdon [30, Terminology 3.1], Brannan, et al. [8, Definition 3.1]). Let  $\psi$  be a faithful state on a finite dimensional  $C^*$ -algebra  $B$  as above and  $\delta > 0$ . The state  $\psi$  is called a  $\delta$ -form on  $B$  if the following equality (so-called *special* in Vicary [40]) is satisfied:

$$\begin{array}{c} | \\ \bigcirc \\ | \end{array} = \delta^2 \quad \Bigg| \quad , \text{ i.e., } mm^\dagger = \delta^2 \text{id}_B. \quad (2.5)$$

And then we call  $(B, \psi)$  a quantum set.

A quantum set  $(B, \psi)$  is said to be *commutative* or *symmetric* (tracial) if  $B$  is commutative or  $\psi$  is tracial respectively, which are formulated in diagrams as below.

$$\begin{array}{ccc} \text{commutative} & & \text{symmetric (tracial)} \\ \begin{array}{c} | \\ \text{---} \\ \bigcap \\ \text{---} \\ | \end{array} = \begin{array}{c} | \\ \text{---} \\ \cup \\ \text{---} \\ | \end{array} & & \begin{array}{c} \text{---} \\ \bigcap \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \cup \\ \text{---} \end{array} \\ yx = xy & & \psi(yx) = \psi(xy) \quad \forall x, y \in B \end{array}$$

We often use  $\tau$  instead of  $\psi$  in the tracial case.

**Remark 2.3.** The notion of  $\delta$ -forms was introduced by Banica [4], and Musto et al. [30] defined quantum sets in the case where  $\psi$  is a trace. Finally, Brannan, et al. [8] defined quantum sets as above. The definition in [30] is  $mm^\dagger = \text{id}_B$ , which does not have  $\delta^2$ . This is because the counit is normalized as  $\psi(1) = \delta^2 = |B|$  in [30], whence  $m^\dagger$  in [30] is our  $m^\dagger/\delta^2$ . Thus these formulations are equivalent.

**Lemma 2.4.** *A finite set with the uniform probability measure corresponds to a commutative quantum set via Gelfand duality. In particular  $\tau = \text{Tr}/n$  is a  $\delta = \sqrt{n}$ -form on  $\mathbb{C}^n$ .*

*Proof.* Let  $X = \{1, \dots, n\}$  be an  $n$ -element set with the uniform probability measure  $\mu$ . The pair  $(X, \mu)$  corresponds to the commutative  $C^*$ -algebra  $(C(X), \int \cdot d\mu)$  of (continuous) functions on  $X$  with a tracial state  $\int \cdot d\mu$  via Gelfand duality. Moreover  $(C(X), \int \cdot d\mu)$  is isomorphic to the  $n \times n$  diagonal matrix algebra  $(\mathbb{C}^n, \tau = \text{Tr}/n)$  with normalized trace via  $C(X) \ni \delta_i \mapsto e_i \in \mathbb{C}^n$  where  $\delta_i$  is the indicator function of  $\{i\} \subseteq X$  and  $e_i$  is the matrix unit of  $(i, i)$  entry. Note that  $(e_j e_k)^* e_i = \delta_{jk} \delta_{ki} e_i = \delta_{ji} \delta_{ki} e_i$  and  $\langle e_j | e_i \rangle_\tau = \tau(e_j^* e_i) = \frac{1}{n} \delta_{ji}$ . The comultiplication  $m^\dagger$  is given by  $e_i \mapsto n e_i \otimes e_i$  because

$$\begin{aligned} \langle e_j \otimes e_k | m^\dagger e_i \rangle_{\tau \otimes \tau} &= \langle m(e_j \otimes e_k) | e_i \rangle_\tau = \tau((e_j e_k)^* e_i) = \frac{1}{n} \delta_{ji} \delta_{ki} \\ &= n \langle e_j | e_i \rangle_\tau \langle e_k | e_i \rangle_\tau = \langle e_j \otimes e_k | n e_i \otimes e_i \rangle_{\tau \otimes \tau}. \end{aligned}$$

Thus  $mm^\dagger e_i = m(ne_i \otimes e_i) = ne_i$ , i.e.,  $mm^\dagger = n \text{id}_{\mathbb{C}^n}$ . Therefore  $\tau = \text{Tr}/n$  is a  $\delta = \sqrt{n}$ -form on  $\mathbb{C}^n$ .  $\square$

Although a general quantum set  $(B, \psi)$  is not symmetric, it satisfies the following equality, so-called *balanced symmetric* in Vicary [40, Definition 3.10]:

$$\begin{array}{c} \curvearrowright \\ \text{---} \\ \curvearrowleft \end{array} = \begin{array}{c} \text{---} \\ \diagup \quad \diagdown \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \diagdown \quad \diagup \\ \text{---} \end{array}, \quad (2.6)$$

where  $\curvearrowright = \begin{array}{c} \text{---} \\ \diagdown \quad \diagup \\ \text{---} \end{array} = (\psi m \otimes \text{id})(\text{id} \otimes \sigma)(m^\dagger 1 \otimes \text{id})$  and  $\curvearrowleft$  as well. Equation (2.6) directly follows from the snake equation (2.4) as

$$\begin{array}{c} \curvearrowright \\ \text{---} \\ \curvearrowleft \end{array} = \begin{array}{c} \text{---} \\ \diagup \quad \diagdown \\ \text{---} \end{array} \stackrel{(2.4)}{=} \begin{array}{c} \text{---} \\ \diagdown \quad \diagup \\ \text{---} \end{array}.$$

Thus topological deformations through a cusp are not allowed in nontracial cases, while they are allowed in the tracial case.

Put  $B = \bigoplus_s M_{n_s}$  and  $\psi = \text{Tr}(Q \cdot) = \bigoplus_s \text{Tr}_s(Q_s \cdot)$ , where  $\text{Tr} = \bigoplus_s \text{Tr}_s$  is the canonical unnormalized trace given by the sum of diagonal entries or eigenvalues, and  $Q = \bigoplus_s Q_s \in B$ . Note that  $Q$  is positive definite and  $\text{Tr}(Q) = \sum_s \text{Tr}_s(Q_s) = 1$  if and only if  $\psi$  is a faithful state. Since positive matrices are unitarily diagonalizable, we may assume that  $Q$  is diagonal.

Let  $e_{ij,s}$  be the matrix unit of  $(i, j)$  entry of  $s$ -th direct summand  $M_{n_s} \subseteq B$ , i.e., the matrix with entries 0 except for  $(i, j)$  entry 1 of  $s$ -th direct summand.

**Lemma 2.5.**  $\{\widetilde{e}_{ij,s} := e_{ij,s} Q_s^{-1/2} \mid i, j \leq n_s, s\}$  forms an ONB for  $L^2(B, \psi)$ .

*Proof.* Since  $\{e_{ij,s} \mid i, j \leq n_s, s\}$  forms an ONB for  $L^2(B, \text{Tr})$ , we have

$$\langle e_{kl,r} Q_r^{-1/2} \mid e_{ij,s} Q_s^{-1/2} \rangle_\psi = \text{Tr}(Q(e_{kl,r} Q_r^{-1/2})^* e_{ij,s} Q_s^{-1/2}) = \text{Tr}(e_{kl,r}^* e_{ij,s}) = \delta_{ij,s}^{kl,r}$$

$$\text{where } \delta_{ij,s}^{kl,r} := \begin{cases} 1 & \text{if } (i, j, s) = (k, l, r) \\ 0 & \text{otherwise} \end{cases}. \quad \square$$

We sometimes describe operators with respect to the basis  $\{\widetilde{e}_{ij,s} = e_{ij,s} Q_s^{-1/2}\}_{ij,s}$  as indicated below.

**Lemma 2.6.** *We have*

- $1 = \sum_{ij,s} (Q_s^{1/2})_{ij} \widetilde{e}_{ij,s}$ ,
- $\psi : \widetilde{e}_{ij,s} \mapsto (Q_s^{1/2})_{ji}$ .

- $m : \widetilde{e}_{ij,s} \otimes \widetilde{e}_{kl,r} \mapsto \delta_{rs}(Q_s^{-1/2})_{jk}\widetilde{e}_{il,r}$ .
- $m^\dagger : \widetilde{e}_{ij,s} \mapsto \sum_{u,v \leq n_s} (Q_s^{-1/2})_{vu}\widetilde{e}_{iu,s} \otimes \widetilde{e}_{vj,s}$ .

*Proof.* Simple computations show  $\langle \widetilde{e}_{ij,s} | 1 \rangle = \text{Tr}(Q_s^{1/2} e_{ji,s}) = (Q_s^{1/2})_{ij}$ ,  $\psi(\widetilde{e}_{ij,s}) = \text{Tr}(Q_s^{1/2} e_{ij,s}) = (Q_s^{1/2})_{ji}$ ,  $\widetilde{e}_{ij,s}\widetilde{e}_{kl,r} = e_{ij,s}Q_s^{-1/2}e_{kl,r}Q_r^{-1/2} = \delta_{rs}(Q_s^{-1/2})_{jk}\widetilde{e}_{il,r}$ , and

$$\begin{aligned} \langle \widetilde{e}_{ku,r} \otimes \widetilde{e}_{vl,r} | m^\dagger \widetilde{e}_{ij,s} \rangle_{\psi \otimes \psi} &= \langle \widetilde{e}_{ku,r}\widetilde{e}_{vl,r} | \widetilde{e}_{ij,s} \rangle_{\psi} = \langle (Q_r^{-1/2})_{uv}\widetilde{e}_{kl,r} | \widetilde{e}_{ij,s} \rangle_{\psi} \\ &= (Q_s^{-1/2})_{uv}\delta_{ij,s}^{kl,r} = (Q_s^{-1/2})_{vu}\delta_{ij,s}^{kl,r}. \end{aligned}$$

□

**Remark 2.7.** Brannan et al. [9, Lemma 3.2] uses another unnormalized orthogonal basis  $\{f_{ij,s} := Q_s^{-1/2}e_{ij,s}Q_s^{-1/2}\}$  for diagonal  $Q$  in order to simplify the expression of  $m^\dagger$  and prevent the square root  $Q^{1/2}$  from appearing in the coefficients above. In this thesis, we choose  $\{\widetilde{e}_{ij,s}\}$  because we later use matrix expressions of operators with respect to this ONB to compute quantum automorphism groups.

**Proposition 2.8** (Banica [4, section 1]). *In this terminology,  $\psi$  is a  $\delta$ -form on  $B$  if and only if  $\text{Tr}_s(Q_s^{-1}) = \delta^2$  holds for all indices  $s$ .*

*Proof.* By Lemma 2.6,  $\psi$  is a  $\delta$ -form if and only if it holds for all  $i, j, s$  that

$$\begin{aligned} \delta^2 \widetilde{e}_{ij,s} &= mm^\dagger \widetilde{e}_{ij,s} = m \sum_{u,v \leq n_s} (Q_s^{-1/2})_{vu}\widetilde{e}_{iu,s} \otimes \widetilde{e}_{vj,s} \\ &= \sum_{u,v \leq n_s} (Q_s^{-1/2})_{vu}(Q_s^{-1/2})_{uv}\widetilde{e}_{ij,s} \\ &= \sum_{v \leq n_s} (Q_s^{-1})_{vv}\widetilde{e}_{ij,s} = \text{Tr}_s(Q_s^{-1})\widetilde{e}_{ij,s}, \end{aligned}$$

i.e.,  $\text{Tr}_s(Q_s^{-1}) = \delta^2$  for all  $s$ . □

**Lemma 2.9.** *We have  $\curvearrowleft = Q^{-1}(\cdot)Q = \sigma_i$  and  $\curvearrowright = Q(\cdot)Q^{-1} = \sigma_{-i}$ , where  $\sigma_z : B \rightarrow B$  for  $z \in \mathbb{C}$  are the modular automorphisms  $\sigma_z(x) = Q^{iz}xQ^{-iz}$  for the positive invertible density  $Q \in B$  of the faithful state  $\psi = \text{Tr}(Q\cdot)$ .*

*Proof.* It holds for  $x, y \in B$  that

$$\psi(yx) = \text{Tr}(Qyx) = \text{Tr}(xQy) = \psi(Q^{-1}xQy) = \psi(xQyQ^{-1})$$

$$\text{i.e., } \begin{array}{c} \curvearrowleft \\ \circlearrowleft \\ \textcircled{x} \quad \textcircled{y} \end{array} = \begin{array}{c} \textcircled{Q^{-1}xQ} \quad \textcircled{y} \\ \text{---} \end{array} = \begin{array}{c} \textcircled{x} \quad \textcircled{QyQ^{-1}} \\ \text{---} \end{array}.$$

Comparing above with (2.6), we obtain  $\curvearrowleft = Q^{-1}(\cdot)Q$  and  $\curvearrowright = Q(\cdot)Q^{-1}$  by the faithfulness of  $\psi$ .  $\square$

**Lemma 2.10.** *A  $\delta$ -form  $\psi$  on  $B$  satisfies  $\delta^2 \geq |B| = \dim B$ , with equality if and only if  $\psi$  is tracial.*

*Proof.* For  $\psi = \bigoplus_s \text{Tr}_s(Q_s \cdot)$  as above, Cauchy-Schwarz inequality with respect to  $\text{Tr}_s$  gives us

$$n_s^2 = (\text{Tr}_s(Q_s^{-1/2}Q_s^{1/2}))^2 \leq \text{Tr}_s(Q_s^{-1}) \text{Tr}_s(Q_s) \stackrel{\text{(Proposition 2.8)}}{=} \delta^2 \text{Tr}_s(Q_s).$$

Hence  $1 = \text{Tr}(Q) \geq \sum_s n_s^2/\delta^2 = |B|/\delta^2$  shows  $\delta^2 \geq |B|$ , with equality if and only if

$$Q_s^{1/2} = q_s Q_s^{-1/2} \iff Q_s = q_s 1_s$$

for some constant  $q_s$  for every  $s$ , i.e.,  $\psi$  is tracial.  $\square$

**Proposition 2.11** (Banica [3, Proposition 2.1]). *There exists a unique tracial  $\delta$ -form  $\tau = \tau_B$  on  $B$ , and  $\delta^2 = |B|$ . The trace  $\tau$  is explicitly given by  $\tau = \bigoplus_s \frac{n_s}{|B|} \text{Tr}_s$  with  $Q_s = \frac{n_s}{|B|} 1_s$ . Moreover  $\tau$  is the so-called Plancherel trace, the restriction of the unique tracial state of  $B(L^2(B, \psi))$  via left regular representation  $B \hookrightarrow B(L^2(B, \psi))$ .*

*Proof.* Let  $\tau = \bigoplus_s \text{Tr}_s(Q_s \cdot)$  be a tracial  $\delta$ -form on  $B = \bigoplus_s M_{n_s}$ . Traciality implies  $Q_s = q_s 1_s$  for some  $q_s > 0$  for each  $s$ , and hence  $\delta^2 = \text{Tr}_s(Q_s^{-1}) = q_s^{-1} n_s$  by Proposition 2.8. Then

$$1 = \tau(1) = \sum_s \text{Tr}_s(q_s 1_s) = \sum_s q_s n_s = \sum_s n_s^2/\delta^2 = \frac{|B|}{\delta^2},$$

therefore we have  $\delta^2 = |B|$  and  $Q_s = \frac{n_s}{|B|} 1_s$ . [3, Proposition 2.1] states that a tracial state  $\tau$  satisfies  $mm^\dagger = \delta^2 \text{id}$  if and only if  $\tau$  is the restriction of the unique tracial state of  $B(L^2(B, \psi))$ .  $\square$

**Remark 2.12.** Since commutativity  $xy = yx$  implies traciality  $\tau(xy) = \tau(yx)$ , a commutative quantum set is the pair  $(\mathbb{C}^n, \tau)$  of an  $n \times n$  diagonal matrix algebra  $\mathbb{C}^n$  and its normalized trace  $\tau = \text{Tr}/n$ , which corresponds to the pair of an  $n$ -element set and the uniform probability measure as in Lemma 2.4.

In string diagram notation, involution and adjoint are related via twisted wires. The equality  $x^\dagger = \langle x | = \psi(x^* \cdot) = \psi m(x^* \otimes \text{id}_B)$  shows the identity

$$\begin{array}{c} \textcircled{x^\dagger} \\ | \end{array} = \begin{array}{c} \textcircled{x^*} \\ \curvearrowright \\ | \end{array}, \text{ hence } \begin{array}{c} | \\ \curvearrowleft \\ \textcircled{x^\dagger} \end{array} = \begin{array}{c} | \\ \textcircled{x^*} \end{array}. \quad (2.7)$$

This gives a characterization of  $*$ -preserving (also called real) operators in terms of string diagrams.



**Lemma 2.13.** *Let  $(B, \psi)$  be a quantum set. Then an operator  $f : B \rightarrow B$  is  $*$ -preserving if and only if the following equality holds:*

$$\left| \begin{array}{c} \text{---} \\ \circlearrowleft \text{ } f^\dagger \\ \text{---} \end{array} \right| = \left| \begin{array}{c} \text{---} \\ \circlearrowright \text{ } f \\ \text{---} \end{array} \right|. \quad (2.8)$$

*Proof.* For  $x \in B$ ,  $f(x^*)^*$  is formulated in string diagrams as

$$f(x^*)^* = \left( \left| \begin{array}{c} \text{---} \\ \circlearrowright \text{ } f \\ \circlearrowleft \text{ } x^* \\ \text{---} \end{array} \right| \right)^* \stackrel{(2.7)}{=} \left( \left| \begin{array}{c} \text{---} \\ \circlearrowleft \text{ } x^\dagger \\ \circlearrowright \text{ } f \\ \text{---} \end{array} \right| \right)^* \stackrel{(2.7)}{=} \left| \begin{array}{c} \text{---} \\ \circlearrowright \text{ } x \\ \circlearrowleft \text{ } f^\dagger \\ \text{---} \end{array} \right|.$$

Therefore  $f(x^*)^* = f(x) \forall x \in B$  is exactly equal to the desired equality.  $\square$

**Remark 2.14.** Note that bending strings in the other direction can result in different operators. To bend strings means to precompose one end of  $m^\dagger 1 = \cup$  or to postcompose one end of  $\psi m = \cap$ , and different choices of the end can have different outputs as follows:

$$\left| \begin{array}{c} \text{---} \\ \circlearrowleft \text{ } x^\dagger \\ \text{---} \end{array} \right| \stackrel{(2.7)}{=} \left| \begin{array}{c} \text{---} \\ \circlearrowleft \text{ } x^\dagger \\ \text{---} \\ \circlearrowright \text{ } x^* \\ \text{---} \end{array} \right| \stackrel{\text{Lemma 2.9}}{=} Qx^*Q^{-1} \neq x^* = \left| \begin{array}{c} \text{---} \\ \circlearrowright \text{ } x^* \\ \text{---} \end{array} \right|,$$

$$\left| \begin{array}{c} \text{---} \\ \circlearrowright \text{ } f^\dagger \\ \circlearrowleft \text{ } x \\ \text{---} \end{array} \right| \stackrel{(\text{flip})}{=} \left| \begin{array}{c} \text{---} \\ \circlearrowleft \text{ } x \\ \circlearrowright \text{ } f^\dagger \\ \text{---} \end{array} \right| \stackrel{\text{Lemma 2.9}}{=} Qf(Qx^*Q^{-1})^*Q^{-1} \neq f(x^*)^*.$$

In particular,  $f^\dagger$  is not necessarily  $*$ -preserving even if  $f : B \rightarrow B$  is  $*$ -preserving. Indeed  $f^\dagger$  is  $*$ -preserving if and only if

$$\left| \begin{array}{c} \text{---} \\ \circlearrowright \text{ } f \\ \text{---} \end{array} \right| = f^\dagger, \text{ i.e., } f = \left| \begin{array}{c} \text{---} \\ \circlearrowleft \text{ } f^\dagger \\ \text{---} \end{array} \right| \quad (2.9)$$

is satisfied, but the RHS is not necessarily equal to  $*$ -preserving  $f = f((\cdot)^*)^*$  as above.

**Proposition 2.15.** *Given a  $*$ -preserving operator  $f : B \rightarrow B$ ,  $f^\dagger$  is also  $*$ -preserving if and only if  $f$  commutes with  $\prec = Q^{-1}(\cdot)Q$ .*

*Proof.* If  $f^\dagger$  is also  $*$ -preserving, then (2.9) and the adjoint of (2.8) shows

$$\left| \begin{array}{c} \text{---} \\ \circlearrowright \text{ } f \\ \text{---} \end{array} \right| \stackrel{(2.9)}{=} f^\dagger \stackrel{(2.8)}{=} \left| \begin{array}{c} \text{---} \\ \circlearrowleft \text{ } f \\ \text{---} \end{array} \right|.$$

By bending the bottom string counterclockwise (precompose the left end of  $\cup$ ) and the top string clockwise (postcompose the left end of  $\cap$ ), we obtain

$$\begin{array}{c} \diagup \\ \circlearrowleft \\ \text{\scriptsize } f \\ \circlearrowright \\ \diagdown \end{array} = \begin{array}{c} \diagdown \\ \circlearrowright \\ \text{\scriptsize } f \\ \circlearrowleft \\ \diagup \end{array}.$$

Conversely if  $f$  commutes with  $\curvearrowright$ , then we can go back to

$$\begin{array}{c} \diagup \\ \circlearrowleft \\ \text{\scriptsize } f \\ \circlearrowright \\ \diagdown \end{array} = \begin{array}{c} \diagdown \\ \circlearrowright \\ \text{\scriptsize } f \\ \circlearrowleft \\ \diagup \end{array} \stackrel{(2.8)}{=} f^\dagger.$$

□

In the case of  $B = B(H)$  for a finite dimensional Hilbert space  $H$ , operators in  $B(H) \cong H \otimes H^*$  can be expressed by strings of  $H$  and  $H^*$  under the identification  $H \otimes H^* \ni |v\rangle \otimes \langle w| \leftrightarrow |v\rangle \langle w| \in B(H)$ . This identification is formulated in string diagrams as

$$B(H) \ni T \leftrightarrow \begin{array}{c} \uparrow \\ \circlearrowleft \\ \text{\scriptsize } T \\ \circlearrowright \\ \downarrow \end{array} \in H \otimes H^*.$$

Recall that the strings of  $H$  are oriented from bottom to top and those of  $H^*$  from top to bottom.

**Proposition 2.16** (Musto, Reutter, Verdon [30, Definition 2.5]). *By the identification above, the canonical operators of  $(B(H), \tau = \tau_{B(H)})$  is formulated in string diagrams of  $H \otimes H^*$  as follows:*


$$\text{id}_H = \cup, \quad m = \begin{array}{c} \diagup \\ \diagdown \\ \curvearrowright \end{array}, \quad \tau = \frac{\text{Tr}}{|H|} = \frac{1}{|H|} \curvearrowleft, \quad m^\dagger = |H| \begin{array}{c} \diagdown \\ \diagup \\ \curvearrowleft \end{array}.$$

*Proof.* The equality about  $\text{id}_H$  is by the identification. Since the multiplication in  $B(H)$  is the composition, the equality about  $m$  directly follows from the snake equation (2.2). Let  $\{v_i\}_i$  be an ONB for  $H$ . Then

$$\begin{array}{c} \curvearrowright \\ \circlearrowleft \\ \text{\scriptsize } v_i \\ \circlearrowright \\ \text{\scriptsize } v_j^\dagger \end{array} = \langle v_j | v_i \rangle = \delta_{ij}$$

shows the equality about  $\tau$ . Note that  $H \otimes H^*$  is equipped with the inner product

$$\begin{aligned} \langle v_1 \otimes w_1^\dagger | v_0 \otimes w_0^\dagger \rangle_{H \otimes H^*} &= \langle v_1 | v_0 \rangle_H \langle w_1^\dagger | w_0^\dagger \rangle_{H^*} = \langle v_1 | v_0 \rangle_H \langle w_0 | w_1 \rangle_H \\ &= \text{Tr}(|w_1\rangle \langle v_1| |v_0\rangle \langle w_0|) = \text{Tr}((|v_1\rangle \langle w_1|)^\dagger (|v_0\rangle \langle w_0|)) \\ &= \langle (|v_1\rangle \langle w_1|) | (|v_0\rangle \langle w_0|) \rangle_{\text{Tr}}, \end{aligned}$$

hence the diagram  is the adjoint of  $m$  with respect to  $\text{Tr}$ . Therefore the adjoint of  $m$  with respect to  $\tau = \text{Tr}/|H|$  is as stated.  $\square$

Considering  $H = L^2(B, \psi) \cong B$ , we have the same result for strings of  $B$ .

**Corollary 2.17.** *By an identification*

$$B(H) = B(L^2(B, \psi)) \ni T \leftrightarrow \begin{array}{c} \textcircled{T} \\ \cup \end{array} \in B \otimes B$$

for  $H = L^2(B, \psi) \cong B$ , the canonical operators of  $(B(H), \tau_{B(H)} = \text{Tr}_{B(H)}/|B|)$  is formulated in string diagrams of  $B \otimes B$  as follows:

$$\text{id}_B = \cup, \quad m_{B(H)} = \begin{array}{c} \diagup \\ \diagdown \end{array}, \quad \tau_{B(H)} = \frac{1}{|B|} \begin{array}{c} \diagdown \\ \diagup \end{array}, \quad m_{B(H)}^\dagger = |B| \begin{array}{c} \diagdown \\ \diagup \end{array}.$$



*Proof.* The statement directly follows from the previous proposition by the identification

$$B = L^2(B, \psi) \ni y = |y\rangle \leftrightarrow (y^*)^\dagger = \langle y^*| \in L^2(B, \psi)^* \quad (2.10)$$

because  $\text{Tr}(|x\rangle \langle y^*|) = \langle y^*|x\rangle_\psi = \psi(yx) = \begin{array}{c} \textcircled{x} \\ \textcircled{y} \end{array}$  for any  $x, y \in B$ . Since

$$\cup = \sum_i b_i^\dagger \otimes b_i \stackrel{(2.10)}{\leftrightarrow} \sum_i b_i^* \otimes b_i = \sum_i \boxed{b_i^\dagger} / \boxed{b_i} = \begin{array}{c} \diagdown \\ \diagup \end{array}$$

holds for an ONB  $\{b_i\}$  for  $L^2(B, \psi)$ ,  $m^\dagger$  with respect to  $\tau_{B(H)}$  is as stated.  $\square$

The balancing loop in the trace is caused by the discrepancy between the inner products  $\langle \cdot | \cdot \rangle_{\text{Tr}_{B(H)}}$  and  $\langle \cdot | \cdot \rangle_{\psi \otimes \psi}$  on  $B(L^2(B, \psi)) = B \otimes B$ . If we replace  with , then we obtain a nontracial  $B(L^2(B, \psi))$ .

**Corollary 2.18.** *By the same identification  $B(H) = B(L^2(B, \psi)) = B \otimes B$  as in Corollary 2.17,  $\tilde{\psi} := \delta^{-2} \begin{array}{c} \diagdown \\ \diagup \end{array}$  is a  $\delta^2$ -form on  $B(L^2(B, \psi))$  with canonical operators*

$$\text{id}_B = \cup, \quad m_{B(H)} = \begin{array}{c} \diagup \\ \diagdown \end{array}, \quad \tilde{\psi} = \delta^{-2} \begin{array}{c} \diagdown \\ \diagup \end{array}, \quad m_{B(H)}^\dagger = \delta^2 \begin{array}{c} \diagdown \\ \diagup \end{array}.$$

*Proof.* The unit and the multiplication are those in Corollary 2.17. In the same way as Proposition 2.16, we have  $\langle \cdot | \cdot \rangle_{\delta^2 \tilde{\psi}} = \langle \cdot | \cdot \rangle_{\psi \otimes \psi}$ , and hence  $\tilde{\psi}$  is faithful and  $m_{B(H)}^\dagger$  with respect to  $\tilde{\psi}$  is as stated. Since  $\begin{array}{c} \textcircled{\phantom{x}} \\ \textcircled{\phantom{y}} \end{array} = \delta^2$ ,  $\tilde{\psi}$  is a state and we have  $m_{B(H)} m_{B(H)}^\dagger = (\delta^2)^2 \text{id}_{B(H)}$ .  $\square$

Note that  $m_B^\dagger : B \rightarrow B \otimes B$  with  $m_{B(H)}$  as above is a  $*$ -homomorphism that corresponds to the left regular representation of  $B$  (cf. Vicary [40, Lemma 3.19, 3.20]). If we identify  $L^2(B, \psi)^*$  with the left tensorand  $B$  instead of the right one, then  $m_B^\dagger$  corresponds to the right regular representation. The Frobenius equality (2.3) means that the left and right regular representations are  $*$ -homomorphisms.

## 2.2 Quantum graphs

Recall that the adjacency matrix  $A$  of a multiplicity-free finite classical graph  $(V, E)$  is nothing but an operator  $A : C(V) \rightarrow C(V)$  that is idempotent with respect to the entrywise product, which we call Schur product. Quantum graphs as adjacency matrix is defined in this manner as follows.

**Definition 2.19** ([30, 8]). A *quantum set* is  $(B, \psi)$  consisting of a finite-dimensional  $C^*$ -algebra  $B$  with a  $\delta$ -form  $\psi : B \rightarrow \mathbb{C}$ , where the  $\delta$ -form is defined as a faithful state satisfying  $mm^\dagger = \delta^2 \text{id}_B$  for  $\delta \geq 0$ .

**Definition 2.20** ([30, 8, 9]). Let  $(B, \psi)$  be a quantum set. We define the *Schur product*  $S \bullet T$  and the involution  $T^*$  of  $S, T \in B(L^2(B, \psi))$  by

$$S \bullet T := \delta^{-2} m(S \otimes T) m^\dagger = \delta^{-2} \begin{array}{c} \text{---} \\ \circlearrowleft \text{---} \\ \text{---} \\ \circlearrowright \text{---} \\ \text{---} \\ \circlearrowright \text{---} \\ \text{---} \\ \circlearrowleft \text{---} \\ \text{---} \end{array} ; \quad T^* := (T(\cdot)^*)^* = \begin{array}{c} \text{---} \\ \circlearrowright \text{---} \\ \text{---} \\ \circlearrowleft \text{---} \\ \text{---} \end{array} ,$$

with which  $B(L^2(B, \psi))$  forms a  $*$ -algebra isomorphic to  $B^{\text{op}} \otimes B$ . See for example [28, Lemma 2.13] about the identity of the involution and the diagram. The correspondence is given by

$$B(L^2(B, \psi)) \ni T \leftrightarrow p_T := \delta^{-2} \begin{array}{c} \text{---} \\ \boxed{\sigma_{i/2}} \\ \text{---} \\ \boxed{T} \\ \text{---} \end{array} \in B^{\text{op}} \otimes B$$

where  $\sigma_{i/2} = Q^{-1/2}(\cdot)Q^{1/2} : B \rightarrow B$  is a modular automorphism and  $p_T = \Psi'_{0,1/2}(T)$  defined in [17, Definition 5.1]. See [23] for the tracial setting and [17, 42] for the details in general setting.

We say that  $T : B \rightarrow B$  is *real* if  $T^* = T$  (i.e.,  $*$ -preserving. cf. [30]);  $T$  is *Schur idempotent* if  $T \bullet T = T$ ; and  $T$  is a *Schur projection* if it is real and Schur idempotent.

We often use the realness of  $T : B \rightarrow B$  in the form of

$$\begin{array}{c} \text{---} \\ \circlearrowright \text{---} \\ \text{---} \\ \circlearrowleft \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \circlearrowleft \text{---} \\ \text{---} \\ \circlearrowright \text{---} \\ \text{---} \end{array} \quad \text{or} \quad \begin{array}{c} \text{---} \\ \circlearrowleft \text{---} \\ \text{---} \\ \circlearrowright \text{---} \\ \text{---} \end{array} = \begin{array}{c} \text{---} \\ \circlearrowright \text{---} \\ \text{---} \\ \circlearrowleft \text{---} \\ \text{---} \end{array} . \quad (2.11)$$

Note that if  $T$  is real, then  $T^\dagger$  is real if and only if  $T$  commutes with modular automorphisms  $\sigma_z$  (c.f. [28, Proposition 2.15], [42, Lemma 2.1]). This means that we cannot always replace  $T$  with  $T^\dagger$  in (2.11).

**Definition 2.21** (KMS adjoint). Wasilewski [42] pointed out that the *KMS inner product*  $\langle x|y \rangle = \psi(x^* \sigma_{-i/2}(y))$  on  $B$  behaves better than the GNS inner product  $\langle x|y \rangle_\psi = \psi(x^* y)$  when we define nontracial quantum Cayley graphs. They coincide if  $\psi$  is tracial. The *KMS adjoint* is the adjoint of an operator on (tensor powers of)  $B$  with respect to the KMS inner product.

The relation between the GNS adjoint  $T^\dagger$  and the KMS adjoint  $T^\ddagger$  of  $T : B^{\otimes m} \rightarrow B^{\otimes n}$  is given by  $T^\ddagger = \sigma_{i/2}^{\otimes m} T^\dagger \sigma_{-i/2}^{\otimes n}$ . Define  $\lrcorner := \sigma_{i/2}$ ,  $\rceil := \sigma_{-i/2}$ , and  $\frown := \cap \smile = \lrcorner \cap \rceil$ , where the cusp stands for the operator in the middle of the straight string  $\text{id}_B$  and the loops  $\sigma_{\pm i}$ . Then the KMS inner product is drawn as  $\langle x|y \rangle = \text{cusp}(x^* y)$  and the relation

of the KMS adjoint and the involution is  $T^* = \text{cusp}(T^\ddagger)$ . Thus in terms of the KMS adjoint, the realness (2.11) of  $T$  is replaced by

$$\text{cusp}(T^\ddagger) = \text{cusp}(T) \text{ or } \text{cusp}(T) = \text{cusp}(T^\ddagger).$$

A benefit of KMS adjoint is that  $T^\ddagger$  is real if and only if  $T$  is real. Indeed, the flip invariance  $\text{cusp} = \text{cusp} = \text{cusp}$  implies the equivalence between the realness of  $T$  and that of  $T^\ddagger$  by flipping the strings:

$$\text{cusp}(T) = \text{cusp}(T^\ddagger) \iff \text{cusp}(T) = \text{cusp}(T^\ddagger). \quad (2.12)$$

Since the GNS adjoint is easier to treat in string diagrams, we stick to the GNS inner product in this thesis.

**Definition 2.22** (Musto, Reutter, Verdon [30, Definition 5.1], Brannan et al. [8, Definition 3.4]). We define a *quantum adjacency matrix* on a quantum set  $(B, \psi)$  as an operator  $A : B \rightarrow B$  satisfying *Schur idempotence*

$$\text{cusp}(A A) = \delta^2 \text{cusp}(A), \text{ i.e., } A \bullet A = A, \quad (2.13)$$

and then we call  $\mathcal{G} = (B, \psi, A)$ , or simply  $A$ , a quantum graph on  $(B, \psi)$ .

We denote the GNS space of a quantum graph  $\mathcal{G} = (B, \psi, A)$  by  $L^2(\mathcal{G}) := L^2(B, \psi)$ .

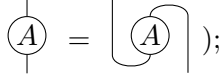
**Remark 2.23.** The notion of quantum adjacency matrix is first introduced by Musto, Reutter, Verdon [30, Definition 5.1], who defined undirected quantum graphs on tracial quantum sets. Following [30], Brannan et al. [8, Definition 3.4] defined undirected quantum graphs on general quantum sets. The weakest definition assigning only Schur idempotence appears in Brannan, Eifler, Voigt, Weber [9, Definition 3.3].

### 2.3 Basic properties of quantum graphs

**Definition 2.24.** Let  $\mathcal{G} = (B, \psi, A)$  be a quantum graph.

[8]  $\mathcal{G}$  is tracial (or symmetric) if  $\psi$  is tracial, i.e.,  $\psi = \tau_B$ ;

[30]  $\mathcal{G}$  is real if  $A$  is real  $A^* = A$ . The realness is equivalent to the complete positivity by the Schur idempotence of  $A$  (cf. [28, Proposition 2.23], [42, Remark 3.2]);

[15]  $\mathcal{G}$  is *self-transposed* (or GNS symmetric [42]) if  $\psi((Ax)y) = \psi(x(Ay))$  ( $\iff$ )  


[30]  $\mathcal{G}$  is undirected if  $A$  is both real and self-adjoint;

[42]  $\mathcal{G}$  is KMS symmetric if  $A$  is both real and KMS self-adjoint  $A = A^\ddagger$ ;

[30]  $\mathcal{G}$  is reflexive (or has all loops) if  $A \bullet \text{id} = \text{id}$ ;

[30]  $\mathcal{G}$  is irreflexive (or has no loops) if  $A \bullet \text{id} = 0$ ;

[23]  $\mathcal{G}$  has no partial loops if  $A \bullet \text{id} = \text{id} \bullet A$ ;

[28]  $\mathcal{G}$  is  $d$ -regular if  $A1_B = d1_B = A^\dagger 1_B$ . The  $d \in \mathbb{C}$  is the degree of  $\mathcal{G}$ ;

- $\mathcal{G}$  is Schur central if  $A \bullet \cdot = \cdot \bullet A$ , i.e.,  $A$  is central with respect to the Schur product.

**Remark 2.25.** In the classical case  $(\mathbb{C}^n, \tau)$ , *Schur product*  $f \bullet g$  of operators  $f, g \in M_n \cong B(\mathbb{C}^n)$  is defined as the entrywise product. In fact it is realized as

$$f \bullet g = m(f \otimes g)m^\dagger / \delta^2.$$

That is why the condition (2.13) is called Schur idempotence. Since a matrix is Schur idempotent if and only if it is  $\{0, 1\}$ -valued, quantum graphs  $A$  on  $(\mathbb{C}^n, \tau)$  are exactly equal to the adjacency operators of classical multiplicity-free graphs on  $n$  vertices. Then  $A$  is always real because  $A$  is real-valued and  $*$  is just the complex conjugate, and  $A$  is undirected if and only if the graph  $(V, E)$  is undirected, i.e., any edge  $(v, w) \in E$  has its opposite  $(w, v) \in E$ . It seems natural to call the graph symmetric instead of self-transposed, but it may be confused with the symmetry (traciality) of a quantum set, so we use the term self-transposed. A classical graph is called reflexive if it has all self-loops  $(v, v)$  for  $v \in V$ , and irreflexive if it has no self-loops. Thus reflexivity is characterized by the Schur product of  $A$  and  $\text{id}_{\mathbb{C}^n}$ , which outputs the diagonal entries  $A_{v,v}$ .

Recall that the *indegree* (resp. *outdegree*) of a vertex of a classical directed graph is the number of edges into (resp. out of) the vertex, and the

graph is called *d-regular* if the indegrees and outdegrees of all vertices are equal to  $d$ . Note that a classical graph is *d-regular* if and only if the adjacency operator  $A$  and  $A^\dagger$  have the constant function 1 as an eigenvector of eigenvalue  $d$ .

**Lemma 2.26.** *Let  $(B, \psi, A)$  be a quantum graph. Every couple of the following three conditions imply the other. Equivalently, all couples of the following are equivalent to each other.*

- (1)  $A$  is self-adjoint;
- (2)  $A$  is self-transposed;
- (3)  $A$  is real.

*In particular,  $A$  is undirected if and only if (1), (2), and (3) hold.*

*Proof.* (1)(2)  $\implies$  (3) We have

$$\left| \begin{array}{c} \circlearrowleft \\ A^\dagger \end{array} \right| \stackrel{(1)}{=} \left| \begin{array}{c} \circlearrowright \\ A \end{array} \right| \stackrel{(2)}{=} \begin{array}{c} | \\ \circlearrowleft \\ A \end{array} .$$

Thus  $A$  is real.

(2)(3)  $\implies$  (1) By using the Hilbert adjoint of real condition, we have

$$\begin{array}{c} | \\ \circlearrowleft \\ A^\dagger \end{array} \stackrel{(3)}{=} \left| \begin{array}{c} \circlearrowright \\ A \end{array} \right| \stackrel{(2)}{=} \begin{array}{c} | \\ \circlearrowleft \\ A \end{array} .$$

Thus  $A$  is self-adjoint.

(3)(1)  $\implies$  (2) We have

$$\left| \begin{array}{c} \circlearrowright \\ A \end{array} \right| \stackrel{(1)}{=} \left| \begin{array}{c} \circlearrowleft \\ A^\dagger \end{array} \right| \stackrel{(3)}{=} \begin{array}{c} | \\ \circlearrowleft \\ A \end{array} .$$

Thus  $A$  is self-transposed. □

Recall that an operator  $A : B \rightarrow B'$  between  $C^*$ -algebras is called positive if it preserves the positive cone consisting of positive semidefinite elements  $A(B^+) \subset B'^+$ , and called completely positive if its amplification  $A \otimes \text{id}_{M_n} : B \otimes M_n \cong M_n(B) \rightarrow B' \otimes M_n \cong M_n(B')$  is positive for arbitrary positive integer  $n$ . We can deduce the following equivalence from Schur idempotence.

**Proposition 2.27.** *Let  $\mathcal{G} = (B, \psi, A)$  be a quantum graph. TFAE:*

- (1)  $A$  is real;
- (2)  $A$  is positive;

(3)  $A$  is completely positive.

*Proof.* (3)  $\implies$  (2) Obvious by definition. (2)  $\implies$  (1) Since the positive cone  $B^+$  of  $B$  spans the subspace  $B^{sa}$  of self-adjoint operators,  $A(B^+) \subset B^+$  implies  $A(B^{sa}) \subset B^{sa}$ , i.e.,  $A$  is real.

(1)  $\implies$  (3) Assume that  $A$  is a real quantum graph on  $(B, \psi)$ . Then  $A \otimes \text{id}_{M_n}$  is also a quantum graph on  $(B \otimes M_n, \psi \otimes \tau_{M_n})$  for arbitrary  $n$ , and it is real since the involution is  $(b \otimes x)^* = b^* \otimes x^*$  in  $B \otimes M_n$ . Replacing  $(B \otimes M_n, \psi \otimes \tau_{M_n}, A \otimes \text{id}_{M_n})$  by  $(B, \psi, A)$ , it suffices to show that  $A$  is positive. We take an arbitrary  $x \in B$  and check that  $A(x^*x)$  is positive semidefinite:

$$A(x^*x) = \begin{array}{c} \textcircled{A} \\ | \\ \boxed{x^*x} \end{array} = \begin{array}{c} \textcircled{A} \\ / \quad \backslash \\ \boxed{x^*} \quad \boxed{x} \end{array} = \delta^{-2} \begin{array}{c} \textcircled{A} \quad \textcircled{A} \\ / \quad \backslash \\ \boxed{x^*} \quad \boxed{x} \end{array} = \delta^{-2} \begin{array}{c} \textcircled{A} \quad \textcircled{A} \\ / \quad \backslash \\ \boxed{x^*} \quad \boxed{x} \end{array} .$$

Decomposing the identity string in the middle of the diagram into  $\text{id}_B = \sum_i |b_i\rangle \langle b_i|$  by an ONB  $\{b_i\}_{i=1}^{|B|}$  for  $L^2(B, \psi)$ , we obtain

$$\begin{aligned} A(x^*x) &= \delta^{-2} \sum_i \begin{array}{c} \textcircled{A} \quad \boxed{b_i^\dagger} \quad \textcircled{A} \\ / \quad \backslash \\ \boxed{x^*} \quad \boxed{b_i} \quad \boxed{x} \end{array} = \delta^{-2} \sum_i \begin{array}{c} \textcircled{A} \quad \textcircled{A} \\ / \quad \backslash \\ \boxed{x^*b_i} \quad \boxed{b_i^*x} \end{array} \\ &= \delta^{-2} \sum_i A(x^*b_i)A(b_i^*x) = \delta^{-2} \sum_i A(b_i^*x)^*A(b_i^*x) \geq 0. \end{aligned}$$

Therefore  $A$  is positive.  $\square$

**Lemma 2.28.** *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular real quantum graph. It follows that  $d \in \mathbb{R}$ .*

*Proof.* We have  $d = \langle 1_B | A 1_B \rangle = \langle 1_B | A^* 1_B \rangle = \langle 1_B | (A 1_B)^* \rangle = \bar{d}$ .  $\square$

**Definition 2.29** (Weaver [43]). A quantum relation on a von Neumann algebra  $B \subset B(H)$  is a weak\*-closed  $B'$ - $B'$ -bimodule  $\mathcal{S} \subset B(H)$ , where we regard  $B(H)$  as the dual of the trace class  $TC(H) = \{T \in B(H) \mid \text{Tr}(|T|) < \infty\}$  via the coupling  $(S, T) \mapsto \text{Tr}(ST)$ .

[43, Theorem 2.7] showed that the quantum relations are independent of the choice of  $H$ , i.e., there is a canonical correspondence between quantum relation on isomorphic von Neumann algebras  $B \subset B(H)$ .

We chose  $H = L^2(B, \psi)$  for a quantum set  $(B, \psi)$ , then a quantum relation on  $B = \lambda(B) \subset B(H)$  is a  $\rho(B)$ - $\rho(B)$ -bimodule  $\mathcal{S} \subset B(H)$  where  $\lambda$  (resp.  $\rho$ ) is the left (resp. right) regular representation with respect to  $\psi$ .



Quantum relations on a quantum set  $(B, \psi)$  are identified with  $B$ - $B$ -bimodules  $\mathcal{S} \subset B \otimes B$  via the identification:

$$\iota : B(L^2(B, \psi)) \ni T \mapsto \iota(T) = \begin{array}{c} \downarrow \\ \boxed{T} \\ \uparrow \end{array} \in B \otimes B. \quad (2.14)$$

See for example [27], [12, Appendix F] about bimodules over von Neumann algebras, and [30] about the one-to-one correspondence above.

The linear isomorphism  $\iota$  is the linear extension of  $\iota(|x\rangle\langle y|) = \sigma_{-i}(y^*) \otimes x$  for  $x, y \in B$ . We endow  $B(L^2(B, \psi))$  with a Hilbert space structure via  $\iota$ , i.e.,

$$\langle S|T \rangle = \langle \iota(S)|\iota(T) \rangle_{\psi \otimes \psi} = \Psi(S^\dagger T) = \delta^2 \langle 1|S^* \bullet T|1 \rangle, \quad (2.15)$$

where  $\Psi = \delta^2 \langle 1|\text{id}_B \bullet \cdot|1 \rangle = \begin{array}{c} \downarrow \\ \boxed{1} \\ \uparrow \end{array}$  is an extension of  $\delta^2 \psi$  on  $\rho(B)$  to  $B(L^2(B, \psi))$ .

Let  $P : L^2(B, \psi)^{\otimes 2} \rightarrow L^2(B, \psi)^{\otimes 2}$  be the orthogonal projection onto the  $B$ - $B$ -bimodule  $\mathcal{S} \subset B \otimes B = L^2(B, \psi)^{\otimes 2}$ . Then  $P$  is  $B$ - $B$ -bimodule map, i.e.,  $P(x\xi y) = xP(\xi)y$  for  $x, y \in B$  and  $\xi \in B \otimes B$ .

There is a one-to-one correspondence (cf. [30]) between  $B$ - $B$ -bimodule projections  $P$  on  $B \otimes B$  and real quantum graphs  $(B, \psi, A)$  as follows:

$$P = P_A := \delta^{-2} \begin{array}{c} \downarrow \\ \boxed{A} \\ \uparrow \end{array}; \quad A = A_P = \delta^2 \begin{array}{c} \circ \\ \downarrow \\ \boxed{P} \\ \uparrow \\ \circ \end{array}. \quad (2.16)$$

Note that  $P_A = \iota \widetilde{P}_A \iota^{-1}$  is the reformulation of left Schur product by  $A$ :

$$\widetilde{P}_A = A \bullet (\cdot) : B(L^2(B, \psi)) \ni T \mapsto A \bullet T \in B(L^2(B, \psi)).$$

Here are typical examples of quantum graphs.

**Example 2.30** (cf. Brannan et al. [8, Remark 3.6]).

- Let  $(V, E)$  be a simple classical graph, and  $A : C(V) \rightarrow C(V)$  the adjacency matrix. Then  $(C(V), \tau, A)$  is a quantum graph.
- Let  $(B, \psi)$  be a quantum set. The (reflexive) *complete graph* on  $(B, \psi)$  is given by  $A = \delta^2 \psi(\cdot)1$ , which is an undirected reflexive  $\delta^2$ -regular quantum graph. Indeed the definition of the unit and counit shows

$$\begin{array}{c} \circ \\ \downarrow \\ \circ \end{array} = \begin{array}{c} \downarrow \\ \circ \\ \downarrow \end{array}; \quad \begin{array}{c} \downarrow \\ \circ \\ \downarrow \end{array} = \begin{array}{c} \downarrow \\ \circ \\ \downarrow \end{array}; \quad \left( \begin{array}{c} \downarrow \\ \circ \\ \downarrow \end{array} \right)^\dagger = \begin{array}{c} \downarrow \\ \circ \\ \downarrow \end{array}; \quad \begin{array}{c} \downarrow \\ \circ \\ \downarrow \end{array} = \begin{array}{c} \downarrow \\ \circ \\ \downarrow \end{array}.$$



We have by the irreflexivity that

$$\begin{aligned}
 \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ | \end{array} &= \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ \text{---} \\ | \end{array} + \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ \text{---} \\ | \end{array} + \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} + \begin{array}{c} | \\ \text{---} \\ | \end{array} \\
 &= \delta^2 \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} + \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} + \delta^2 \begin{array}{c} | \\ \text{---} \\ | \end{array} = \delta^2 \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} + \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} .
 \end{aligned}$$

Hence it suffices to show that the final term  $m(\text{id}_B \otimes A)m^\dagger$  is zero. Indeed reality and irreflexivity implies that

$$\begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} \stackrel{\text{(real)}}{=} \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} = \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} \stackrel{\text{(irreflexive)}}{=} 0,$$

where the third equality follows from topological calculation using the coassociativity, associativity, snake equation (2.4) and Frobenius equation (2.3). Therefore  $A_{\text{ref}} = A_{\text{irref}} + \text{id}_B$  is a reflexive quantum graph. Similarly given reflexive quantum graph  $A_{\text{ref}}$ , it follows that  $A_{\text{irref}} = A_{\text{ref}} - \text{id}_B$  is an irreflexive quantum graph. The equality of their spectra follows from

$$\lambda \text{id}_B - A_{\text{irref}} = (\lambda + 1)\text{id}_B - A_{\text{ref}} \quad \forall \lambda \in \mathbb{C}.$$

□

**Proposition 2.33.** *Let  $(B, \psi, A)$  be a real reflexive quantum graph. Then*

$$A^c := \text{id}_B + \delta^2 \psi(\cdot)1 - A$$

*is also a real reflexive quantum graph on  $(B, \psi)$ , the so-called reflexive complement of  $A$ .*

*Proof.* Since  $\text{id}_B$ ,  $\delta^2 \psi(\cdot)1$ , and  $A$  are real reflexive quantum graphs on  $(B, \psi)$ , linearity shows that  $A^c$  is also real and reflexive. We have by distributing the unit and the counit that

$$\begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} = \begin{array}{c} | \\ \text{---} \\ | \end{array} \begin{array}{c} \text{---} \\ \text{---} \\ | \end{array} + 2\delta^2 \begin{array}{c} | \\ \text{---} \\ | \end{array} + \delta^4 \begin{array}{c} | \\ \text{---} \\ | \end{array} .$$

Since  $A - \text{id}_B$  is an irreflexive real quantum graph by Proposition 2.31, we obtain

$$= \delta^2 \boxed{\text{id} - A} + \delta^4 \begin{array}{c} | \\ \circ \\ | \end{array} = \delta^2 \begin{array}{c} | \\ \circ \\ | \end{array} \text{A}^c.$$

□

The degree of a regular classical graph is at most the size of the vertex set. The value  $\delta^2$  plays the role of the size of a quantum set, and it bounds the degree.

**Lemma 2.34.** *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular real quantum graph. Then  $0 \leq d \leq \delta^2$ . In particular,  $d = 0$  if and only if  $A = 0$ , and  $d = \delta^2$  if and only if  $A = \delta^2 \psi(\cdot)1_B$ .*

*Proof.* We use the correspondence between  $A$  and a projection  $p_A \in B^{\text{op}} \otimes B$ . Note that the reflexive complete graph  $(B, \psi, J = \delta^2 \psi(\cdot)1_B)$  corresponds to the maximal projection  $p_J = 1 \otimes 1 \in B^{\text{op}} \otimes B$ . Since  $0 \leq p_A \leq p_J$  and  $\psi^{\otimes 2}$  is a state on  $B^{\text{op}} \otimes B$ , we have

$$0 \leq d = \psi(A1_B) = \psi^{\otimes 2}(p_A) \leq \psi^{\otimes 2}(p_J) = \psi(J1_B) = \delta^2.$$

Since  $\psi^{\otimes 2}$  is faithful,  $d = 0$  holds if and only if  $A = 0$ , and  $d = \delta^2$  holds if and only if  $A = J$ . □

Gromada [23, section 2.3] pointed out that the value  $\delta^2 \langle 1_B | A | 1_B \rangle = \delta^2 \psi(A1_B)$  is the number of edges. This value is strictly positive whenever  $A$  is nonzero and real:

**Lemma 2.35.** *Let  $\mathcal{G} = (B, \psi, A)$  be a real quantum graph. Then  $\langle 1_B | A | 1_B \rangle \geq 0$  with equality if and only if  $A = 0$ .*

*Proof.* Similarly to the proof of Lemma 2.34, we have

$$\langle 1_B | A | 1_B \rangle = \psi^{\otimes 2}(p_A) \geq 0.$$

Since  $\psi^{\otimes 2}$  is faithful,  $\langle 1_B | A | 1_B \rangle = 0$  holds if and only if  $A = 0$ . □

For later use, we show that the eigenspace for any real eigenvalue of a real quantum graph is spanned by self-adjoint elements:

**Lemma 2.36.** *Let  $(B, \psi, A)$  be a real quantum graph and  $x \in B$  be an eigenvector for an eigenvalue  $\lambda$  of  $A$ . Then  $x^*$  is an eigenvector for the eigenvalue  $\bar{\lambda}$  of  $A$ . In particular if  $\lambda \in \text{spec}(A) \cap \mathbb{R}$ , then the eigenspace  $\ker(\lambda \text{id} - A)$  and the generalized eigenspace  $\ker(\lambda \text{id} - A)^{\dim B}$  are spanned by self-adjoint elements.*

*Proof.* Taking the involution of  $(\lambda \text{id} - A)x = 0$ , we get  $(\bar{\lambda} \text{id} - A)x^* = (\lambda x)^* - (Ax)^* = ((\lambda \text{id} - A)x)^* = 0$ . If  $\lambda$  is real, then both  $x$  and  $x^*$  are eigenvectors for  $\lambda$ , hence  $\Re x = \frac{x+x^*}{2}$ ,  $\Im x = \frac{x-x^*}{2i}$  are also eigenvectors for  $\lambda$ . Since  $x$  is arbitrary,  $\ker(\lambda \text{id} - A)$  is spanned by self-adjoint elements. Similarly  $\ker(\lambda \text{id} - A)^{\dim B}$  is so.  $\square$

### 3 Quantum isomorphisms of quantum graphs

#### 3.1 Quantum isomorphisms

**Definition 3.1** (Musto, Reutter, Verdon [30, Definition 3.11, 4.3]). A *quantum function*  $(H, P) : (B', \psi') \rightarrow (B, \psi)$  between quantum sets  $(B, \psi)$  and  $(B', \psi')$  is a pair  $(H, P)$  of a finite dimensional Hilbert space  $H$  and a linear operator  $P : B \otimes H \rightarrow H \otimes B'$  denoted in string diagrams by

$$P = \begin{array}{c} H \quad B' \\ \swarrow \quad \searrow \\ \textcircled{P} \\ \nearrow \quad \nwarrow \\ B \quad H \end{array}$$

satisfying

$$\begin{array}{c} \textcircled{P} \\ \circlearrowleft \end{array} = \text{---} \circlearrowleft \quad \begin{array}{c} \textcircled{P} \quad \textcircled{P} \\ \swarrow \quad \searrow \\ \textcircled{P} \end{array} = \begin{array}{c} \textcircled{P} \\ \swarrow \quad \searrow \end{array} \quad \begin{array}{c} \textcircled{P} \\ \circlearrowright \end{array} = \begin{array}{c} \textcircled{P} \\ \swarrow \quad \searrow \end{array}, \quad (3.1)$$

which respectively means that  $P$  preserves the unit, multiplication, and involution. A quantum function  $(H, P)$  is called a *quantum bijection* if it also satisfies

$$\begin{array}{c} \textcircled{P} \\ \circlearrowright \end{array} = \text{---} \circlearrowright \quad \begin{array}{c} \textcircled{P} \quad \textcircled{P} \\ \swarrow \quad \searrow \\ \textcircled{P} \end{array} = \begin{array}{c} \textcircled{P} \\ \swarrow \quad \searrow \end{array}, \quad (3.2)$$

which respectively means that  $P$  preserves the counit and comultiplication. If  $|H| = \dim H = 1$ , then a quantum function (resp. quantum bijection)  $(H, P)$  is called a classical function (resp. classical bijection).

**Remark 3.2.** In the case of  $|H| = 1$ , we may forget the oriented strings of  $H$ . Then (3.1) exactly says that

$$P(1) = 1, \quad P(x)P(y) = P(xy), \quad P(x^*)^* = P(x) \quad \forall x, y \in B,$$

i.e.,  $P : B \rightarrow B'$  is a  $*$ -homomorphism. Similarly (3.2) says that  $P : B \rightarrow B'$  is a cohomomorphism. This is why  $(H, P)$  is called classical if  $|H| = 1$ .

Note that the quantum function  $(H, P) : (B', \psi') \rightarrow (B, \psi)$  and ‘homomorphism’  $P : B \otimes H \rightarrow H \otimes B'$  have opposite direction. This is based on the Gelfand duality, where a set function  $f : X \rightarrow Y$  corresponds to a unital  $*$ -homomorphism  $\cdot \circ f : C(Y) \rightarrow C(X)$ .

**Remark 3.3.** Alternatively we may consider

$$\tilde{P} = \begin{array}{c} \uparrow \uparrow \uparrow \\ \boxed{\tilde{P}} \\ \downarrow \end{array} := \begin{array}{c} \swarrow \quad \searrow \\ \textcircled{P} \\ \nearrow \quad \nwarrow \end{array} : B \rightarrow H \otimes B' \otimes H^* \cong B' \otimes B(H)$$

(cf. [30, proof of Theorem 3.28]). Then  $(H, P)$  is a quantum function if and only if  $P : B \rightarrow B' \otimes B(H)$  is a  $*$ -homomorphism. Note that  $H \otimes B' \otimes H^* \cong B' \otimes B(H)$  is equipped with the following operators by Proposition 2.16:

$$1' \otimes \text{id}_H = \begin{array}{c} \downarrow \\ \cup \end{array}, \quad m = \begin{array}{c} \nearrow \searrow \\ \nearrow \searrow \\ \nearrow \searrow \end{array}, \quad \psi' \otimes \frac{\text{Tr}}{|H|} = \frac{1}{|H|} \begin{array}{c} \curvearrowright \\ \curvearrowleft \end{array}, \quad m^\dagger = |H| \begin{array}{c} \curvearrowleft \\ \curvearrowright \end{array}.$$

Thus indeed (3.1) implies that  $\tilde{P}$  is a  $*$ -homomorphism. Although string diagrams like  $\curvearrowright$  do not work well for infinite dimensional  $H$ , the formulation in terms of  $\tilde{P}$  is valid. The formulation of quantum isomorphisms by Brannan et al. [8, section 4] is derived from this viewpoint.

**Remark 3.4.** By the snake equations (2.4), the  $*$ -preserving condition in (3.1) has an equivalent formulation:

$$\begin{array}{c} \curvearrowright \\ \textcircled{P^\dagger} \end{array} = \begin{array}{c} \nearrow \searrow \\ \textcircled{P} \\ \nearrow \searrow \end{array} \iff \begin{array}{c} \nearrow \searrow \\ \textcircled{P^\dagger} \\ \nearrow \searrow \end{array} = \begin{array}{c} \curvearrowleft \\ \textcircled{P} \end{array}. \quad (3.3)$$

**Definition 3.5** (Musto, Reutter, Verdon [30, Definition 3.18]). Let  $(H, P), (H', P') : (B', \psi') \rightarrow (B, \psi)$  be quantum functions. An *intertwiner*  $f : (H, P) \rightarrow (H', P')$  is an operator  $f : H \rightarrow H'$  satisfying

$$\begin{array}{c} \textcircled{f} \\ \nearrow \searrow \\ \textcircled{P} \\ \nearrow \searrow \end{array} = \begin{array}{c} \nearrow \searrow \\ \textcircled{P'} \\ \nearrow \searrow \\ \textcircled{f} \end{array}.$$

The category QSet of quantum sets is defined as a 2-category that consists of

- **Objects:** quantum sets  $(B, \psi)$ ;
- **1-morphisms:** quantum functions  $(H, P) : (B', \psi') \rightarrow (B, \psi)$ ;
- **2-morphisms:** intertwiners  $f : (H, P) \rightarrow (H', P')$ .

Given quantum sets  $(B, \psi), (B', \psi')$ , we define the category QBij $((B', \psi'), (B, \psi))$  as a category consisting of

- **Objects:** quantum bijections  $(H, P) : (B', \psi') \rightarrow (B, \psi)$ ;
- **Morphisms:** intertwiners  $f : (H, P) \rightarrow (H', P')$ .

**Lemma 3.6** (Tracial case by Musto, Reutter, Verdon [30, Theorem 4.8]).  
For a quantum function  $(H, P) : (B', \psi') \rightarrow (B, \psi)$ , TFAE:

- (1)  $(H, P)$  is a quantum bijection;
- (2)  $P$  is a unitary operator.

*Proof.* (1)  $\implies$  (2) By the involution and multiplication preserving conditions in (3.1) and the counit preserving condition in (3.2), we have

$$P^\dagger P = \begin{array}{c} \circlearrowleft \\ P^\dagger \\ \circlearrowright \\ P \\ \circlearrowleft \\ \circlearrowright \end{array} \stackrel{(3.3)}{=} \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \\ P \\ \circlearrowleft \\ \circlearrowright \end{array} \stackrel{(3.1)}{=} \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \end{array} \stackrel{(3.2)}{=} \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \end{array} = \begin{array}{c} | \\ | \end{array} = \text{id}_{B \otimes H}.$$

Similarly by the involution and unit preserving conditions in (3.1) and the comultiplication preserving condition in (3.2), we have

$$P P^\dagger = \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \\ P^\dagger \\ \circlearrowleft \\ \circlearrowright \end{array} \stackrel{(3.3)}{=} \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \\ P \\ \circlearrowleft \\ \circlearrowright \end{array} \stackrel{(3.2)}{=} \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \end{array} \stackrel{(3.1)}{=} \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \end{array} = \begin{array}{c} | \\ | \end{array} = \text{id}_{H \otimes B'}.$$

Therefore  $P$  is unitary.

(2)  $\implies$  (1) Since  $P$  is a unitary quantum function, we have

$$\begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \end{array} \stackrel{(3.1)}{=} \begin{array}{c} | \\ | \end{array} \stackrel{(\text{unitary})}{=} \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \\ P^\dagger \\ \circlearrowleft \\ \circlearrowright \end{array}.$$

By postcomposing  $P^\dagger$  and taking the adjoint, we obtain (3.2):

$$\begin{array}{c} | \\ | \end{array} = \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \end{array}.$$

Next, we show the comultiplication preserving condition in (3.2). Considering the composition of  $P$  and the adjoint of (3.2), we have

$$\begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \\ P^\dagger \\ \circlearrowleft \\ \circlearrowright \end{array} \stackrel{(3.1)}{=} \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \\ P \\ \circlearrowleft \\ P^\dagger \\ \circlearrowright \end{array} \stackrel{(\text{unitary})}{=} \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \\ P^\dagger \\ \circlearrowleft \\ \circlearrowright \end{array} \stackrel{(\text{unitary})}{=} \begin{array}{c} | \\ | \end{array} \begin{array}{c} \circlearrowleft \\ \circlearrowright \end{array}.$$

By postcomposing  $P^\dagger$  and taking the adjoint again, we obtain (3.2):

$$\begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \\ P \\ \circlearrowleft \\ \circlearrowright \end{array} = \begin{array}{c} \circlearrowleft \\ P \\ \circlearrowright \end{array}.$$

Therefore  $(H, P)$  is a quantum bijection.  $\square$



**Definition 3.7** (Musto, Reutter, Verdon [30, Definition 5.11]). Let  $\mathcal{G} = (B, \psi, A)$  and  $\mathcal{G}' = (B', \psi', A')$  be quantum graphs. A *quantum* (resp. *classical*) *isomorphism*  $(H, P) : \mathcal{G}' \rightarrow \mathcal{G}$  is a quantum (resp. classical) bijection  $(H, P) : (B', \psi') \rightarrow (B, \psi)$  satisfying

Quantum graphs  $\mathcal{G}, \mathcal{G}'$  are said to be quantum (resp. classical) isomorphic if there is a nonzero quantum (resp. classical) isomorphism  $(H, P) : \mathcal{G}' \rightarrow \mathcal{G}$ .

**Remark 3.8.** Quantum isomorphism is denoted by  $\cong_q$ . Recall that we assume  $H$  to be finite-dimensional. If quantum graphs are quantum isomorphic via possibly infinite dimensional  $H$ , then they are said to be  *$C^*$ -algebraically quantum isomorphic* ( $\cong_{C^*}$ ) in Brannan et al. [8, Definition 4.4]. The authors of [8] also defined *quantum commuting isomorphism* ( $\cong_{qc}$ ), and *algebraic quantum isomorphism* ( $\cong_{A^*}$ ) for quantum graphs,  $\cong_q, \cong_{qc} \Rightarrow \cong_{C^*} \Leftrightarrow \cong_{A^*}$  ([8, Corollary 4.8]).

Since quantum bijections are unitary, finiteness of  $|H|$  implies  $|B| = |B'|$  for  $(B, \psi, A) \cong_q (B', \psi', A')$ . It is shown in [8, Example 4.13] that there are  $C^*$ -quantum isomorphic quantum graphs with distinct dimensions, hence our  $\cong_q$  is strictly stronger than  $\cong_{C^*}$ .

**Definition 3.9.** Given quantum graphs  $\mathcal{G}, \mathcal{G}'$ , the category  $\text{QIso}(\mathcal{G}', \mathcal{G})$  of quantum isomorphisms is a category that consists of

- **Objects:** quantum isomorphisms  $(H, P) : \mathcal{G}' \rightarrow \mathcal{G}$ ;
- **Morphisms:** intertwiners  $f : (H, P) \rightarrow (H', P')$ .

We denote  $\text{QIso}(\mathcal{G}, \mathcal{G})$  by  $\text{QAut}(\mathcal{G})$ .

**Remark 3.10.** Since tensoring with zero annihilates everything, any couple of quantum graphs have a trivial quantum isomorphism  $0 = (H = 0, P = 0)$ .

**Remark 3.11.** Let  $\mathcal{G} = (B, \psi, A), \mathcal{G}' = (B', \psi', A')$  be quantum graphs, and  $\{e_i\}_{i=1}^m, \{e'_k\}_{k=1}^n$  be ONB's for  $L^2(B, \psi), L^2(B', \psi')$  with  $|B| = m, |B'| = n$ . Note that a quantum isomorphism  $(H, P) : \mathcal{G}' \rightarrow \mathcal{G}$  can be described by operators  $P_i^k \in B(H)$  as follows:

Then  $\tilde{P} : B \rightarrow B' \otimes B(H)$  as in Remark 3.3 is explicitly described as  $\tilde{P}e_i = \sum_k e'_k \otimes P_i^k$ . In this setting  $\tilde{P}$  is a unital  $*$ -homomorphism since  $P$

is a quantum function, and the matrix  $(P_i^k)_{k,i} \in M_{n,m}(B(H))$  is unitary since  $P$  is a quantum bijection (hence unitary by Lemma 3.6), and  $\tilde{P}A = (A' \otimes \text{id}_{B(H)})\tilde{P}$  since  $P$  is a quantum isomorphism. Note that  $m, n$  need not be equal if we allow infinite-dimensional  $H$ . By considering universal such  $P_i^k$ 's, we reach the notion of the quantum automorphism group of a quantum graph as below and the bigalois extension between two quantum graphs introduced in [8, Definition 4.1], which we later use in section 4.

### 3.2 Quantum automorphism groups

**Definition 3.12** (Woronowicz [46, Definition 1.1], [47, Definition 1.1]). A *compact quantum group* (CQG) is a pair  $(\mathcal{A}, \Delta)$  of a separable unital  $C^*$ -algebra  $\mathcal{A}$  and a  $*$ -homomorphism  $\Delta : \mathcal{A} \rightarrow \mathcal{A} \otimes \mathcal{A}$ , so-called comultiplication, satisfying

**(coassociativity)**  $(\Delta \otimes \text{id}_{\mathcal{A}})\Delta = (\text{id}_{\mathcal{A}} \otimes \Delta)\Delta$ ;

**(cancellation property)**  $(\mathcal{A} \otimes 1)\Delta(\mathcal{A})$  and  $(1 \otimes \mathcal{A})\Delta(\mathcal{A})$  are dense in  $\mathcal{A} \otimes \mathcal{A}$ .

The quantum symmetry group  $A_{\text{aut}}(B)$  of a finite quantum space  $B$  was introduced by Wang [41]. The quantum automorphism group of a quantum graph is a quantum subgroup (quotient algebra) of such a quantum symmetry group of the base space.

**Definition 3.13** (Brannan et al. [8, Definition 3.7]). Let  $\mathcal{G} = (B, \psi, A)$  be a quantum graph and fix an ONB  $\{e_i\}_i$  for  $L^2(B, \psi)$ . The quantum automorphism group of  $\mathcal{G}$  is a CQG  $\text{Qut}(\mathcal{G}) = (A_{\text{aut}}(\mathcal{G}), \Delta)$  defined as follows:

- The group algebra  $A_{\text{aut}}(\mathcal{G})$  is the universal unital  $C^*$ -algebra generated by the coefficients  $u_i^k$  of a unitary  $u = (u_i^k)_{k,i} \in M_n(A_{\text{aut}}(\mathcal{G}))$  that makes the operator

$$\rho : B \ni e_i \mapsto \sum_k e_k \otimes u_i^k \in B \otimes A_{\text{aut}}(\mathcal{G})$$

a unital  $*$ -homomorphism satisfying  $\rho A = (A \otimes \text{id})\rho$ . This  $\rho$  and  $u$  are called the fundamental representation;

- The comultiplication  $\Delta : A_{\text{aut}}(\mathcal{G}) \rightarrow A_{\text{aut}}(\mathcal{G}) \otimes A_{\text{aut}}(\mathcal{G})$  is defined as a  $*$ -homomorphism satisfying

$$\Delta u_i^k = \sum_j u_j^k \otimes u_i^j.$$

We denote the universal  $*$ -algebra generated by  $u_i^k$  as above by  $\mathcal{O}(\text{Qut}(\mathcal{G})) \subset A_{\text{aut}}(\mathcal{G})$ . We have additional operators associated to  $A_{\text{aut}}(\mathcal{G})$ , a counit  $\epsilon$  and

antipode  $S$  defined as a  $*$ -homomorphism  $\epsilon : A_{aut}(\mathcal{G}) \rightarrow \mathbb{C}$  and a homomorphism  $S : \mathcal{O}(\text{Qut}(\mathcal{G})) \rightarrow \mathcal{O}(\text{Qut}(\mathcal{G}))^{op}$  satisfying

$$\epsilon u_i^k = \delta_{ik}; \quad S u_i^k = u_k^{i*}.$$

Then  $(\mathcal{O}(\text{Qut}(\mathcal{G})), \Delta, \epsilon, S)$  satisfy

$$\begin{aligned} (\Delta \otimes \text{id})\Delta &= (\text{id} \otimes \Delta)\Delta; \\ (\epsilon \otimes \text{id})\Delta &= \text{id} = (\text{id} \otimes \epsilon)\Delta; \\ m(\epsilon \otimes \text{id})\Delta &= \epsilon(\cdot)1 = m(\text{id} \otimes \epsilon)\Delta. \end{aligned}$$

Such a quadruple  $(\mathcal{O}(\text{Qut}(\mathcal{G})), \Delta, \epsilon, S)$  is called a Hopf  $*$ -algebra.

**Remark 3.14.** Note that  $\rho A = (A \otimes \text{id})\rho$  is equivalent to  $uA = Au$ .

The *quantum symmetric group*  $\text{Qut}(B, \psi)$  of a quantum set  $(B, \psi)$  is defined in the same way without the assumption  $\rho A = (A \otimes \text{id})\rho$ . It follows that  $C(\text{Qut}(B, \psi, A)) = C(\text{Qut}(B, \psi)) / \langle uA = Au \rangle$  for a quantum graph  $(B, \psi, A)$ , where we denote by  $\mathcal{A} / \langle \mathcal{R} \rangle$  the quotient of a  $C^*$ -algebra  $\mathcal{A}$  by the self-adjoint closed ideal generated by the relations  $\mathcal{R}$ .

**Lemma 3.15.** *The quantum automorphism groups of the quantum set  $(B, \psi)$ , the trivial graph  $(B, \psi, \text{id})$ , and the complete graph  $(B, \psi, \delta^2\psi(\cdot)1)$  are the same:  $\text{Qut}(B, \psi) = \text{Qut}(B, \psi, \text{id}_B) = \text{Qut}(B, \psi, \delta^2\psi(\cdot)1)$ .*

*Proof.* It suffices to show  $uA = Au$  for  $A = \text{id}, \delta^2\psi(\cdot)1$  from other assumptions on  $\text{Qut}(B, \psi)$ . For  $A = \text{id}$ ,  $uid = idu$  is trivial. For  $A = \delta^2\psi(\cdot)1$ , consider a faithful representation  $C(\text{Qut}(B, \psi)) \subset B(H)$  and  $P = \sum_{i,k} |e_k\rangle u_i^k \langle e_i| : B \otimes H \rightarrow H \otimes B$  as in Remark 3.11. By definition of  $u$ ,  $P$  is a (possibly infinite-dimensional) unitary quantum function, hence a quantum bijection by Lemma 3.6, whose proof does not need the finiteness of  $|H|$ . Thus (3.1) and (3.2) shows

i.e.,  $uA = Au$  in  $M_n(C(\text{Qut}(B, \psi)))$ .  $\square$

**Example 3.16.** • Wang's *quantum symmetry group*  $A_{aut}(B)$  [41] is the quantum automorphism group of the tracial quantum set  $(B, \psi)$ .

- In particular, the *quantum symmetric group*  $S_N^+ = (C(S_N^+), \Delta)$  is the quantum automorphism group of the trivial and complete classical graphs on  $N$  vertices. Its generators form the universal *magic unitary*  $u = (u_i^k)$ , i.e., a unitary matrix with entries of projections that are mutually orthogonal and sum up to 1 on each row and column.

- The *hyperoctahedral quantum group*  $H_N^+$  [6] is the quantum automorphism group of the  $N$ -dimensional hyperoctahedron (and the  $N$  segments of axes as its complement), whose algebra  $C(H_N^+)$  is generated by the universal coefficients of a magic unitary

$$u = \begin{pmatrix} p_{11} & q_{11} & \cdots & p_{1N} & q_{1N} \\ q_{11} & p_{11} & \cdots & q_{1N} & p_{1N} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ p_{N1} & q_{N1} & \cdots & p_{NN} & q_{NN} \\ q_{N1} & p_{N1} & \cdots & q_{NN} & p_{NN} \end{pmatrix}.$$

The authors of [30] investigated the relationship between the category  $\text{QAut}(\mathcal{G})$  and the quantum automorphism group  $\text{Qut}(\mathcal{G})$  for classical graphs, but they did not introduce the quantum automorphism group of quantum graphs. Here we show the straightforward generalization of the following theorem.

**Theorem 3.17** (Musto, Reutter, Verdon, [30, Proposition 5.19]). *If  $\mathcal{G}$  is a classical graph on  $(\mathbb{C}^n, \tau)$ , then we have an isomorphism of categories*

$$\text{Rep}_{\text{fin}}(A_{\text{aut}}(\mathcal{G})) \cong \text{QAut}(\mathcal{G})$$

where  $\text{Rep}_{\text{fin}}(A_{\text{aut}}(\mathcal{G}))$  is the category of finite dimensional  $*$ -representations of the  $C^*$ -algebra  $A_{\text{aut}}(\mathcal{G})$ , and  $\text{QAut}(\mathcal{G})$  is the category of quantum automorphisms on  $\mathcal{G}$ .

**Theorem 3.18.** *If  $\mathcal{G}$  is a quantum graph on  $(B, \psi)$ , then we have an isomorphism of categories*

$$\text{Rep}_{\text{fin}}(A_{\text{aut}}(\mathcal{G})) \cong \text{QAut}(\mathcal{G})$$

where  $\text{Rep}_{\text{fin}}(A_{\text{aut}}(\mathcal{G}))$  is the category of finite dimensional  $*$ -representations of the  $C^*$ -algebra  $A_{\text{aut}}(\mathcal{G})$ , and  $\text{QAut}(\mathcal{G})$  is the category of quantum automorphisms on  $\mathcal{G}$ .

*Proof.* As is explained in Remark 3.11, the CQG algebra  $A_{\text{aut}}(\mathcal{G})$  is generated by the universal coefficients of a unitary  $u = (u_i^k)$  that satisfies exactly the same relation as the unitary  $P = (P_i^k)$  of a quantum automorphism  $(H, P)$  on  $\mathcal{G} = (B, \psi, A)$ . Therefore given a quantum isomorphism  $(H, P)$  in  $\text{QAut}(\mathcal{G})$ , the universality of  $A_{\text{aut}}(\mathcal{G})$  shows the existence of a  $*$ -representation  $\pi_P : A_{\text{aut}}(\mathcal{G}) \ni u_i^k \mapsto P_i^k \in B(H)$ . Conversely a  $*$ -representation  $\pi : A_{\text{aut}}(\mathcal{G}) \rightarrow B(H)$  defines operators  $P_i^k = \pi(u_i^k)$ , which induces a quantum automorphism  $P_\pi = \sum_j |e_k\rangle P_i^k \langle e_i|$ . By construction, it is trivial that  $P_{\pi_P} = P$  and  $\pi_{P_\pi} = \pi$ . For quantum automorphisms  $(H, P), (H', P')$ , an operator  $f : H \rightarrow H'$  is an intertwiner  $(H, P) \rightarrow (H', P')$  in  $\text{QAut}(\mathcal{G}) \iff (f \otimes \text{id}_B)P = P'(\text{id}_B \otimes f) \iff$

$f\pi(u_i^k) = fP_i^k = P_i^k f = \pi'(u_i^k)f \ (\forall i, k) \iff f\pi(\cdot) = \pi'(\cdot)f \iff f$  is an intertwiner  $\pi \rightarrow \pi'$  in  $\text{Rep}_{\text{fin}}(A_{\text{aut}}(\mathcal{G}))$ . Therefore the intertwiners also coincide.  $\square$

Since finiteness of  $|H|$  is not used in the proof of Theorem 3.18, if we allow ‘ $\text{QAut}(\mathcal{G})$ ’ to include infinite dimensional quantum isomorphisms as in Remark 3.11, then  $\text{Rep}(A_{\text{aut}}(\mathcal{G})) \cong \text{‘QAut}(\mathcal{G})\text{’}$  is obtained.

## 4 Quantum graphs on $M_2$

### 4.1 Tracial quantum graphs

Let  $(B = \bigoplus_s M_{n_s}, \tau)$  be a quantum set with the unique tracial  $\sqrt{|B|}$ -form  $\tau = \frac{1}{|B|} \bigoplus_s n_s \text{Tr}_s$ . We always assume that *quantum graphs* are undirected in this chapter.

Let  $A = (A_{ij,s}^{kl,r})_{i,j \leq n_s, s}^{k,l \leq n_r, r}$  be a reflexive quantum graph on  $(B, \tau)$  parametrized as

$$A_{ij,s}^{kl,r} = \langle \widetilde{e}_{kl,r} | A \widetilde{e}_{ij,s} \rangle, \text{ i.e., } A = \sum_{ijsklr} |\widetilde{e}_{kl,r}\rangle A_{ij,s}^{kl,r} \langle \widetilde{e}_{ij,s}|$$

where  $\left\{ \widetilde{e}_{ij,s} = \sqrt{\frac{|B|}{n_s}} e_{ij,s} \right\}$  is an ONB for  $L^2(B, \tau)$ . Thus  $A$  is a self-adjoint  $(\overline{A_{ij,s}^{kl,r}} = A_{kl,r}^{ij,s})$  operator satisfying the following:

$$\text{Schur idempotent} \iff \frac{1}{\sqrt{n_s n_r}} \sum_{u,v} A_{iu,s}^{kv,r} A_{uj,s}^{vl,r} = A_{ij,s}^{kl,r};$$

$$\text{reflexive} \iff \frac{1}{n_s} \sum_u A_{iu,s}^{ku,s} = \delta_{ik};$$

$$\text{undirected (self-transposed)} \iff A_{ij,s}^{kl,r} = A_{lk,r}^{ji,s},$$

where the RHS of these equivalences are quantified by  $\forall i, j, s, k, l, r$ .

Note that these relations are independent for different pairs  $(r, s)$  and  $(r', s')$ .

### 4.2 Tracial quantum graphs on $M_2$

Let  $A = (A_{ij}^{kl})_{i,j=1,2}^{k,l=1,2}$  be a quantum adjacency matrix on  $(M_2, \text{Tr}/2)$  with respect to the orthonormal basis  $\{\widetilde{e}_{ij} = \sqrt{2}e_{ij}\}$ . Then

$$\frac{1}{2} \left( A_{i1}^{k1} A_{1j}^{l1} + A_{i1}^{k2} A_{1j}^{l2} + A_{i2}^{k1} A_{2j}^{l1} + A_{i2}^{k2} A_{2j}^{l2} \right) = A_{ij}^{kl} \quad \forall i, j, k, l = 1, 2; \quad (4.1)$$

$$\frac{1}{2} \left( A_{i1}^{k1} + A_{i2}^{k2} \right) = \delta_{ik} \quad \forall i, k = 1, 2; \quad (4.2)$$

$$\overline{A_{kl}^{ij}} = A_{ij}^{kl} = A_{lk}^{ji} \quad \forall i, j, k, l = 1, 2. \quad (4.3)$$

By the latter two conditions (4.2)(4.3),  $A$  is of the following form where  $x, p \in \mathbb{R}$  and  $y, z \in \mathbb{C}$ :

$$\begin{pmatrix} A_{11}^{11} & A_{11}^{12} & A_{21}^{11} & A_{21}^{12} \\ A_{11}^{12} & A_{11}^{22} & A_{21}^{12} & A_{21}^{22} \\ A_{12}^{11} & A_{12}^{21} & A_{22}^{11} & A_{22}^{21} \\ A_{12}^{21} & A_{12}^{22} & A_{22}^{21} & A_{22}^{22} \end{pmatrix} = \begin{pmatrix} p & \bar{y} & y & x \\ y & 2-p & z & -y \\ \bar{y} & \bar{z} & 2-p & -\bar{y} \\ x & -\bar{y} & -y & p \end{pmatrix}$$

Regularity  $A1 = d1$  holds for some  $d \in \mathbb{R}$  if and only if

$$\begin{aligned} d1 &= A(e_{11} + e_{22}) \\ &= (A_{11}^{11} + A_{22}^{11})e_{11} + (A_{11}^{12} + A_{22}^{12})e_{12} + (A_{11}^{21} + A_{22}^{21})e_{21} + (A_{11}^{22} + A_{22}^{22})e_{22} \\ &= (p+x)e_{11} + (\bar{y}-\bar{y})e_{12} + (y-y)e_{21} + (x+p)e_{22} = (p+x)1, \end{aligned}$$

i.e., this is automatically  $p+x = d$ -regular.

If  $y = 0$ , then we have  $\text{spec}(A) = \{p \pm x, 2 - p \pm |z|\}$ .

**Theorem 4.1.** *A reflexive quantum graph  $A$  on  $(M_2, \tau)$  is classically (and quantum) isomorphic to exactly one of the following  $d$ -regular quantum graphs.*

$$d = 1) \text{ Trivial graph } A_1 = \text{id}_B = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{pmatrix}, \text{spec}(A_1) = \{1, 1, 1, 1\}.$$

$$d = 2) A_2 = \begin{pmatrix} 2 & & & \\ & 0 & & \\ & & 0 & \\ & & & 2 \end{pmatrix}, \text{spec}(A_2) = \{2, 2, 0, 0\}.$$

$$d = 3) A_3 = \begin{pmatrix} 1 & & 2 \\ & 1 & \\ & & 1 \\ 2 & & & 1 \end{pmatrix}, \text{spec}(A_3) = \{3, 1, 1, -1\}.$$

$$d = 4) \text{ Complete graph } A_4 = 4\tau(\cdot)1 = \begin{pmatrix} 2 & & & 2 \\ & 0 & & \\ & & 0 & \\ 2 & & & 2 \end{pmatrix}, \text{spec}(A_4) = \{4, 0, 0, 0\}.$$

*Proof.* By Schur idempotence (4.1), we get the following equations:

$$2p = p^2 + |y|^2 + (2-p)^2 + |y|^2 \quad (4.4)$$

$$2(2-p) = p(2-p) - |y|^2 + p(2-p) - |y|^2 \iff (p-1)(2-p) = |y|^2 \quad (4.5)$$

$$2x = |y|^2 + x^2 + |y|^2 + |z|^2 \quad (4.6)$$

$$2z = y^2 + xz + y^2 + zx \iff (1-x)z = y^2 \quad (4.7)$$

$$2y = py + yx - y(2-p) + \bar{y}z \quad (4.8)$$

By (4.5) and (4.7), we get  $p \in [1, 2]$  and  $(p-1)(2-p) = |y|^2 = |1-x||z|$ . Hence

$$(4.4) \iff (p-1+2-p)^2 = 1^2 = 1 \quad (\text{automatic})$$

$$(4.6) \iff (|1-x| + |z|)^2 = 1 \iff |1-x| + |z| = 1$$

[0] If  $y = 0$ , (4.8) is automatic, (4.5)  $\iff p = 1$  or  $2$ , and (4.7)  $\iff (1-x)z = 0$ .

- If  $x = 1$ , then  $|z| = 1$  by (4.6).
- If  $z = 0$ , then  $|1 - x| = 1$  by (4.6), hence  $x = 0, 2$

Therefore we have the solutions in Table I, where  $\mathbb{T} = \{z \in \mathbb{C} \mid |z| = 1\}$ .

Table I: Solutions  $p, x, z$  for  $y = 0$  with the degree  $d$  and the spectrum of  $A$

$p$	$x$	$z$	$d = p + x$	$\text{Spec}(A) = \{p \pm x, 2 - p \pm  z \}$
1	0	0	1	$\{1, 1, 1, 1\}$
1	1	$\mathbb{T}$	2	$\{2, 0, 2, 0\}$
1	2	0	3	$\{3, -1, 1, 1\}$
2	0	0	2	$\{2, 2, 0, 0\}$
2	1	$\mathbb{T}$	3	$\{3, 1, 1, -1\}$
2	2	0	4	$\{4, 0, 0, 0\}$

[1] If  $y \neq 0$ , (4.7) implies  $z \neq 0$  and hence

$$\begin{aligned}
(4.8) \quad &\iff (x - 2(2 - p))y + \bar{y}z = 0 \stackrel{y \neq 0}{\iff} (x - 2(2 - p))y^2 + |y|^2z = 0 \\
&\iff ((x - 2(2 - p))(1 - x) + (p - 1)(2 - p))z = 0 \\
&\iff (x - (3 - p))(x - (2 - p)) = 0 \iff x = 3 - p \text{ or } 2 - p \quad (4.9)
\end{aligned}$$

By (4.5), we may put  $y = \theta\sqrt{(p - 1)(2 - p)}$  for some  $\theta \in \mathbb{T}$ . Then (4.7) implies

$$z = \frac{y^2}{1 - x} = \theta^2 \frac{(p - 1)(2 - p)}{1 - x}.$$

If  $x = 2 - p$  in (4.9), then  $d = p + x = 2$  and

$$z = \theta^2 \frac{(p - 1)(2 - p)}{p - 1} = \theta^2(2 - p) = \theta^2(4 - d - p),$$

which satisfies (4.6):  $|1 - x| + |z| = (p - 1) + (2 - p) = 1$ , hence all conditions are satisfied.

If  $x = 3 - p$  in (4.9), then  $d = p + x = 3$  and

$$z = \theta^2 \frac{(p - 1)(2 - p)}{p - 2} = \theta^2(1 - p) = \theta^2(4 - d - p),$$

which satisfies (4.6):  $|1 - x| + |z| = (2 - p) + (p - 1) = 1$ , hence all conditions are satisfied.

Therefore we obtain two families of quantum graphs for each  $d = 2, 3$



parametrized by  $(p, \theta) \in (1, 2) \times \mathbb{T}$  under  $|y| = \sqrt{(p-1)(2-p)} \neq 0$ :

$$d=2) \quad A_{p,\theta}^{(2)} = \begin{pmatrix} p & \bar{\theta}|y| & \theta|y| & 2-p \\ \theta|y| & 2-p & \theta^2(2-p) & -\theta|y| \\ \bar{\theta}|y| & \bar{\theta}^2(2-p) & 2-p & -\bar{\theta}|y| \\ 2-p & -\bar{\theta}|y| & -\theta|y| & p \end{pmatrix}$$

$$d=3) \quad A_{p,\theta}^{(3)} = \begin{pmatrix} p & \bar{\theta}|y| & \theta|y| & 3-p \\ \theta|y| & 2-p & \theta^2(1-p) & -\theta|y| \\ \bar{\theta}|y| & \bar{\theta}^2(1-p) & 2-p & -\bar{\theta}|y| \\ 3-p & -\bar{\theta}|y| & -\theta|y| & p \end{pmatrix}$$

If we take the limits  $p \rightarrow 1$  or  $2$ , these graphs converges to  $y = 0$  cases above. Hence we may include them as  $p \in [1, 2]$ .

Those graphs  $\{A_{p,\theta}^{(d)} \mid \theta \in \mathbb{T}\}$  arising from the sign  $\theta$  are mutually isomorphic via inner automorphism of  $M_2$  by  $u_\theta = \begin{pmatrix} 1 & 0 \\ 0 & \theta \end{pmatrix}$ :

**Lemma 4.2.** *It follows that*

$$A_{p,\theta}^{(d)} = \text{ad}(u_\theta^*) A_{p,1}^{(d)} \text{ad}(u_\theta). \quad (4.10)$$

Moreover those graphs  $\{A_{p,1}^{(d)} \mid p \in [1, 2]\}$  are also mutually isomorphic via inner automorphism of  $M_2$  by  $v_p = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1+\sqrt{2-p}} & \sqrt{1-\sqrt{2-p}} \\ -\sqrt{1-\sqrt{2-p}} & \sqrt{1+\sqrt{2-p}} \end{pmatrix}$ :

**Lemma 4.3.** *It follows that*

$$\text{ad}(v_p^*) A_{p,1}^{(3)} \text{ad}(v_p) = A_{1,1}^{(3)} \quad \text{and} \quad \text{ad}(v_p) A_{3-p,1}^{(2)} \text{ad}(v_p^*) = A_{2,1}^{(2)}. \quad (4.11)$$

Therefore up to inner automorphism, there is a unique reflexive quantum graph on  $M_2$  for every degree  $d \in \{1, 2, 3, 4\}$ . Since an inner automorphism is a classical isomorphism (1-dimensional quantum isomorphism) and  $\text{spec}(A)$  is invariant under quantum isomorphism, the complete system of representatives for the classical and quantum isomorphism classes of quantum graphs on  $M_2$  is given by the following.

$p$	$x$	$z = y$	$d = p + x$	$\text{spec}(A) = \{p \pm x, 2 - p \pm  z \}$
1	0	0	1	$\{1, 1, 1, 1\}$
2	0	0	2	$\{2, 2, 0, 0\}$
1	2	0	3	$\{3, -1, 1, 1\}$
2	2	0	4	$\{4, 0, 0, 0\}$

Recall that  $A$  above are of the form

$$A = \begin{pmatrix} p & \bar{y} & y & x \\ y & 2-p & z & -y \\ \bar{y} & \bar{z} & 2-p & -\bar{y} \\ x & -\bar{y} & -y & p \end{pmatrix} = \begin{pmatrix} p & 0 & 0 & x \\ 0 & 2-p & 0 & 0 \\ 0 & 0 & 2-p & 0 \\ x & 0 & 0 & p \end{pmatrix},$$

therefore the table indicates the quantum graphs in the statement.  $\square$

Therefore reflexive quantum graph on  $M_2$  can be  $d$ -regular for  $d \in \{1, 2, 3, 4\}$ . Hence irreflexive quantum graph on  $M_2$  can be  $d$ -regular for  $d \in \{0, 1, 2, 3\}$ .

In the rest of this section, we prove the lemmas in the proof above.

*Proof of Lemma 4.2.* The adjoint action  $\text{ad}(u_\theta) \begin{pmatrix} a & b \\ c & d \end{pmatrix} = u_\theta \begin{pmatrix} a & b \\ c & d \end{pmatrix} u_\theta^* = \begin{pmatrix} a & \bar{\theta}b \\ \theta c & d \end{pmatrix}$  has a diagonal unitary matrix expression

$$\text{ad}(u_\theta) = \begin{pmatrix} 1 & & 0 \\ & \bar{\theta} & \\ 0 & & \theta \\ & & & 1 \end{pmatrix}$$

with respect to the ONB  $(\widetilde{e}_{11}, \widetilde{e}_{12}, \widetilde{e}_{21}, \widetilde{e}_{22})$ . Hence

$$\text{ad}(u_\theta^*)A \text{ad}(u_\theta) = \begin{pmatrix} 1 & & 0 \\ & \theta & \\ 0 & & \bar{\theta} \\ & & & 1 \end{pmatrix} A \begin{pmatrix} 1 & & 0 \\ & \bar{\theta} & \\ 0 & & \theta \\ & & & 1 \end{pmatrix}$$

is the entrywise product of  $A$  and

$$\begin{pmatrix} 1 & \bar{\theta} & \theta & 1 \\ \theta & 1 & \theta^2 & \theta \\ \bar{\theta} & \bar{\theta}^2 & 1 & \bar{\theta} \\ 1 & \bar{\theta} & \theta & 1 \end{pmatrix}.$$

Therefore we have  $A_{p,\theta}^{(d)} = \text{ad}(u_\theta^*)A_{p,1}^{(d)} \text{ad}(u_\theta)$ .  $\square$

*Proof of Lemma 4.3.* The operator  $\text{ad}(v_p)$  has a unitary matrix expression

$$\text{ad}(v_p) = \frac{1}{2} \begin{pmatrix} 1 + \sqrt{2-p} & \sqrt{p-1} & \sqrt{p-1} & 1 - \sqrt{2-p} \\ -\sqrt{p-1} & 1 + \sqrt{2-p} & -(1 - \sqrt{2-p}) & \sqrt{p-1} \\ -\sqrt{p-1} & -(1 - \sqrt{2-p}) & 1 + \sqrt{2-p} & \sqrt{p-1} \\ 1 - \sqrt{2-p} & -\sqrt{p-1} & -\sqrt{p-1} & 1 + \sqrt{2-p} \end{pmatrix}$$

with respect to the ONB  $(\widetilde{e}_{11}, \widetilde{e}_{12}, \widetilde{e}_{21}, \widetilde{e}_{22})$ , and we can directly compute (4.11).

Abstractly  $v_p$  is a unitary matrix such that  $\text{ad}(v_p)$  maps the eigenvector  $\begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$  for the eigenvalue  $-1$  of  $A_{1,1}^{(3)}$  to the eigenvector  $\begin{pmatrix} -\sqrt{2-p} & \sqrt{p-1} \\ \sqrt{p-1} & \sqrt{2-p} \end{pmatrix}$  for the eigenvalue  $-1$  of  $A_{p,1}^{(3)}$ . Since  $\text{spec}(A_{p,1}^{(3)}) = \{3, 1, 1, -1\}$  and  $\text{ad}(v_p)$

also preserves the eigenvector  $1_{M_2}$  for the eigenvalue 3, the orthogonality of eigenspaces implies

$$\text{ad}(v_p^*)A_{p,1}^{(3)}\text{ad}(v_p) = A_{1,1}^{(3)}. \quad (4.12)$$

By the correspondence between a quantum graph  $A$  and its reflexive complement as in Proposition 2.33

$$A^c := \text{id}_B + |B|\tau(\cdot)1_B - A,$$

we do not need the latter equality in (4.11) for the proof of Theorem 4.1 because the complement preserves isomorphism classes of quantum graphs, and the graphs of degree 2 and 3 are mutual complements. But here we show (4.11) explicitly. In this case

$$\begin{aligned} (A_{p,\theta}^{(d)})^c &= \text{id} + 4\tau(\cdot)1 - A_{p,\theta}^{(d)} \\ &= \begin{pmatrix} 1 & & 0 \\ & 1 & \\ 0 & & 1 \end{pmatrix} + \begin{pmatrix} 2 & & 2 \\ & 0 & \\ 2 & & 2 \end{pmatrix} - \begin{pmatrix} p & \bar{\theta}|y| & \theta|y| & d-p \\ \theta|y| & 2-p & \theta^2(4-d-p) & -\theta|y| \\ \bar{\theta}|y| & \bar{\theta}^2(4-d-p) & 2-p & -\bar{\theta}|y| \\ d-p & -\bar{\theta}|y| & -\theta|y| & p \end{pmatrix} \\ &= \begin{pmatrix} 3-p & -\bar{\theta}|y| & -\theta|y| & 2-d+p \\ -\theta|y| & p-1 & -\theta^2(4-d-p) & \theta|y| \\ -\bar{\theta}|y| & -\bar{\theta}^2(4-d-p) & p-1 & \bar{\theta}|y| \\ 2-d+p & \bar{\theta}|y| & \theta|y| & 3-p \end{pmatrix} \\ &= A_{3-p,-\theta}^{(5-d)}, \end{aligned} \quad (4.13)$$

where the last equality follows from  $p-1 = 2 - (3-p)$ ,  $2-d+p = (5-d) - (3-p)$ , and  $-(4-d-p) = 4 - (5-d) - (3-p)$ . Note that the complement and the conjugation by  $\text{ad}(u)$  for unitary  $u \in B$  commute as

$$\begin{aligned} \text{ad}(u^*)A^c\text{ad}(u) &= \text{ad}(u^*)\text{ad}(u) + |B|\tau(u \cdot u^*)u^*1u - \text{ad}(u^*)A\text{ad}(u) \\ &= \text{id} + |B|\tau(\cdot)1 - \text{ad}(u^*)A\text{ad}(u) \\ &= (\text{ad}(u^*)A\text{ad}(u))^c, \end{aligned} \quad (4.14)$$

thereby

$$\begin{aligned} \text{ad}(v_p)A_{3-p,1}^{(2)}\text{ad}(v_p^*) &\stackrel{(4.13)}{=} \text{ad}(v_p)\left(A_{p,-1}^{(3)}\right)^c\text{ad}(v_p^*) \\ &\stackrel{(4.14)}{=} \left(\text{ad}(v_p)A_{p,-1}^{(3)}\text{ad}(v_p^*)\right)^c \\ &\stackrel{(4.10)}{=} \left(\text{ad}(v_p u_{-1}^*)A_{p,1}^{(3)}\text{ad}(u_{-1}v_p^*)\right)^c \end{aligned}$$

$$\begin{aligned}
\text{and since } u_{-1}v_p^* &= \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{1+\sqrt{2-p}} & -\sqrt{1-\sqrt{2-p}} \\ -\sqrt{1-\sqrt{2-p}} & -\sqrt{1+\sqrt{2-p}} \end{pmatrix} = v_p u_{-1}, \\
&= \left( \text{ad}(u_{-1}^* v_p^*) A_{p,1}^{(3)} \text{ad}(v_p u_{-1}) \right)^c \\
&\stackrel{(4.12)}{=} \left( \text{ad}(u_{-1}^*) A_{1,1}^{(3)} \text{ad}(u_{-1}) \right)^c \\
&\stackrel{(4.10)}{=} \left( A_{1,-1}^{(3)} \right)^c \stackrel{(4.13)}{=} A_{2,1}^{(2)}.
\end{aligned}$$

□

### 4.3 Nontracial quantum graphs on $M_2$

By unitary diagonalization, a faithful state on  $M_2$  is a unitary conjugate of one of the Powers states  $\omega_q = \text{Tr}(Q \cdot)$  where  $q \in (0, 1]$  and  $Q = \frac{1}{1+q^2} \begin{pmatrix} 1 & 0 \\ 0 & q^2 \end{pmatrix}$ .

Note that  $\omega_1 = \tau_{M_2}$ , hence we may assume  $q \in (0, 1)$ .

**Lemma 4.4.** *The Powers state  $\omega_q$  is a  $\delta = q + q^{-1}$ -form on  $M_2$ . Hence  $(M_2, \omega_q)$  is a quantum set.*

*Proof.* It follows from Proposition 2.8 that

$$\delta^2 = \text{Tr}(Q^{-1}) = (1+q^2)(1+q^{-2}) = (q+q^{-1})^2.$$

□

Note that we have  $Q = \begin{pmatrix} q\delta & 0 \\ 0 & q^{-1}\delta \end{pmatrix}^{-1}$ .

Let  $e_{ij}$  be the  $(i, j)$  matrix unit in  $M_2$ . By Lemma 2.5,  $\{\widetilde{e}_{ij} := e_{ij} Q^{-1/2}\}_{ij}$  forms an ONB for  $L^2(M_2, \omega_q)$ . Explicitly these are

$$\begin{aligned}
\widetilde{e}_{11} &= \sqrt{1+q^2} e_{11} = \sqrt{q\delta} e_{11}; & \widetilde{e}_{12} &= \sqrt{1+q^{-2}} e_{12} = \sqrt{q^{-1}\delta} e_{12}; \\
\widetilde{e}_{21} &= \sqrt{1+q^2} e_{21} = \sqrt{q\delta} e_{21}; & \widetilde{e}_{22} &= \sqrt{1+q^{-2}} e_{22} = \sqrt{q^{-1}\delta} e_{22}.
\end{aligned}$$

Then we have

$$\begin{aligned}
1 &= (q\delta)^{-1/2} \widetilde{e}_{11} + (q^{-1}\delta)^{-1/2} \widetilde{e}_{22}; & m(\widetilde{e}_{ij} \otimes \widetilde{e}_{kl}) &= Q_{jk}^{-1/2} \widetilde{e}_{il}; \\
m^\dagger \widetilde{e}_{ij} &= (q\delta)^{1/2} \widetilde{e}_{i1} \otimes \widetilde{e}_{1j} + (q^{-1}\delta)^{1/2} \widetilde{e}_{i2} \otimes \widetilde{e}_{2j}; & \omega_q(\widetilde{e}_{ij}) &= Q_{ij}^{1/2}.
\end{aligned}$$

For a quantum graph  $(M_2, \omega_q, A)$ , we put  $A_{ij}^{kl} = \langle \widetilde{e}_{kl} | A \widetilde{e}_{ij} \rangle$  and

$$A = \begin{pmatrix} A_{11}^{11} & A_{11}^{12} & A_{21}^{11} & A_{22}^{11} \\ A_{11}^{12} & A_{11}^{22} & A_{21}^{12} & A_{22}^{12} \\ A_{11}^{21} & A_{11}^{22} & A_{21}^{21} & A_{22}^{21} \\ A_{11}^{22} & A_{11}^{22} & A_{21}^{22} & A_{22}^{22} \end{pmatrix}.$$

Rewriting the diagrammatic definitions as equations of the coefficients, this operator  $A$  is:

- a) self-adjoint if and only if  $A_{ij}^{kl} = \overline{A_{kl}^{ij}}$ .
- b) real if and only if  $A_{ij}^{kl} = \overline{A_{ji}^{lk}} Q_{ii}^{1/2} Q_{jj}^{-1/2} Q_{kk}^{-1/2} Q_{ll}^{1/2}$ .
- c) Schur idempotent if and only if  $\delta^2 A_{ij}^{kl} = \sum_{u,v} Q_{uu}^{-1/2} Q_{vv}^{-1/2} A_{iu}^{kv} A_{uj}^{vl}$   
 $= q\delta A_{i1}^{k1} A_{1j}^{l1} + \delta A_{i2}^{k1} A_{2j}^{l1} + \delta A_{i1}^{k2} A_{1j}^{l2} + q^{-1}\delta A_{i2}^{k2} A_{2j}^{l2}$ .
- d) reflexive if and only if  $\delta^2 \delta_i^k = \sum_u Q_{uu}^{-1} A_{iu}^{ku} = q\delta A_{i1}^{k1} + q^{-1}\delta A_{i2}^{k2}$ .

**Theorem 4.5.** *An undirected reflexive quantum graph  $(M_2, \omega_q, A)$  with  $q \in (0, 1), \delta = q + q^{-1}$  is exactly one of the following.*

- 1) The trivial quantum graph  $A_1 = \text{id}_B = \begin{pmatrix} 1 & & 0 \\ & 1 & \\ 0 & & 1 \end{pmatrix}$ , which is 1-regular

with  $\text{spec}(A) = \{1, 1, 1, 1\}$ .

- 2)  $A_2 = \begin{pmatrix} q^{-1}\delta & & \\ & 0 & \\ & & 0 \\ & & & q\delta \end{pmatrix}$ , which is irregular with  $\text{spec}(A) = \{q^{-1}\delta, q\delta, 0, 0\}$ .

- 3)  $A_3 = \begin{pmatrix} 1 & & \delta \\ & 1 & \\ \delta & & 1 \end{pmatrix}$ , which is irregular with  $\text{spec}(A) = \{1+\delta, 1, 1, 1-\delta\}$ .

- 4) The complete quantum graph  $A_4 = \delta^2 \omega_q(\cdot)1 = \begin{pmatrix} q^{-1}\delta & & \delta \\ & 0 & \\ \delta & & 0 \\ & & & q\delta \end{pmatrix}$ , which

is  $\delta^2$ -regular with  $\text{spec}(A) = \{\delta^2, 0, 0, 0\}$ .

*Proof.* By (a) and (b) we put

$$\begin{aligned} p &= A_{11}^{11} \stackrel{(a)}{=} \overline{A_{11}^{11}}; & t &= A_{12}^{12} \stackrel{(a)}{=} \overline{A_{12}^{12}} \stackrel{(b)}{=} A_{21}^{21}; \\ p' &= A_{22}^{22} \stackrel{(a)}{=} \overline{A_{22}^{22}}; & x &= A_{22}^{11} \stackrel{(b)}{=} \overline{A_{22}^{11}} \stackrel{(a)}{=} A_{11}^{22}; \\ y &= A_{12}^{11} \stackrel{(a)}{=} \overline{A_{11}^{12}} \stackrel{(b)}{=} q A_{11}^{21} \stackrel{(a)}{=} q \overline{A_{21}^{11}} \stackrel{(b)}{=} q^2 A_{12}^{11}; \\ y' &= A_{21}^{22} \stackrel{(a)}{=} \overline{A_{22}^{21}} \stackrel{(b)}{=} q^{-1} A_{22}^{12} \stackrel{(a)}{=} q^{-1} \overline{A_{12}^{22}} \stackrel{(b)}{=} q^{-2} A_{21}^{22}; \\ z &= A_{12}^{21} \stackrel{(a)}{=} \overline{A_{21}^{12}} \stackrel{(b)}{=} q^2 A_{12}^{21}. \end{aligned}$$

Then  $y = q^2y, y' = q^{-2}y', z = q^2z$  and  $0 < q < 1$  imply  $y = y' = z = 0$ . Thus

$$A = \begin{pmatrix} A_{11}^{11} & A_{12}^{11} & A_{21}^{11} & A_{22}^{11} \\ A_{11}^{12} & A_{12}^{12} & A_{21}^{12} & A_{22}^{12} \\ A_{11}^{21} & A_{12}^{21} & A_{21}^{21} & A_{22}^{21} \\ A_{11}^{22} & A_{12}^{22} & A_{21}^{22} & A_{22}^{22} \end{pmatrix} = \begin{pmatrix} p & 0 & 0 & x \\ 0 & t & 0 & 0 \\ 0 & 0 & t & 0 \\ x & 0 & 0 & p' \end{pmatrix}$$

where  $p, t, p', x \in \mathbb{R}$ . By (d):  $\delta\delta_i^k = qA_{i1}^{k1} + q^{-1}A_{i2}^{k2}$ , we have

$$\delta = qp + q^{-1}t; \quad \delta = qt + q^{-1}p'. \quad (4.15)$$

By  $(c_{ij}^{kl})$ :  $\delta A_{ij}^{kl} = qA_{i1}^{k1}A_{1j}^{l1} + A_{i2}^{k1}A_{2j}^{l1} + A_{i1}^{k2}A_{1j}^{l2} + q^{-1}A_{i2}^{k2}A_{2j}^{l2}$ , we obtain

$$\begin{array}{ll} (c_{11}^{11}) & \delta p = qp^2 + q^{-1}t^2 \\ (c_{12}^{12}) & \delta t = qpt + q^{-1}tp' \\ (c_{22}^{22}) & \delta p' = qt^2 + q^{-1}p'^2 \\ (c_{22}^{11}) & \delta x = x^2 \end{array}$$

Substituting (4.15) for  $t$  in  $(c_{11}^{11})$ ,

$$\begin{aligned} \delta p &= qp^2 + q(\delta - qp)^2 = q(p^2 + \delta^2 - 2q\delta p + q^2p^2) \\ \delta^2 - (q^{-1} + 2q)\delta p + (1 + q^2)p^2 &= 0. \end{aligned}$$

Since  $1 + q^2 = q\delta$ , division by  $\delta$  deduces

$$\delta - (\delta + q)p + qp^2 = (\delta - qp)(1 - p) = 0.$$

Thus (4.15) implies

$$(p, t, p') = (1, 1, 1), (q^{-1}\delta, 0, q\delta).$$

These solutions also satisfy  $(c_{12}^{12})$  and  $(c_{22}^{22})$ . Independently  $(c_{22}^{11})$  shows  $x = 0, \delta$ . Therefore undirected quantum graphs are the four graphs in the statement:

$$(p, t, p', x) = A_1(1, 1, 1, 0), A_2(q^{-1}\delta, 0, q\delta, 0), A_3(1, 1, 1, \delta), A_4(q^{-1}\delta, 0, q\delta, \delta).$$

Now  $A$  is  $d$ -regular if and only if  $(q\delta)^{1/2}1_{M_2} = q\widetilde{e}_{11} + \widetilde{e}_{22}$  is an eigenvector of eigenvalue  $d$  for  $A$ :

$$A \begin{pmatrix} q \\ 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} pq + x \\ 0 \\ 0 \\ xq + p' \end{pmatrix} = d \begin{pmatrix} q \\ 0 \\ 0 \\ 1 \end{pmatrix},$$

i.e.,  $d = p + q^{-1}x = xq + p'$ . Thus  $A_1$  is 1-regular,  $A_4$  is  $\delta^2$ -regular, and  $A_2, A_3$  are irregular.  $\square$

## 5 Quantum automorphism groups of quantum graphs on $M_2$

### 5.1 Quantum automorphism groups of tracial $(M_2, \tau, A)$

For each  $d = 1, 2, 3, 4$ , let  $\mathcal{G}_d = (M_2, \tau, A_d)$  be the  $d$ -regular quantum graph as in Theorem 4.1.

**Theorem 5.1.** *The quantum automorphism groups of the 1-regular (trivial) or 4-regular (complete) quantum graphs on  $(M_2, \tau)$  are the special orthogonal group  $SO(3)$ :*

$$\text{Qut}(\mathcal{G}_1) = \text{Qut}(\mathcal{G}_4) \cong SO(3).$$

*Proof.* By Lemma 3.15, we have  $\text{Qut}(\mathcal{G}_1) = \text{Qut}(\mathcal{G}_4) = \text{Qut}(M_2, \tau) = (A_{\text{aut}}(M_2), \Delta)$ . On the other hand Sołtan [37, Theorem 5.2] shows  $(A_{\text{aut}}(M_2), \Delta) \cong SO(3)$ . So we are done.  $\square$

In order to compute  $\text{Qut}(\mathcal{G}_2)$ , we take a closer look at Sołtan's description. Concretely [37, Theorem 5.2] shows

$$\begin{aligned} C(\text{Qut}(M_2, \tau)) &\cong C(SO(3)) \\ &= C^* \langle S, T, R \text{ normal, commuting} \mid ST = -R^2, |S| + |T| = 1 \rangle, \end{aligned}$$

where  $C^* \langle \mathcal{S} \mid \mathcal{R} \rangle$  denotes the universal  $C^*$ -algebra with generators  $\mathcal{S}$  satisfying the relations  $\mathcal{R}$ . This is the universal coefficient algebra with fundamental representation with respect to  $(\widetilde{e}_{11}, \widetilde{e}_{12}, \widetilde{e}_{21}, \widetilde{e}_{22})$ :

$$u = (u_{ij}^{kl}) = \begin{pmatrix} 1 - K & -R & -R^* & K \\ C & S & T^* & -C \\ C^* & T & S^* & -C^* \\ K & R & R^* & 1 - K \end{pmatrix}$$

where  $K = R^*R + T^*T$ ,  $C = SR^* - RT$ . The generators  $S, T, R$  are obtained as the coordinate functions for  $s, t, r$  of  $SO(3)$  subgroup of  $SU(3)$  as follows:

$$v^* SO(3)v = \left\{ \left( \begin{array}{ccc} s & \bar{t} & \sqrt{2}(r\bar{t} - s\bar{r}) \\ t & \bar{s} & \sqrt{2}(t\bar{r} - r\bar{s}) \\ \sqrt{2}r & \sqrt{2}\bar{r} & |s|^2 - |t|^2 \end{array} \right) \middle| \begin{array}{l} st = -r^2 \\ |s| + |t| = 1 \end{array} \right\} \subset SU(3)$$

where  $v = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ -i & i & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} \in U(3)$ . In other words, a choice of  $S, T, R$  in  $C(SO(3))$  is given by

$$S(x) = (v^* x v)_{11}, \quad T(x) = (v^* x v)_{21}, \quad R(x) = (v^* x v)_{31} / \sqrt{2}.$$

for  $x \in SO(3) = \{x \in M_3(\mathbb{R}) \mid x^T x = x x^T = I, \det x = 1\}$ .

**Theorem 5.2.** *The quantum automorphism groups of the 2-regular or 3-regular quantum graphs on  $(M_2, \tau)$  are the subgroup of  $SO(3)$  that is isomorphic to the orthogonal group  $O(2)$ :*

$$\text{Qut}(\mathcal{G}_2) = \text{Qut}(\mathcal{G}_3) \cong O(2)$$

*Proof.* Since  $\mathcal{G}_3 = \mathcal{G}_2^c$ , we have  $\text{Qut}(\mathcal{G}_2) = \text{Qut}(\mathcal{G}_3)$ . It suffices to compute  $C(SO(3)) / \langle A_2 u = u A_2 \rangle$ . Then  $A_2 u = u A_2$  implies

$$\begin{pmatrix} 1-K & -R & -R^* & K \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ K & R & R^* & 1-K \end{pmatrix} = \begin{pmatrix} 1-K & 0 & 0 & K \\ C & 0 & 0 & -C \\ C^* & 0 & 0 & -C^* \\ K & 0 & 0 & 1-K \end{pmatrix},$$

hence  $C = R = 0$ . Since  $C = SR^* - RT$ , the additional relation is  $R = 0$ . Then  $ST = -R^2 = 0$ , and  $|S| + |T| = 1$  implies  $|S| = 1$  or  $|T| = 1$ . Therefore it follows that

$$\begin{aligned} \text{Qut}(\mathcal{G}_2) &\cong \left\{ \begin{pmatrix} t & 0 & 0 \\ 0 & \bar{t} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & \bar{t} & 0 \\ t & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \middle| |t| = 1 \right\} \\ &\stackrel{(\text{ad } v)}{\cong} \left\{ \begin{pmatrix} x & 0 \\ 0 & \det x \end{pmatrix} \middle| x \in O(2) \right\} \cong O(2). \end{aligned}$$

where  $v$  is as above. □

## 5.2 Quantum automorphism groups of nontracial $(M_2, \omega_q, A)$

For each  $d = 1, 2, 3, 4$ , let  $\mathcal{G}_d$  be the quantum graph on  $(M_2, \omega_q)$  for  $q \in (0, 1)$  with adjacency operator  $A_d$  as in Theorem 4.5.

**Theorem 5.3.** *The quantum automorphism groups of the trivial and complete graphs  $\mathcal{G}_1, \mathcal{G}_4$  are the quantum special orthogonal group  $SO_q(3)$ :*

$$\text{Qut}(\mathcal{G}_1) = \text{Qut}(\mathcal{G}_4) \cong SO_q(3).$$

*Proof.* Similarly to Theorem 5.1, the quantum automorphism group of trivial and complete graphs are the quantum symmetry group  $\text{Qut}(M_2, \omega_q)$ , and hence the statement follows from  $\text{Qut}(M_2, \omega_q) \cong SO_q(3)$  by Sołtan [37, Theorem 4.3]. □

Concretely [37, Theorem 4.3] shows that

$$C(\text{Qut}(M_2, \omega_q)) \cong C(SO_q(3)) = C^* \langle A, G, L \rangle$$



is generated by the universal coefficients of the fundamental representation with respect to  $(\widetilde{e}_{11}, \widetilde{e}_{12}, \widetilde{e}_{21}, \widetilde{e}_{22})$ :

$$u = (u_{ij}^{kl}) = \begin{pmatrix} 1 - q^2K & -A & -qA^* & qK \\ qC & L & -q^2G^* & -C \\ C^* & -G & L^* & -q^{-1}C^* \\ qK & q^{-1}A & A^* & 1 - K \end{pmatrix}$$

where  $K = A^*A + G^*G$ ,  $C = q^{-1}LA^* + q^2AG^*$ . By Podleś [35, Proposition 3.1], their defining relations are the following:

$$\begin{aligned} L^*L &= (1 - K)(1 - q^{-2}K) & LL^* &= (1 - q^2K)(1 - q^4K) & G^*G &= GG^* = K^2 \\ A^*A &= C^*C = K - K^2 & AA^* &= CC^* = q^2K - q^4K^2 & A^2 &= q^{-1}LG \\ LG &= q^4GL & LA &= q^2AL & AG &= q^2GA \\ LG^* &= q^4G^*L & A^*L &= q^{-1}(1 - K)C & LK &= q^4KL \\ GK &= KG & AK &= q^2KA & CK &= q^2KC \\ AC &= CA \end{aligned}$$

**Theorem 5.4.** *The quantum automorphism groups of  $\mathcal{G}_2, \mathcal{G}_3$  are the torus subgroup  $\mathbb{T}$  of  $SO_q(3)$ :*

$$\text{Qut}(\mathcal{G}_2) = \text{Qut}(\mathcal{G}_3) \cong \mathbb{T} < SO_q(3).$$

*Proof.* Since  $\mathcal{G}_3 = \mathcal{G}_2^c$ , we have  $\text{Qut}(\mathcal{G}_2) = \text{Qut}(\mathcal{G}_3)$ . It suffices to compute  $C(SO(3)) / \langle A_2u = uA_2 \rangle$ . Then  $A_2u = uA_2$  implies

$$\begin{pmatrix} q^{-1}(1 - q^2K) & -q^{-1}A & -A^* & K \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ q^2K & A & qA^* & q(1 - K) \end{pmatrix} = \begin{pmatrix} q^{-1}(1 - q^2K) & 0 & 0 & q^2K \\ C & 0 & 0 & -qC \\ q^{-1}C^* & 0 & 0 & -C^* \\ K & 0 & 0 & q(1 - K) \end{pmatrix},$$

hence  $A = C = 0, K = q^2K$ . Then  $K = 0$  by  $0 < q < 1$ , and  $G^*G = K - A^*A = 0$  implies  $G = 0$ . Therefore we have

$$C(\text{Qut}(\mathcal{G}_2)) = C^* \langle L | L^*L = LL^* = 1 \rangle \cong C(\mathbb{T})$$

where the last isomorphism is via  $L \mapsto z = (\text{id}_{\mathbb{T}} : \mathbb{T} \rightarrow \mathbb{C})$ . Note that the coproduct  $\Delta$  of  $\text{Qut}(\mathcal{G}_2)$  is now characterized by


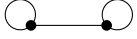
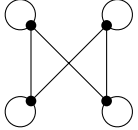
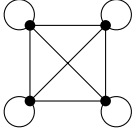
$$\Delta(L) = -qC \otimes A + L \otimes L + G \otimes q^2G^* - q^{-1}A \otimes C = L \otimes L,$$

which is isomorphic to the unitary torus  $\mathbb{T} = (C(\mathbb{T}), \Delta : z \mapsto z \otimes z)$ . Therefore  $\text{Qut}(\mathcal{G}_2) = \mathbb{T}$ .  $\square$

### 5.3 Quantum isomorphisms between quantum graphs on $M_2$ and $\mathbb{C}^4$

Recall that a regular undirected reflexive classical graph on four vertices is isomorphic to one of the graphs  $\mathcal{G}'_d = (\mathbb{C}^4, \tau_{\mathbb{C}^4}, A'_d)$  of degree  $d = 1, 2, 3, 4$  as in Table II.

Table II: Regular reflexive graphs on four vertices up to permutation

	$d = 1$	$d = 2$	$d = 3$	$d = 4$
$\mathcal{G}'_d$				
$A'_d$	$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \end{pmatrix}$	$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix}$
Spec	$\{1, 1, 1, 1\}$	$\{2, 2, 0, 0\}$	$\{3, 1, 1, -1\}$	$\{4, 0, 0, 0\}$

By the identity of their spectra, we can expect the quantum isomorphism between  $\mathcal{G}_d$  on  $(M_2, \tau = \text{Tr}/2)$  and  $\mathcal{G}'_d$  on  $(\mathbb{C}^4, \tau_{\mathbb{C}^4} = \text{Tr}/4)$ , and indeed this is the case.

Recall that  $\{\widetilde{e}_{ij} = \sqrt{2}e_{ij}\}_{i,j=1}^2$  is an ONB for  $L^2(M_2, \tau)$  and  $\{\widetilde{e}_r = 2e_r\}_{r=1}^4$  is an ONB for  $L^2(\mathbb{C}^4, \tau_{\mathbb{C}^4})$  where  $e_{ij}, e_r$  are matrix units.

Before considering concrete quantum isomorphisms  $(H, P) : \mathcal{G}' \rightarrow \mathcal{G}$  for some  $H$ , we compute the relations of the universal coefficients of quantum isomorphisms:

**Definition 5.5** ([8, Definition 4.1]). Let  $\mathcal{G} = (B, \psi, A), \mathcal{G}' = (B', \psi', A')$  be quantum graphs and  $\{e_i\}, \{e'_k\}$  be ONB's for  $L^2(B, \psi), L^2(B', \psi')$ . The bigalois extension from  $\mathcal{G}'$  to  $\mathcal{G}$  is the  $*$ -algebra  $\mathcal{O}(G^+(\mathcal{G}', \mathcal{G}))$  generated by the universal coefficients  $(P_i^k)$  that make

$$P := \sum_{ik} |e'_k\rangle P_i^k \langle e_i| : B \rightarrow B' \otimes \mathcal{O}(G^+(\mathcal{G}', \mathcal{G}))$$

a quantum isomorphism as in Remark 3.11, i.e.,  $P$  is a unital  $*$ -homomorphism, the matrix  $(P_i^k)$  is unitary, and  $PA = (A' \otimes \text{id}_{\mathcal{O}})P$ .

Recall that such  $(P_i^k)$  is unitary if and only if  $P$  satisfies the counit and comultiplication preserving conditions by Lemma 3.6. If both  $\mathcal{G}$  and  $\mathcal{G}'$  are trivial  $A^{(\iota)} = \text{id}_{B^{(\iota)}}$ , then the compatibility with adjacency operators  $PA = (A' \otimes \text{id}_{\mathcal{O}})P$  is trivial. If both  $\mathcal{G}$  and  $\mathcal{G}'$  are complete  $A^{(\iota)} = \delta^{(\iota)2} \psi^{(\iota)}(\cdot)1_{B^{(\iota)}}$ , then the compatibility with adjacency operators follows from the compatibility with unit and counit if  $\delta = \delta'$ .

**Lemma 5.6.** *If both  $\mathcal{G}$  and  $\mathcal{G}'$  are real reflexive quantum graphs equipped with  $\delta = \delta'$ -forms  $\psi, \psi'$ , then  $\mathcal{O}(G^+(\mathcal{G}', \mathcal{G})) = \mathcal{O}(G^+(\mathcal{G}'^c, \mathcal{G}^c))$  holds for the reflexive complement  $\mathcal{G}^c = (B, \psi, A^c = \text{id}_B + \delta^2\psi(\cdot)1_B - A)$ .*

*Proof.* Since  $\mathcal{G}$  and  $\mathcal{G}'$  are real reflexive,  $\mathcal{G}^c$  and  $\mathcal{G}'^c$  are real reflexive quantum graphs by Proposition 2.33. Since  $\delta = \delta'$ , we have

$$PA^c - (A'^c \otimes \text{id}_{\mathcal{O}})P = -PA + (A' \otimes \text{id}_{\mathcal{O}})P.$$

Thus  $\mathcal{O}(G^+(\mathcal{G}', \mathcal{G})) = \mathcal{O}(G^+(\mathcal{G}'^c, \mathcal{G}^c))$ . □

**Proposition 5.7.** *The bigalois extension  $\mathcal{O}_d := \mathcal{O}(G^+(\mathcal{G}'_d, \mathcal{G}_d))$  is given by*

$$\begin{aligned} \mathcal{O}_1 = \mathcal{O}_4 &= * \left\langle S_1, S_2, S_3, S_4 \left| \begin{array}{l} S_r S_r^* S_r = S_r, \quad S_r S_r^* + S_r^* S_r = 1, \\ \sum_{r=1}^4 S_r^* S_r = 2, \quad \sum_{r=1}^4 S_r = 0, \\ S_s^* S_r = -S_s^* S_s S_r^* S_r \quad \forall r \neq s \end{array} \right. \right\rangle; \\ \mathcal{O}_2 = \mathcal{O}_3 &= \mathcal{O}_1 / \langle S_1 + S_2 = S_3 + S_4 = 0 \rangle = * \left\langle S_1, S_3 \left| \begin{array}{l} S_r S_r^* S_r = S_r, \\ S_r S_r^* + S_r^* S_r = 1, \\ S_1^* S_1 + S_3^* S_3 = 1 \end{array} \right. \right\rangle, \end{aligned}$$

where  $*\langle \mathcal{S} | \mathcal{R} \rangle$  denotes the  $*$ -algebra generated by  $\mathcal{S}$  under the relations  $\mathcal{R}$ . The generators arise as the universal coefficients of quantum isomorphism  $P : M_2 \rightarrow \mathbb{C}^4 \otimes \mathcal{O}_d$  in the following way:

$$\begin{aligned} P\widetilde{e}_{11} &= \sum_{r=1}^4 \widetilde{e}_r \otimes \frac{S_r S_r^*}{\sqrt{2}}; & P\widetilde{e}_{12} &= \sum_{r=1}^4 \widetilde{e}_r \otimes \frac{S_r}{\sqrt{2}}; \\ P\widetilde{e}_{21} &= \sum_{r=1}^4 \widetilde{e}_r \otimes \frac{S_r^*}{\sqrt{2}}; & P\widetilde{e}_{22} &= \sum_{r=1}^4 \widetilde{e}_r \otimes \frac{S_r^* S_r}{\sqrt{2}}. \end{aligned} \quad (5.1)$$

Note that the first two defining relations mean that each  $S_r$  is a partial isometry where its source and range are mutual orthocomplements.

*Proof.* Let  $(P_{ij}^r)_{i,j \leq 2}^{r \leq 4}$  be the generators of  $\mathcal{O} = \mathcal{O}_d$  that make  $P = \sum_{ijr} |\widetilde{e}_r\rangle P_{ij}^r \langle \widetilde{e}_{ij} | : M_2 \rightarrow \mathbb{C}^4 \otimes \mathcal{O}$  a quantum isomorphism. The coefficients satisfy the following relations by (3.1), (3.2):

**(unit)**  $P1_{M_2} = 1_{\mathbb{C}^4} \otimes 1_{\mathcal{O}}$ , so  $1_{M_2} = \frac{1}{\sqrt{2}}(\widetilde{e}_{11} + \widetilde{e}_{22})$  and  $1_{\mathbb{C}^4} = \frac{1}{2} \sum_r \widetilde{e}_r$  implies

$$\sqrt{2}(P_{11}^r + P_{22}^r) = 1_{\mathcal{O}} \quad \forall r. \quad (5.2)$$

**(multiplication)**  $P(\widetilde{e}_{ij}\widetilde{e}_{kl}) = P(\widetilde{e}_{ij})P(\widetilde{e}_{kl})$ , so  $\widetilde{e}_{ij}\widetilde{e}_{kl} = \sqrt{2}\delta_{jk}\widetilde{e}_{il}$  and  $\langle \widetilde{e}_r | m_{\mathbb{C}^4} = 2 \langle \widetilde{e}_r | \otimes \langle \widetilde{e}_r |$  implies

$$\sqrt{2}\delta_{jk}P_{il}^r = 2P_{ij}^r P_{kl}^r \quad \forall i, j, k, l, r. \quad (5.3)$$

**(involution)**  $P(\widetilde{e}_{ij}^*)^* = P(\widetilde{e}_{ij})$  implies

$$P_{ji}^{r*} = P_{ij}^r \quad \forall i, j, r. \quad (5.4)$$

**(count)**  $\tau_{\mathbb{C}^4}P = \tau_{M_2} \otimes 1_{\mathcal{O}}$ , so  $\tau_{M_2} = \frac{1}{\sqrt{2}}(|\widetilde{e}_{11}\rangle + |\widetilde{e}_{22}\rangle|)$  and  $\tau_{\mathbb{C}^4} = \frac{1}{2} \sum_r \langle \widetilde{e}_r |$  imply

$$\sum_r \sqrt{2}P_{11}^r = \sum_r \sqrt{2}P_{22}^r = 2, \quad \sum_r \sqrt{2}P_{12}^r = \sum_r \sqrt{2}P_{21}^r = 0. \quad (5.5)$$

**(comultiplication)**  $m_{\mathbb{C}^4}^\dagger P = m_{\mathcal{O}}(P \otimes P)m_{M_2}^\dagger$ , so  $m_{M_2}^\dagger \widetilde{e}_{ij} = \sqrt{2}(\widetilde{e}_{i1} \otimes \widetilde{e}_{1j} + \widetilde{e}_{i2} \otimes \widetilde{e}_{2j})$  and  $(\langle \widetilde{e}_s | \otimes \langle \widetilde{e}_r |)m_{\mathbb{C}^4}^\dagger = 2\delta_{rs} \langle \widetilde{e}_r |$  imply

$$2P_{ij}^r = \sqrt{2}(P_{i1}^r P_{1j}^r + P_{i2}^r P_{2j}^r) \quad \forall i, j, r; \quad (5.6)$$

$$0 = P_{i1}^s P_{1j}^r + P_{i2}^s P_{2j}^r \quad \forall i, j, r, s (r \neq s). \quad (5.7)$$

Put  $S_r = \sqrt{2}P_{12}^r$ , then (5.4) and (5.3) show

$$S_r^* = \sqrt{2}P_{21}^r, \quad S_r^* S_r = \sqrt{2}P_{22}^r, \quad S_r S_r^* = \sqrt{2}P_{11}^r.$$

and

$$(S_r^* S_r)^2 = 2P_{22}^r P_{22}^r = S_r^* S_r, \quad (S_r S_r^*)^2 = 2P_{11}^r P_{11}^r = S_r S_r^*.$$

Thus every  $S_r$  is a partial isometry  $S_r S_r^* S_r = S_r$  with source projection  $\sqrt{2}P_{22}^r$  and range projection  $\sqrt{2}P_{11}^r$ . By (5.2), these two projections are mutual orthocomplement

$$S_r^* S_r + S_r S_r^* = 1_{\mathcal{O}}.$$

By (5.5), we have

$$\sum_r S_r^* S_r = \sum_r S_r S_r^* = 2, \quad \sum_r S_r = 0.$$

Since we have

$$\sum_r S_r S_r^* = \sum_r (1 - S_r^* S_r) = 4 - \sum_r S_r^* S_r,$$

the equality  $\sum_r S_r S_r^* = 2$  is redundant. Now (5.6) follows from (5.3):

$$\sqrt{2}(P_{i1}^r P_{1j}^r + P_{i2}^r P_{2j}^r) \stackrel{(5.3)}{=} P_{ij}^r + P_{ij}^r = 2P_{ij}^r.$$

Multiplying (5.7) by  $\sqrt{2}P_{2i}^s$  from left and by  $\sqrt{2}P_{j2}^r$  from right reduces (5.7) to

$$0 = P_{21}^s P_{12}^r + P_{22}^s P_{22}^r = S_s^* S_r + S_s^* S_s S_r^* S_r,$$

and multiplying by their adjoints recovers (5.7). Hence  $S_s^* S_r = -S_s^* S_s S_r^* S_r$ .

Since both  $\mathcal{G}_1$  and  $\mathcal{G}'_1$  are trivial graphs, the above are all the defining relations of  $\mathcal{O}_1$ . Since  $A_4^{(i)} = A_1^{(i)c}$ ,  $A_3^{(i)} = A_2^{(i)c}$  and both  $\tau_{M_2}$  and  $\tau_{\mathbb{C}^4}$  are 2-forms, we have  $\mathcal{O}_4 = \mathcal{O}_1$ ,  $\mathcal{O}_3 = \mathcal{O}_2$  by Lemma 5.6.

In the case of  $\mathcal{O}_2$ , subtracting  $P$  from  $PA_2 = (A'_2 \otimes \text{id}_{\mathcal{O}})P$  gives  $P(A_2 - \text{id}_{M_2}) = ((A' - \text{id}_{\mathbb{C}^4}) \otimes \text{id}_{\mathcal{O}})P$ . By matrix presentation with respect to the ONB's,

$$(P_{ij}^r)(A_2 - \text{id}_{M_2}) = (A'_2 - \text{id}_{\mathbb{C}^4})(P_{ij}^r)$$

$$\begin{pmatrix} S_1 S_1^* & S_1 & S_1^* & S_1^* S_1 \\ S_2 S_2^* & S_2 & S_2^* & S_2^* S_2 \\ S_3 S_3^* & S_3 & S_3^* & S_3^* S_3 \\ S_4 S_4^* & S_4 & S_4^* & S_4^* S_4 \end{pmatrix} \begin{pmatrix} 1 & & & 0 \\ & -1 & & \\ & & -1 & \\ 0 & & & 1 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} S_1 S_1^* & S_1 & S_1^* & S_1^* S_1 \\ S_2 S_2^* & S_2 & S_2^* & S_2^* S_2 \\ S_3 S_3^* & S_3 & S_3^* & S_3^* S_3 \\ S_4 S_4^* & S_4 & S_4^* & S_4^* S_4 \end{pmatrix}$$

$$\begin{pmatrix} S_1 S_1^* & -S_1 & -S_1^* & S_1^* S_1 \\ S_2 S_2^* & -S_2 & -S_2^* & S_2^* S_2 \\ S_3 S_3^* & -S_3 & -S_3^* & S_3^* S_3 \\ S_4 S_4^* & -S_4 & -S_4^* & S_4^* S_4 \end{pmatrix} = \begin{pmatrix} S_2 S_2^* & S_2 & S_2^* & S_2^* S_2 \\ S_1 S_1^* & S_1 & S_1^* & S_1^* S_1 \\ S_4 S_4^* & S_4 & S_4^* & S_4^* S_4 \\ S_3 S_3^* & S_3 & S_3^* & S_3^* S_3 \end{pmatrix}.$$

Hence  $S_2 = -S_1$ ,  $S_4 = -S_3$ , and  $\mathcal{O}_2 = \mathcal{O}_1 / \langle S_1 + S_2 = S_3 + S_4 = 0 \rangle$ . Then  $\sum_{r=1}^4 S_r^* S_r = 2$  reduces to

$$S_1^* S_1 + S_3^* S_3 = 1_{\mathcal{O}},$$

and  $\sum_{r=1}^4 S_r = 0$  follows automatically. Finally  $S_s^* S_r = -S_s^* S_s S_r^* S_r$  is automatic for  $\{r, s\} = \{1, 2\}, \{3, 4\}$ , and the rest  $\{r, s\}$  follows from

$$\begin{aligned} -S_1^* S_1 S_3^* S_3 &= -S_1^* S_1 (1 - S_1^* S_1) = 0; \\ S_1^* S_3 &= S_1^* S_3 S_3^* S_3 = S_1^* (1 - S_1 S_1^*) S_3 = 0. \end{aligned}$$

□

In order to show quantum isomorphism, we construct a nonzero  $*$ -representation of the bigalois extension on a Hilbert space.

**Theorem 5.8.** *The bigalois extension  $\mathcal{O}_d$  ( $d = 1, 2, 3, 4$ ) admits a two-dimensional  $*$ -representation  $\pi : \mathcal{O}_d \rightarrow M_2$  defined by*

$$\pi(S_1) = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad \pi(S_2) = \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix}; \quad \pi(S_3) = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}; \quad \pi(S_4) = \begin{pmatrix} 0 & 0 \\ -1 & 0 \end{pmatrix}.$$

*Proof.* It suffices to show that  $\pi$  is a  $*$ -homomorphism for  $d = 2$  because  $\mathcal{O}_2 = \mathcal{O}_3$  is a quotient of  $\mathcal{O}_1 = \mathcal{O}_4$ . By definition  $\pi(S_r)$  is a partial isometry with orthogonal source and range,  $\mathbb{C} \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $\mathbb{C} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ , which span  $\mathbb{C}^2$ . Trivially  $\pi(S_1) + \pi(S_2) = \pi(S_3) + \pi(S_4) = 0$  is satisfied, and we also have

$$\pi(S_1)^* \pi(S_1) + \pi(S_3)^* \pi(S_3) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = 1_{M_2}.$$

Thus  $\pi$  defines a unital  $*$ -homomorphism  $\mathcal{O}_2 \rightarrow M_2$ .  $\square$

**Corollary 5.9.** *For every  $d = 1, 2, 3, 4$ , the quantum graph  $\mathcal{G}_d$  on  $(M_2, \tau)$  and the classical graph  $\mathcal{G}'_d$  on four vertices are quantum isomorphic.*

*Proof.* By definition, a  $*$ -representation of the bigalois extension on a finite dimensional Hilbert space  $H$  is equivalent to a quantum isomorphism between the quantum graphs via  $H$ . In other words (5.1) with  $S_r$  replaced by  $\pi(S_r)$  is a quantum isomorphism  $(H = \mathbb{C}^2, \pi(P)) : \mathcal{G}'_d \rightarrow \mathcal{G}_d$ .  $\square$

**Definition 5.10** (Brannan et al. [8, Definition 3.11]). Quantum groups  $G, G'$  are said to be monoidally equivalent if their representation categories  $\text{Rep}(G)$  and  $\text{Rep}(G')$  are unitarily monoidally equivalent as strict  $C^*$ -tensor categories, i.e., there is an fully faithful essentially surjective functor  $\text{Rep}(G) \rightarrow \text{Rep}(G')$  that preserves the trivial representation, composition, involution, and tensor product of intertwiners.

Brannan et al. [8, Theorem 4.7] proved that a quantum isomorphism between quantum graphs induces a monoidal equivalence between their quantum automorphism groups. Applying this to our result, we obtain the following.

**Corollary 5.11. (1)** *The special orthogonal group  $SO(3)$  is monoidally equivalent to the quantum symmetric group  $S_4^+$ .*

**(2)** *The orthogonal group  $O(2)$  is monoidally equivalent to the hyperoctahedral quantum group  $H_2^+ < S_4^+$ .*

*Proof. (1)* Note that  $\text{Qut}(\mathcal{G}'_1)$  is the quantum symmetric group  $S_4^+$ . It follows from  $\mathcal{G}_1 \cong_q \mathcal{G}'_1$  that  $\text{Qut}(\mathcal{G}_1) = SO(3)$  is monoidally equivalent to  $\text{Qut}(\mathcal{G}'_1) = S_4^+$ .

**(2)** By Banica, Bichon, Collins [6, Definition 2.1],  $\text{Qut}(\mathcal{G}'_2)$  is the hyperoctahedral quantum group  $H_2^+ < S_4^+$ . It follows from  $\mathcal{G}_2 \cong_q \mathcal{G}'_2$  that  $\text{Qut}(\mathcal{G}_2) = O(2)$  is monoidally equivalent to  $\text{Qut}(\mathcal{G}'_2) = H_2^+$ .  $\square$

In the case of  $d = 1, 4$ , we can also construct a quantum isomorphism using the symmetry of the 24-cell and four-dimensional hypercube.

**Theorem 5.12.** *The bigalois extension  $\mathcal{O}_d$  ( $d = 1, 4$ ) admits a four-dimensional  $*$ -representation  $\rho : \mathcal{O}_d \rightarrow M_4$  defined by*

$$\begin{aligned} \rho(S_1) &= \frac{\sqrt{2}}{6} \begin{pmatrix} 0 & 0 & 0 & 0 \\ -3 & -1 & -1 & -1 \\ 0 & 2 & 2 & 2 \\ 3 & -1 & -1 & -1 \end{pmatrix}; & \rho(S_2) &= \frac{\sqrt{2}}{6} \begin{pmatrix} -1 & 3 & -1 & 1 \\ 0 & 0 & 0 & 0 \\ -1 & -3 & -1 & 1 \\ -2 & 0 & -2 & 2 \end{pmatrix}; \\ \rho(S_3) &= \frac{\sqrt{2}}{6} \begin{pmatrix} 2 & -2 & 0 & 2 \\ 1 & -1 & 3 & 1 \\ 0 & 0 & 0 & 0 \\ -1 & 1 & 3 & -1 \end{pmatrix}; & \rho(S_4) &= \frac{\sqrt{2}}{6} \begin{pmatrix} -1 & -1 & 1 & -3 \\ 2 & 2 & -2 & 0 \\ 1 & 1 & -1 & -3 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \end{aligned}$$

We have a conceptually easier presentation of  $\rho(S_r)$ 's:

$$\begin{aligned}\rho(S_1) &= \frac{\sqrt{2}}{2} \begin{pmatrix} 0 \\ -1 \\ 0 \\ 1 \end{pmatrix} (1 \ 0 \ 0 \ 0) + \frac{\sqrt{2}}{6} \begin{pmatrix} 0 \\ -1 \\ 2 \\ -1 \end{pmatrix} (0 \ 1 \ 1 \ 1); \\ \rho(S_2) &= \frac{\sqrt{2}}{2} \begin{pmatrix} 1 \\ 0 \\ -1 \\ 0 \end{pmatrix} (0 \ 1 \ 0 \ 0) + \frac{\sqrt{2}}{6} \begin{pmatrix} -1 \\ 0 \\ -1 \\ -2 \end{pmatrix} (1 \ 0 \ 1 \ -1); \\ \rho(S_3) &= \frac{\sqrt{2}}{2} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} (0 \ 0 \ 1 \ 0) + \frac{\sqrt{2}}{6} \begin{pmatrix} 2 \\ 1 \\ 0 \\ -1 \end{pmatrix} (1 \ -1 \ 0 \ 1); \\ \rho(S_4) &= \frac{\sqrt{2}}{2} \begin{pmatrix} -1 \\ 0 \\ -1 \\ 0 \end{pmatrix} (0 \ 0 \ 0 \ 1) + \frac{\sqrt{2}}{6} \begin{pmatrix} -1 \\ 2 \\ 1 \\ 0 \end{pmatrix} (1 \ 1 \ -1 \ 0).\end{aligned}$$

The four vectors in  $\rho(S_r)$  are mutually orthogonal and normalized by the coefficients. Put these orthonormal vectors  $w_r, e_r, w_r^\perp, e_r^\perp$ , so that we have

$$\rho(S_r) = w_r e_r^\dagger + w_r^\perp e_r^{\perp\dagger}.$$

The row vectors  $e_r^\perp$  in the second term correspond to a mutually orthogonal choice of the diagonal lines of the surface cubes of the hypercube. And the two row vectors  $e_r, e_r^\perp$  span the plane  $L_r$  containing the two parallel diagonal lines of the opposite surface cubes as in Figure 1. The two column vectors  $w_r, w_r^\perp$  span its orthocomplement  $L_r^\perp$ , which is the plane containing one of the four hexagons given by a partition of the 24 vertices of the 24-cell as in Figure 1.

*Proof.* Since the four vectors in  $\rho(S_r)$  are orthonormal,  $\rho(S_r)$  is a partial isometry  $\rho(S_r)\rho(S_r)^*\rho(S_r) = \rho(S_r)$  satisfying  $\rho(S_r)\rho(S_r)^* + \rho(S_r)^*\rho(S_r) = 1$ . We have by direct computation that  $\sum_{r=1}^4 \rho(S_r) = 0$ . Since  $\rho(S_r)^*\rho(S_r)$  is the projection onto the plane  $L_r = \mathbb{C}e_r + \mathbb{C}e_r^\perp$ , we obtain  $\sum_{r=1}^4 \rho(S_r)^*\rho(S_r) = 2$  because the row vectors  $\{e_r\}_r$  and  $\{e_r^\perp\}_r$  are both ONB's for  $\mathbb{C}^4$ . Finally it suffices to show

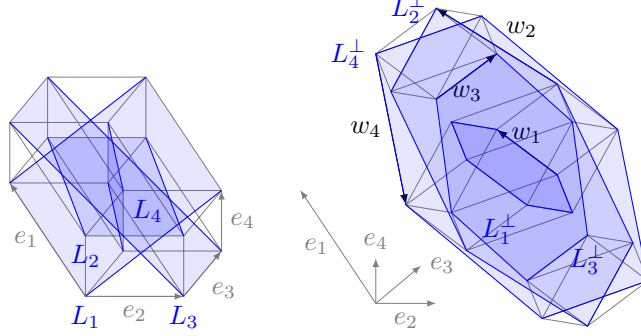
$$\rho(S_s)\rho(S_s)^*\rho(S_r) = -\rho(S_s)\rho(S_r)^*\rho(S_r)$$

for all  $r \neq s$ , which is equivalent to

$$\rho(S_s)^*\rho(S_r) = -\rho(S_s)^*\rho(S_s)\rho(S_r)^*\rho(S_r).$$

By direct computation, we obtain

$$\begin{aligned}\rho(S_s)\rho(S_s)^*\rho(S_r) &= (w_s w_s^\dagger + w_s^\perp w_s^{\perp\dagger})(w_r e_r^\dagger + w_r^\perp e_r^{\perp\dagger}) \\ &= \begin{pmatrix} w_s & w_s^\perp \end{pmatrix} \begin{pmatrix} \langle w_s | w_r \rangle & \langle w_s | w_r^\perp \rangle \\ \langle w_s^\perp | w_r \rangle & \langle w_s^\perp | w_r^\perp \rangle \end{pmatrix} \begin{pmatrix} e_r^\dagger \\ e_r^{\perp\dagger} \end{pmatrix},\end{aligned}$$

Figure 1: Positions of  $L_r$  in a hypercube and  $L_r^\perp$  in a 24-cell

The hypercube is  $[0, 1]^4$  centered in  $\mathbb{R}^4$ . The 24-cell is the convex hull of  $\{\pm e_i \pm e_j\}_{i \neq j}$ . For simplicity the 24-cell is drawn only on the hyperplanes of the first coordinate  $x_1 = \pm 1, 0$ , which are octahedrons and a cuboctahedron.

and similarly

$$\begin{aligned} \rho(S_s)\rho(S_r)^*\rho(S_r) &= (w_s e_s^\dagger + w_s^\perp e_s^{\perp\dagger})(e_r e_r^\dagger + e_r^\perp e_r^{\perp\dagger}) \\ &= \begin{pmatrix} w_s & w_s^\perp \end{pmatrix} \begin{pmatrix} \langle e_s | e_r \rangle & \langle e_s | e_r^\perp \rangle \\ \langle e_s^\perp | e_r \rangle & \langle e_s^\perp | e_r^\perp \rangle \end{pmatrix} \begin{pmatrix} e_r^\dagger \\ e_r^{\perp\dagger} \end{pmatrix}. \end{aligned}$$

Since  $\{e_r\}_r, \{e_r^\perp\}_r, \{w_r\}_r, \{w_r^\perp\}_r$  are chosen to be ONB's, we have

$$\langle e_s | e_r \rangle = \langle e_s^\perp | e_r^\perp \rangle = \langle w_s | w_r \rangle = \langle w_s^\perp | w_r^\perp \rangle = 0$$

for all  $s \neq r$ . Thus it reduces to show  $\langle w_s | w_r^\perp \rangle = -\langle e_s | e_r^\perp \rangle$  for all  $s \neq r$ . It indeed holds that

$$\begin{aligned} \langle w_1 | w_r^\perp \rangle &= -\frac{1}{\sqrt{3}} = -\langle e_1 | e_r^\perp \rangle \quad (r = 2, 3, 4); \\ \langle w_2 | w_4^\perp \rangle &= -\frac{1}{\sqrt{3}} = -\langle e_2 | e_4^\perp \rangle; \quad \langle w_2 | w_r^\perp \rangle = \frac{1}{\sqrt{3}} = -\langle e_2 | e_r^\perp \rangle \quad (r = 1, 3); \\ \langle w_3 | w_2^\perp \rangle &= -\frac{1}{\sqrt{3}} = -\langle e_3 | e_2^\perp \rangle; \quad \langle w_3 | w_r^\perp \rangle = \frac{1}{\sqrt{3}} = -\langle e_3 | e_r^\perp \rangle \quad (r = 1, 4); \\ \langle w_4 | w_3^\perp \rangle &= \frac{1}{\sqrt{3}} = -\langle e_4 | e_3^\perp \rangle; \quad \langle w_4 | w_r^\perp \rangle = -\frac{1}{\sqrt{3}} = -\langle e_4 | e_r^\perp \rangle \quad (r = 1, 2). \end{aligned}$$

Therefore  $\rho$  defines a  $*$ -homomorphism  $\mathcal{O}_1 \rightarrow M_4$ .  $\square$

## Concluding Remarks

For future perspective, it is natural to consider the classification of general directed quantum graphs on  $M_2$  and to ask which quantum subgroup of



$SO_q(3) = \text{Qut}(M_2, \omega_q)$  is obtained as a quantum automorphism group of them. Such a classification will help us to approach a quantum graph version of the Frucht property: whether a quantum group acting on a quantum graph is isomorphic to the quantum automorphism group of some quantum graph. Its classical graph version is discussed by Banica, McCarthy [2] with several counterexamples.

Since we introduced the regularity of quantum graphs, it is natural to ask whether the spectrum of a regular quantum graph can characterize its properties (connected, bipartite, expander, etc.) similarly to classical cases. It is the next step to investigate the connectedness of quantum graphs on  $M_n$  introduced by Chávez-Domínguez, Swift [13].

## 6 Spectral bound for regular quantum graphs

In classical graph theory,  $d$ -regular graphs are known to have spectral radius  $d$  (cf. [14]) and hence it makes sense to argue whether the second largest eigenvalue is  $d$  and the smallest eigenvalue is  $-d$ . Here, we introduce the notion of graph gradient to prove this spectral bound for regular quantum graphs.

### 6.1 Graph gradient of quantum graphs

**Definition 6.1.** Let  $(B, \psi, A)$  be a quantum graph. Define a linear operator  $\nabla = \nabla_A : B \rightarrow B \otimes B$  by

$$\nabla_A = \delta^{-2}(A^\dagger \otimes \text{id}_B - \text{id}_B \otimes A)m^\dagger = \delta^{-2} \left( \begin{array}{c} \text{---} \\ | \\ \textcircled{A^\dagger} \\ | \\ \text{---} \end{array} \Big| - \Big| \begin{array}{c} \text{---} \\ | \\ \textcircled{A} \\ | \\ \text{---} \end{array} \right).$$

We call  $\nabla_A$  the graph gradient.

This gradient coincides with the classical one in the following manner.

**Lemma 6.2.** Let  $(V, E \subset V \times V)$  be a classical directed graph corresponding to  $(C(V) = \mathbb{C}^n, \tau, A)$  with  $A_{ij} = \chi_E(j, i)$  where  $\chi_E$  is the indicator function of  $E$ . The classical graph gradient  $\nabla_E : C(V) \rightarrow C(E)$  (the so-called coboundary operator in [14]) is defined by

$$\nabla_E f(i, j) = f(j) - f(i) \quad f \in C(V), \quad (i, j) \in E.$$

It holds that  $\nabla_A = \iota \circ \nabla_E$ , where  $\iota : C(E) \rightarrow C(V) \otimes C(V) = C(V \times V)$  is the extension of functions on  $E$  to  $V \times V$  with outside zero.

*Proof.* Note that the evaluation map  $C(V) \ni f \mapsto f(i) \in \mathbb{C}$  at  $i \in V$  is given by  $n \langle e_i | = n\tau(e_i \cdot)$  for the tracial  $\sqrt{n}$ -form  $\tau$  and  $m^\dagger e_k = ne_k \otimes e_k$ . By direct computation we have for  $f \in C(V)$  and  $i, j \in V$  that

$$\begin{aligned} \nabla_A f(i, j) &= n^2(\langle e_i | \otimes \langle e_j |) \nabla_A f \\ &= n^2 n^{-1} \left( \langle e_i | A^\dagger \otimes \langle e_j | - \langle e_i | \otimes \langle e_j | A \right) n \sum_k f(k) e_k \otimes e_k \\ &= n^2(\langle e_i | A^\dagger f(j) | e_j \rangle n^{-1} - n^{-1} \langle e_j | A f(i) | e_i \rangle) \\ &= n \sum_{(k, j) \in E} \langle e_i | e_k \rangle f(j) - n \sum_{(i, k) \in E} \langle e_j | e_k \rangle f(i) \\ &= (f(j) - f(i)) \chi_E(i, j) = (\iota \nabla_E f)(i, j). \end{aligned}$$

□

The graph gradient  $\nabla_A$  is the commutator of the right regular representation  $\rho(\cdot)$  and  $A$  via the identification (2.14)  $\iota : B(L^2(\mathcal{G})) \cong B \otimes B$ :

**Proposition 6.3.** *Let  $(B, \psi, A)$  be a real quantum graph. For  $x \in B$ , we have*

$$\delta^2 \iota^{-1}(\nabla_A x) = [\rho(x), A] := \rho(x)A - A\rho(x).$$

*Proof.* By direct computation, we get

$$\delta^2 \iota^{-1}(\nabla_A x) = \begin{array}{c} \text{---} \\ | \\ \textcircled{A^\dagger} \\ | \\ \textcircled{x} \end{array} - \begin{array}{c} \textcircled{A} \\ | \\ \textcircled{x} \end{array} = \begin{array}{c} \textcircled{A} \\ | \\ \textcircled{x} \end{array} - \begin{array}{c} \textcircled{A} \\ | \\ \textcircled{x} \end{array} = [\rho(x), A].$$

□

Recall the one-to-one correspondence (2.16) between real quantum graphs  $A$  on  $(B, \psi)$  and ‘edge space’  $B$ - $B$ -bimodules  $\mathcal{S} = \text{range } P_A \subset B \otimes B$  represented by orthogonal projection  $P_A$  onto  $\mathcal{S} \subset L^2(B, \psi)^{\otimes 2}$ . Similarly to the classical case,  $\nabla_A$  is a map to the edge space.

**Proposition 6.4.** *Let  $(B, \psi, A)$  be a real quantum graph. Then the following holds.*

- (1) *The range of  $\nabla_A$  is included in  $\text{range } P_A$ , i.e.,  $P_A \nabla_A = \nabla_A$ .*
- (2) *The operator  $\nabla_A$  is a  $\mathbb{C}$ -derivation, i.e.,  $\nabla_A(xy) = (\nabla_A x)y + x(\nabla_A y)$  for all  $x, y \in B$  and  $\nabla_A(\lambda) = 0$  for any  $\lambda \in \mathbb{C} \subset B$ .*

*Proof.* (1) Note that the real condition (2.11) implies

$$\begin{array}{c} \textcircled{A^\dagger} \\ | \\ \textcircled{x} \end{array} = \begin{array}{c} \textcircled{A} \\ | \\ \textcircled{x} \end{array} = \delta^2 P_A(1 \otimes \cdot); \quad \begin{array}{c} \textcircled{A} \\ | \\ \textcircled{x} \end{array} = \begin{array}{c} \textcircled{A} \\ | \\ \textcircled{x} \end{array} = \delta^2 P_A(\cdot \otimes 1).$$

Thus we have  $\nabla_A = P_A(1 \otimes \cdot - \cdot \otimes 1)$ , and

$$P_A \nabla_A = P_A^2(1 \otimes \cdot - \cdot \otimes 1) = \nabla_A$$

by idempotence of  $P_A$ .

(2) Now we have  $\nabla_A 1 = P_A(1 \otimes 1 - 1 \otimes 1) = 0$ . It remains to show  $\nabla_A(xy) = (\nabla_A x)y + x(\nabla_A y)$  for  $x, y \in B$ . Indeed by bimodule property  $P_A(xzy) = x(P_A z)y$  for  $x, y \in B, z \in B^{\otimes 2}$ , we obtain

$$\begin{aligned} \nabla_A(xy) &= P_A(1 \otimes xy - xy \otimes 1) \\ &= P_A(1 \otimes xy - x \otimes y + x \otimes y - xy \otimes 1) \\ &= P_A((1 \otimes x - x \otimes 1)y + x(1 \otimes y - y \otimes 1)) \\ &= (\nabla_A x)y + x(\nabla_A y). \end{aligned}$$

□

**Definition 6.5** (Generalization of Ganesan [21] to directed graphs). Let  $\mathcal{G} = (B, \psi, A)$  be a quantum graph. We define the (left) indegree matrix  $D_{\text{in}} : B \rightarrow B$  and (right) outdegree matrix  $D_{\text{out}} : B \rightarrow B$  by

$$D_{\text{in}} = \lambda(A1_B) = \begin{array}{c} | \\ \textcircled{A} \\ | \end{array}; \quad D_{\text{out}} = \rho(A^\dagger 1_B) = \begin{array}{c} | \\ \textcircled{A^\dagger} \\ | \end{array} \quad (\text{if } A:\text{real}) \quad \begin{array}{c} \circ \\ \textcircled{A} \\ | \end{array}$$

where  $\lambda$  (resp.  $\rho$ ) is the left (resp. right) multiplication.

If  $\mathcal{G}$  is undirected, then  $D_{\text{out}} = D_{\text{in}}^*$  by

$$D_{\text{in}}^* x = ((A1)x^*)^* = x(A1)^* = x(A^*1) \stackrel{(\text{undirected})}{=} x(A^\dagger 1) = D_{\text{out}} x.$$

And  $D_{\text{out}} = D_{\text{in}} = d \text{id}_B$  if  $\mathcal{G}$  is  $d$ -regular.

**Lemma 6.6.** Let  $\mathcal{G} = (B, \psi, A)$  be a real quantum graph. Then

$$0 \leq \nabla_A^\dagger \nabla_A = \delta^{-2} (D_{\text{in}} - A + D_{\text{out}} - A^\dagger).$$

Moreover if  $\mathcal{G}$  is  $d$ -regular,

$$0 \leq \nabla_A^\dagger \nabla_A = 2\delta^{-2} \left( d \text{id}_B - \frac{A + A^\dagger}{2} \right).$$

In particular  $\frac{\theta A + \bar{\theta} A^\dagger}{2} \leq d \text{id}_B$  for all  $\theta \in \mathbb{T}$ .

*Proof.* We can compute directly

$$\begin{aligned} \nabla_A^\dagger \nabla_A &= \delta^{-4} m(A \otimes \text{id} - \text{id} \otimes A^\dagger)(A^\dagger \otimes \text{id} - \text{id} \otimes A)m^\dagger \\ &= \delta^{-4} \left( \begin{array}{c} | \\ \boxed{AA^\dagger} \\ | \end{array} + \begin{array}{c} | \\ \boxed{A^\dagger A} \\ | \end{array} - \begin{array}{c} | \\ \textcircled{A} \textcircled{A} \\ | \end{array} - \begin{array}{c} | \\ \textcircled{A^\dagger} \textcircled{A^\dagger} \\ | \end{array} \right) \\ &= \delta^{-2} \left( \delta^{-2} \begin{array}{c} | \\ \textcircled{A} \textcircled{A} \\ | \end{array} + \delta^{-2} \begin{array}{c} | \\ \textcircled{A} \textcircled{A} \\ | \end{array} - A - A^\dagger \right) \\ &= \delta^{-2} \left( \begin{array}{c} | \\ \textcircled{A} \\ | \end{array} + \begin{array}{c} \circ \\ \textcircled{A} \\ | \end{array} - A - A^\dagger \right) \\ &= \delta^{-2} (D_{\text{in}} - A + D_{\text{out}} - A^\dagger). \end{aligned}$$

If it is  $d$ -regular, then  $D_{\text{out}} = D_{\text{in}} = d \text{id}_B$  yields

$$\nabla_A^\dagger \nabla_A = 2\delta^{-2} \left( d \text{id}_B - \frac{A + A^\dagger}{2} \right).$$

Replacing  $A$  by  $\lambda A$  and  $A^\dagger$  by  $\bar{\lambda} A^\dagger$  in  $\nabla_A$ , we deduce  $d \text{id}_B - \frac{\lambda^2 A + \bar{\lambda}^2 A^\dagger}{2} \geq 0$  for any  $\lambda \in \mathbb{T}$ . Since  $\theta = \lambda^2$  ranges all  $\theta \in \mathbb{T}$ , we obtain  $\frac{\theta A + \bar{\theta} A^\dagger}{2} \leq d \text{id}_B$ .  $\square$

**Remark 6.7.** Ganesan [21] defined the graph Laplacian  $L$  by  $L = D - A$  for undirected quantum graphs with right degree matrix  $D = D_{\text{out}}$ . In this case, our Laplacian  $\Delta := \delta^2 \nabla^\dagger \nabla = L^* + L$  is a ‘double’ of usual Laplacian. Usually, the gradient of an undirected classical graph is defined by the gradient as in Lemma 6.2 of an orientation (i.e., a half) of the original graph. This is why we obtained the doubled Laplacian, and such duplication is inevitable because quantum graphs do not always have an orientation as shown below.

**Definition 6.8.** Let  $\mathcal{G} = (B, \psi, A)$  be an undirected quantum graph. We say that a Schur projection  $T : B \rightarrow B$  is an orientation of  $\mathcal{G}$  if  $A \bullet T = T$ ,  $T \bullet T^\dagger = 0$ , and  $\text{range}(T \bullet \cdot) + \text{range}(T^\dagger \bullet \cdot) = \text{range}(A \bullet \cdot)$ .

Note that this definition is equivalent to  $A = T + T^\dagger$  if  $T^\dagger$  is also a Schur projection. The definition states that  $T$  is a directed subgraph (edge subset) of  $A$  over the same quantum set,  $T^\dagger$  is the opposite orientation of  $T$ , and  $T$  and  $T^\dagger$  disjointly cover  $A$ .

If  $\mathcal{G}$  is nonracial, then the GNS adjoint  $T^\dagger$  is not always real, hence not necessarily a Schur projection and  $A = T + T^\dagger$  may not hold. To avoid such a problem, we can instead consider a KMS symmetric quantum graph  $\mathcal{G}$  and the KMS adjoint  $T^\ddagger$  to define an orientation simply by  $A = T + T^\ddagger$ .

**Example 6.9** (A non-orientable quantum graph). Consider 1-regular ir-reflexive undirected quantum graph  $\mathcal{G} = (M_2, \tau = \text{Tr}/2, A = 2E_{\mathbb{C}^2} - \text{id}_{M_2} : \begin{pmatrix} a & b \\ c & d \end{pmatrix} \mapsto \begin{pmatrix} a & -b \\ -c & d \end{pmatrix})$  (c.f. [23, 28]), where  $E_{\mathbb{C}^2}$  is the conditional expectation onto the diagonal subalgebra. Its corresponding projection

$$p_A = \frac{1}{2} \begin{pmatrix} 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \in M_2^{\text{op}} \otimes M_2 = M_4$$

is rank one, hence it does not have an orientation  $T$  whose corresponding projection  $p_T$  must satisfy  $p_A = p_T + p_{T^\dagger}$ .

## 6.2 Spectral bound by the degree

**Proposition 6.10.** *Let  $\mathcal{G}$  be a  $d$ -regular real quantum graph. The spectral radius  $r(A)$  of the adjacency operator satisfies  $r(A) = d$ .*

*Proof.* For a nonzero  $\lambda \in \text{spec}(A)$  and a unit eigenvector  $x \in \ker(\lambda \text{id}_B - A)$ , choose  $\theta \in \mathbb{T}$  so that  $\theta\lambda = |\lambda|$ . Then Lemma 6.6 shows

$$d = d \langle x|x \rangle \geq \frac{\langle x|\theta A + \bar{\theta} A^\dagger|x \rangle}{2} = \frac{\theta \langle x|Ax \rangle + \bar{\theta} \langle Ax|x \rangle}{2} = \frac{\theta\lambda + \bar{\theta}\lambda}{2} = |\lambda|.$$

Thus  $r(A) = \sup_{\lambda \in \text{spec}(A)} |\lambda| \leq d$ . Since  $d \in \text{spec}(A)$ , we have  $r(A) = d$ .  $\square$

**Theorem 6.11.** *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular quantum graph. Then the identity of the operator norm on  $B(L^2(\mathcal{G}))$  and the degree*

$$\|A\|_{\text{op}} = d$$

*holds if either of the following is satisfied:*

- (1)  $\mathcal{G}$  is undirected, whence  $\text{spec}(A) \subset [-d, d]$ ;
- (2) both  $A$  and  $A^\dagger$  are real;
- (3)  $\mathcal{G}$  is real and tracial, i.e.,  $A$  is real and  $\psi = \tau_B$ .

*Proof.* (1) Since  $A$  is normal  $AA^\dagger = A^\dagger A$ , Proposition 6.10 implies  $\|A\|_{\text{op}} = r(A) = d$ . Thus self-adjointness shows  $\text{spec}(A) \subset [-d, d]$ .

(2) We prove this by embedding  $A$  into an undirected  $d$ -regular quantum graph

$$\left( B \otimes \mathbb{C}^2, \tilde{\psi} = \psi \otimes \tau_{\mathbb{C}^2}, \tilde{A} := A \otimes E_{12} + A^\dagger \otimes E_{21} \right) = \left( B \oplus B, \frac{\psi \oplus \psi}{2}, \begin{pmatrix} 0 & A \\ A^\dagger & 0 \end{pmatrix} \right)$$

where  $E_{ij}$  are matrix units in  $M_2$ . By definition  $\tilde{A}$  is self-adjoint. Note that  $A, A^\dagger$  are quantum graphs on  $(B, \psi)$  and  $E_{ij}$  are (quantum) graphs on  $(\mathbb{C}^2, \tau_{\mathbb{C}^2})$ . Then  $A \otimes E_{12}$  and  $A^\dagger \otimes E_{21}$  are quantum graphs on  $(B \otimes \mathbb{C}^2, \psi \otimes \tau_{\mathbb{C}^2})$ . Since the Schur product of  $E_{12}$  and  $E_{21}$  is zero,  $\tilde{A} = A \otimes E_{12} + A^\dagger \otimes E_{21}$  is also a quantum graph.

By assumption,  $A$  and  $A^\dagger$  are real. So are  $A \otimes E_{12}$  and  $A^\dagger \otimes E_{21}$ , hence  $\tilde{A}$  is real.

The regularity follows from  $\tilde{A}(1_B \otimes 1_{\mathbb{C}^2}) = d1_B \otimes e_1 + d1_B \otimes e_2 = d(1_B \otimes 1_{\mathbb{C}^2})$ .

Therefore we have

$$d = \left\| \tilde{A} \right\|_{B(L^2(B \otimes \mathbb{C}^2))} \geq \left\| \tilde{A}|_{L^2(B) \otimes e_2 \rightarrow L^2(B) \otimes e_1} \right\| = \|A\|_{B(L^2(B))}$$

via isometric identifications  $L^2(B) \ni x \mapsto x \otimes \sqrt{2}e_i \in L^2(B) \otimes e_i$  for  $i = 1, 2$ . By  $d \in \text{spec}(A)$ , we obtain  $\|A\| = d$ .

(3) By traciality,  $A^\dagger$  is also real. Thus (3) follows from (2).  $\square$

**Corollary 6.12.** *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular quantum graph. Then we have the identity of the degree and the operator norm with respect to the KMS inner product on  $B$ :*

$$\|A\|_{\text{op}} = d.$$

*Proof.* By (2.12), the realness of  $A$  implies that  $A^\ddagger$  is also real. Thus we have the KMS version of Theorem 6.11 (2): both  $A$  and  $A^\ddagger$  are real. Since the spectral radius does not depend on the inner product structure, we have  $r(A) = d$  by Proposition 6.10. Therefore by the same argument as in the proof of Theorem 6.11, we obtain  $\|A\|_{\text{op}} = d$  over the KMS Hilbert space  $B$ .  $\square$

**Corollary 6.13.** *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular undirected irreflexive quantum graph. Then  $\text{spec}(A) \subset [-d, d]$  and  $0 \leq d \leq \delta^2 - 1$ . Equivalently if  $\mathcal{G}$  is a  $d$ -regular undirected reflexive quantum graph, then  $\text{spec}(A) \subset [-d + 2, d]$  and  $1 \leq d \leq \delta^2$ .*

*Proof.* If  $\mathcal{G}$  is irreflexive, then  $\text{spec } A \subset [-d, d]$  follows from Theorem 6.11. Its reflexive version is given by  $(B, \psi, A + \text{id})$  as a  $(d + 1)$ -regular undirected quantum graph, hence Lemma 2.34 shows that  $0 \leq d \leq \delta^2 - 1$ . If  $\mathcal{G}$  is reflexive, we may replace  $d$  in the previous argument by  $d - 1$  and obtain  $\text{spec}(A - \text{id}) \subset [-d + 1, d - 1]$ , i.e.,  $\text{spec } A \subset [-d + 2, d]$ , and  $1 \leq d \leq \delta^2$ .  $\square$

**Open Problems.** In view of the above, we wonder if  $\|A\|_{\text{op}} = d$  holds with a weaker assumption with respect to the GNS inner product.

Although we showed that some irreflexive quantum graphs do not admit an orientation, there may be a better definition that makes any irreflexive undirected quantum graphs orientable.

As we have the quantum graph Laplacians  $\Delta = \delta^2 \nabla^\dagger \nabla$  and  $L$ , it is natural to consider a quantum Markov semigroup  $e^{-t\Delta}$ , which is the heat semigroup over the quantum graph. We leave it as an open question for future work to investigate the property of  $e^{-t\Delta}$  such as the complete logarithmic Sobolev inequality (cf. [11]).

## 7 Characterization of graph properties

In this section, we introduce graph homomorphisms respecting the adjacency matrices and define the connectedness and bipartiteness of quantum graphs in terms of graph homomorphisms. After that, we give algebraic characterizations of these properties for regular quantum graphs.

### 7.1 Graph properties defined by homomorphisms

**Definition 7.1.** Let  $\mathcal{G} = (B, \psi, A), \mathcal{G}' = (B', \psi', A')$  be quantum graphs. A graph homomorphism  $f^{\text{op}} : \mathcal{G} \rightarrow \mathcal{G}'$  is a unital  $*$ -homomorphism  $f : B' \rightarrow B$  satisfying  $A' \bullet (f^\dagger A f) = f^\dagger A f$ .

We say that  $f^{\text{op}}$  is surjective if  $f$  is injective, and  $f^{\text{op}}$  is injective if  $f$  is surjective.

This definition states that the pushforward  $f^\dagger A f$  of the adjacency matrix of  $\mathcal{G}$  is in the edges of  $\mathcal{G}'$ .

**Definition 7.2.** Let  $\mathcal{G}$  be a quantum graph.

- $\mathcal{G}$  is *disconnected* if there is a surjective graph homomorphism  $\mathcal{G} \rightarrow T_2$ ;
- $\mathcal{G}$  is *connected* if it is not disconnected, i.e., there is no surjective graph homomorphism  $\mathcal{G} \rightarrow T_2$ ;
- $\mathcal{G}$  is *bipartite* if there is a surjective graph homomorphism  $\mathcal{G} \rightarrow K_2$ ;
- $\mathcal{G}$  *has a bipartite component* if there is a graph homomorphism  $\mathcal{G} \rightarrow K_2 \sqcup T_1$  that is onto  $K_2$ , i.e., there is a unital  $*$ -homomorphism  $f : \mathbb{C}^2 \oplus \mathbb{C} \rightarrow B$  satisfying  $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \bullet f^\dagger A f = f^\dagger A f$  and  $f$  is injective on  $\mathbb{C}^2 \oplus 0$ .

If  $\mathcal{G} = (V, E)$  is classical, these definitions agree with classical definitions:  $\mathcal{G}$  is disconnected (resp. bipartite) if there is a decomposition  $V = V_0 \sqcup V_1$  with no edges between  $V_0$  and  $V_1$  (resp. with all edges between  $V_0$  and  $V_1$ ). The equivalence is proved by mapping  $V_0$  and  $V_1$  to the distinct vertices of  $K_2$  or  $T_2$ .

A naive definition of these properties by  $A = \begin{pmatrix} * & 0 \\ 0 & * \end{pmatrix}$  or  $\begin{pmatrix} 0 & * \\ * & 0 \end{pmatrix}$  along some nontrivial decomposition  $B = B_0 \oplus B_1$  of the quantum set is too restrictive for quantum graphs. Indeed there exists a 1-regular undirected irreflexive quantum graph  $(M_2, \tau, A = 2E_{\mathbb{C}^2} - \text{id})$  (c.f. [23, 28]) with  $\text{spec } A = \{-1, -1, 1, 1\}$ , which looks like bipartite and disconnected but has no non-trivial decomposition  $M_2 = B_0 \oplus B_1$ . That is why we defined as above.



The following is the key lemma to prove spectral characterizations of these properties. This lemma allows us to control the decomposition of a self-adjoint operator into positive and negative parts.

**Lemma 7.3.** *Let  $B$  be a  $C^*$ -algebra with a faithful state  $\psi$ , and  $x_{\pm}, y_{\pm} \in B$  be positive elements satisfying*

$$x_+ - x_- = y_+ - y_-$$

with  $\psi(x_+) = \psi(y_+), \psi(x_-) = \psi(y_-)$ . Assume that there is a projection  $p \in B$  such that

$$px_+ = x_+ = x_+p, \quad (1-p)x_- = x_- = x_-(1-p), \quad \psi(p \cdot) = \psi(\cdot p).$$

Then it follows that  $x_+ = y_+, x_- = y_-$ .

*Proof.* We show that  $\xi := y_+ - x_+ = y_- - x_-$  is zero. By assumptions on  $p$ , we have

$$\begin{aligned} p\xi p &= py_+p - x_+ = py_-p \geq 0 \\ (1-p)\xi(1-p) &= (1-p)y_-(1-p) - x_- = (1-p)y_+(1-p) \geq 0 \\ p\xi(1-p) &= py_+(1-p) = py_-(1-p). \end{aligned}$$

By  $\psi(\xi) = \psi(y_+) - \psi(x_+) = 0$  and  $\psi(p\xi(1-p)) = \psi(\xi(1-p)p) = 0$ , we have

$$\begin{aligned} 0 &= \psi(\xi) = \psi(p\xi p) + \psi((1-p)\xi(1-p)) + \psi(p\xi(1-p)) + \psi((1-p)\xi p) \\ &= \psi(p\xi p) + \psi((1-p)\xi(1-p)). \end{aligned}$$

Since  $p\xi p$  and  $(1-p)\xi(1-p)$  are positive, faithfulness of  $\psi$  implies

$$p\xi p = (1-p)\xi(1-p) = 0.$$

By positivity of  $y_+ = x_+ + \xi$ , it follows for all  $t \in \mathbb{R}$  that

$$(p + t(1-p))y_+(p + t(1-p)) = x_+ + t(p\xi(1-p) + (1-p)\xi p)$$

is positive. Since  $p\xi(1-p) + (1-p)\xi p$  is self-adjoint, if it has a nonzero positive or negative part,  $x_+ + t(p\xi(1-p) + (1-p)\xi p)$  cannot be always positive. Therefore  $p\xi(1-p) + (1-p)\xi p = 0$ , hence  $\xi = (p + (1-p))\xi(p + (1-p)) = 0$ .  $\square$

**Lemma 7.4.** *Let  $B$  be a von Neumann algebra with a faithful tracial state  $\tau$ , and  $x_{\pm}, y_{\pm} \in B$  be positive elements satisfying*

$$x_+ - x_- = y_+ - y_-, \quad x_+x_- = x_-x_+ = 0$$

with  $\tau(x_+) = \tau(y_+), \tau(x_-) = \tau(y_-)$ . Then it follows that  $x_+ = y_+, x_- = y_-$ .

*Proof.* Since  $x_+x_- = x_-x_+ = 0$ , the range projection  $p$  of  $x_+$  satisfies  $px_+ = x_+ = x_+p$  and  $(1-p)x_- = x_- = x_-(1-p)$ . Since  $\tau$  is tracial, we also have  $\tau(p \cdot) = \tau(\cdot p)$ . Thus Lemma 7.3 shows  $x_+ = y_+, x_- = y_-$ .  $\square$

**Remark 7.5.** Note that the assumption  $\psi(p \cdot) = \psi(\cdot p)$  is essential in Lemma 7.3. Indeed we have the following counterexample without this property. Let  $B = M_2, \psi = \omega_q \circ \text{ad}(u) = \text{Tr}(u^*Qu \cdot)$  where  $Q = \frac{1}{1+q^2} \begin{pmatrix} 1 & 0 \\ 0 & q^2 \end{pmatrix}, q \in$

$(0, 1), u = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$ . Put

$$x_+ = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \geq 0, \quad x_- = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \geq 0, \quad \xi = \alpha \begin{pmatrix} 1 & \frac{1+q^2}{1-q^2} \\ \frac{1+q^2}{1-q^2} & 1 \end{pmatrix} : \text{s.a.},$$

for  $\alpha \in \left(0, \frac{(q^{-1}-q)^2}{4}\right]$ . It follows that

$$y_{\pm} = x_{\pm} + \xi \geq 0, \quad \psi(\xi) = 0, \text{ i.e., } \psi(x_{\pm}) = \psi(y_{\pm}),$$

and  $x_+, x_-$  are orthogonal projections, but  $\xi \neq 0$ .

*Proof.* We have

$$y_+ = \begin{pmatrix} 1 + \alpha & \frac{1+q^2}{1-q^2}\alpha \\ \frac{1+q^2}{1-q^2}\alpha & \alpha \end{pmatrix},$$

hence  $\text{Tr}(y_+) = 1 + 2\alpha > 0$  and

$$\det y_+ = \alpha + \alpha^2 \left(1 - \left(\frac{1+q^2}{1-q^2}\right)^2\right) = \alpha \left(1 - \alpha \frac{4q^2}{(1-q^2)^2}\right) \geq 0$$

show that  $y_+ \geq 0$ , and  $y_- \geq 0$  as well. By simple computation, we get

$$\psi(\xi) = \text{Tr}(u^*Qu\xi) = \frac{\alpha}{2} \text{Tr} \left( \begin{pmatrix} 1 & \frac{-1+q^2}{1+q^2} \\ \frac{-1+q^2}{1+q^2} & 1 \end{pmatrix} \begin{pmatrix} 1 & \frac{1+q^2}{1-q^2} \\ \frac{1+q^2}{1-q^2} & 1 \end{pmatrix} \right) = 0.$$

$\square$

**Lemma 7.6.** *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular undirected tracial quantum graph. It follows for any self-adjoint  $x \in \ker(d \text{id} - A)$  that  $C^*(x) \subset \ker(d \text{id} - A)$ .*

*Proof.* It suffices to show that  $Ap_i = dp_i$  for the spectral projections  $\{p_1, \dots, p_k\}$  of  $x = \sum_{i=1}^k \lambda_i p_i$  with  $\lambda_1 > \dots > \lambda_k$ . Consider  $\ker(d \text{id} - A) \ni x - \lambda_2 1_B = (\lambda_1 - \lambda_2)p_1 - \sum_{i=2}^k (\lambda_2 - \lambda_i)p_i$ , then

$$(\lambda_1 - \lambda_2)Ap_1 - \sum_{i=2}^k (\lambda_2 - \lambda_i)Ap_i = d(\lambda_1 - \lambda_2)p_1 - d \sum_{i=2}^k (\lambda_2 - \lambda_i)p_i.$$

Since  $(\lambda_1 - \lambda_2)p_1$  and  $\sum_{i=2}^k (\lambda_2 - \lambda_i)p_i$  are positive and have disjoint supports,  $\psi A = d\psi$  shows that we can apply Lemma 7.4. Thus

$$(\lambda_1 - \lambda_2)Ap_1 = d(\lambda_1 - \lambda_2)p_1,$$

hence  $p_1, \sum_{i=2}^k \lambda_i p_i \in \ker(d\text{id} - A)$ . Inductively we get  $p_1, \dots, p_k \in \ker(d\text{id} - A)$ . □

## 7.2 Connected quantum graphs

**Theorem 7.7.** *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular undirected tracial quantum graph. The following are equivalent:*

- (1)  $\mathcal{G}$  is connected.
- (2)  $d \in \text{spec}(A)$  is a simple root, i.e.,  $\dim \ker(d\text{id} - A) = 1$ .

*Proof.* If  $\dim B = 1$ , then  $\mathcal{G}$  is connected and  $d$  is simple. If  $\dim B \geq 2$  and  $d = 0$ , then  $A = 0$  by Lemma 2.35 and  $d$  has multiplicity  $\geq 2$ , whence there is an injective unital  $*$ -homomorphism  $f : \mathbb{C}^2 \rightarrow B$ . Hence neither  $\mathcal{G}$  is connected nor  $d$  is simple. In the sequel of the proof, we may assume  $d > 0$  and  $\dim B \geq 2$ .

((2)  $\implies$  (1)): We show that  $d$  is a multiple root if  $\mathcal{G}$  is disconnected.

We have an injective unital  $*$ -homomorphism  $f : \mathbb{C}^2 \rightarrow B$  such that  $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \bullet f^\dagger A f = f^\dagger A f$ . Put  $x_1 = f(e_1), x_2 = f(e_2) \in B$ , which are mutually orthogonal nonzero projections satisfying  $x_1 + x_2 = 1_B$ . The regularity shows  $Ax_1 + Ax_2 = A1_B = dx_1 + dx_2$ . By  $(f^\dagger A f)_{ij} = 2 \langle e_i | f^\dagger A f | e_j \rangle = 2 \langle x_i | Ax_j \rangle$  and  $\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \bullet f^\dagger A f = f^\dagger A f$ , it follows that

$$\begin{aligned} \langle x_1 | Ax_2 \rangle &= \langle x_2 | Ax_1 \rangle = 0; \\ \langle x_1 | Ax_1 \rangle &= \langle x_1 + x_2 | Ax_1 \rangle = \psi(Ax_1) = d\psi(x_1); \\ \langle x_2 | Ax_2 \rangle &= \langle x_1 + x_2 | Ax_2 \rangle = \psi(Ax_2) = d\psi(x_2). \end{aligned}$$

Thus  $Ax_1 = dx_1 + (dx_2 - Ax_2)$  gives the orthogonal decomposition of  $Ax_1$  along  $\mathbb{C}x_1 \oplus (x_1)^\perp$ . Then we have

$$d^2\psi(x_1) \geq \|Ax_1\|_2^2 = \|dx_1\|_2^2 + \|dx_2 - Ax_2\|_2^2 = d^2\psi(x_1) + \|dx_1 - Ax_2\|_2^2,$$

hence  $\|dx_2 - Ax_2\|_2 = 0$ , i.e.,  $Ax_2 = dx_2$  and  $Ax_1 = dx_1$ . Therefore  $d \in \text{spec}(A)$  has multiplicity more than 1.

((1)  $\implies$  (2)): We show that  $\mathcal{G}$  is disconnected if  $d$  is not simple.

By Lemma 2.36 and the multiplicity of  $d$ , there is a self-adjoint  $x \in \ker(d\text{id} - A) \setminus \mathbb{C}1$ , and Lemma 7.6 allows us to take mutually orthogonal

projections  $x_1, x_2 \in \ker(d \operatorname{id} - A)$  satisfying  $x_1 + x_2 = 1$  as spectral projections of  $x$ . Thus we obtain an injective  $*$ -homomorphism  $f : \mathbb{C}^2 \rightarrow B$  defined by  $f(e_i) = x_i$  for  $i = 1, 2$ . It satisfies

$$2 \langle e_i | f^\dagger A f | e_j \rangle = 2 \langle x_i | A x_j \rangle = 2d \langle x_i | x_j \rangle = 2d\psi(x_i)\delta_{ij}.$$

Thus  $f^\dagger A f = \begin{pmatrix} 2d\psi(x_1) & 0 \\ 0 & 2d\psi(x_2) \end{pmatrix}$ , which gives a surjective graph homomorphism  $f^{\text{op}} : \mathcal{G} \rightarrow T_2$ .  $\square$

### 7.3 Bipartite quantum graphs

**Theorem 7.8.** *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular connected undirected tracial quantum graph. The following are equivalent:*

- (1)  $\mathcal{G}$  is bipartite.
- (2)  $-d \in \operatorname{spec}(A)$ . If  $d = 0$ , we require that the multiplicity of  $0 \in \operatorname{spec}(A)$  is at least two, i.e.,  $\dim B \geq 2$ .

*Proof.* If  $\dim B = 1$ , then  $A = 0$  with simple root  $d = 0$  or  $A = \operatorname{id}_B$  with  $d = 1 \neq -d$ , hence neither bipartite nor  $-d \in \operatorname{spec}(A)$ . We may assume  $\dim B \geq 2$ , then the connectedness implies  $d > 0$  as argued in the proof of Theorem 7.7.

((1)  $\implies$  (2)): We have an injective unital  $*$ -homomorphism  $f : \mathbb{C}^2 \rightarrow B$  such that  $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \bullet f^\dagger A f = f^\dagger A f$ . Put  $x_1 = f(e_1), x_2 = f(e_2) \in B$ , which are mutually orthogonal nonzero projections satisfying  $x_1 + x_2 = 1_B$ . The regularity shows  $Ax_1 + Ax_2 = A1_B = dx_1 + dx_2$ . By  $(f^\dagger A f)_{ij} = 2 \langle e_i | f^\dagger A f | e_j \rangle = 2 \langle x_i | A x_j \rangle$  and  $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \bullet f^\dagger A f = f^\dagger A f$ , it follows that

$$\begin{aligned} \langle x_1 | A x_1 \rangle &= \langle x_2 | A x_2 \rangle = 0; \\ \langle x_1 | A x_2 \rangle &= \langle x_1 + x_2 | A x_2 \rangle = \psi(A x_2) = d\psi(x_2) \\ &= \overline{\langle x_2 | A x_1 \rangle} = d\psi(x_1). \end{aligned}$$

Thus  $\psi(x_1) = \psi(x_2) = 1/2$ , and  $Ax_1 = dx_2 + (dx_1 - Ax_2)$  gives the orthogonal decomposition of  $Ax_1$  along  $\mathbb{C}x_2 \oplus (x_2)^\perp$ . This yields

$$\frac{d^2}{2} = d^2\psi(x_1) \geq \|Ax_1\|_2^2 = \|dx_2\|_2^2 + \|dx_1 - Ax_2\|_2^2 = \frac{d^2}{2} + \|dx_1 - Ax_2\|_2^2,$$

hence  $\|dx_1 - Ax_2\|_2 = 0$ , i.e.,  $Ax_1 = dx_2$  and  $Ax_2 = dx_1$ . Therefore we obtain  $A(x_1 - x_2) = -d(x_1 - x_2)$ , which shows  $-d \in \operatorname{spec}(A)$ .

((2)  $\implies$  (1)): By Lemma 2.36, we can take a self-adjoint  $x \in \ker(d \operatorname{id} + A)$  with  $\|x\|_2 = 1$ . Decompose  $x = x_+ - x_-$  into positive and negative parts  $x_\pm \in B_+$ . Then we have

$$Ax_+ - Ax_- = Ax = -dx = dx_- - dx_+.$$

The self-adjointness of  $A$  implies the orthogonality of eigenvectors  $\psi(x) = \langle 1|x \rangle = 0$ , i.e.,  $\psi(x_+) = \psi(x_-)$ , hence the regularity implies  $\psi(Ax_\pm) = d\psi(x_\pm) = d\psi(x_\mp) = \psi(dx_\mp)$ . Note that the real quantum graph  $A$  is CP; hence  $Ax_\pm$  are positive. Since  $\psi$  is tracial and  $x_\pm$  have disjoint supports, Lemma 7.4 shows

$$Ax_\pm = dx_\mp.$$

Thus  $A(x_+ + x_-) = d(x_+ + x_-)$ . Since  $\mathcal{G}$  is connected, we get  $x_+ + x_- = c1_B$  for some  $c > 0$ . By  $1 = \|x\|_2^2 = \|x_+\|_2^2 + \|x_-\|_2^2 = \|x_+ + x_-\|_2^2 = c^2$ , we have  $c = 1, x_+ + x_- = 1_B$ . Then  $x_+x_- = 0$  shows  $x_\pm^2 = x_\pm(x_\pm + x_\mp) = x_\pm$ , hence  $x_\pm$  are mutually orthogonal projections with  $\psi(x_\pm) = 1/2$ . Thus we obtain an injective  $*$ -homomorphism  $f : \mathbb{C}^2 \rightarrow B$  defined by  $f(e_1) = x_+, f(e_2) = x_-$ . It satisfies

$$\begin{aligned} 2\langle e_i|f^\dagger Af|e_i \rangle &= 2\langle x_\pm|Ax_\pm \rangle = 2d\langle x_\pm|x_\mp \rangle = 0 \quad (i = 1, 2); \\ 2\langle e_1|f^\dagger Af|e_2 \rangle &= 2\langle x_+|Ax_- \rangle = 2d\langle x_+|x_+ \rangle = d. \end{aligned}$$

Thus  $f^\dagger Af = \begin{pmatrix} 0 & d \\ d & 0 \end{pmatrix}$ , which gives a surjective graph homomorphism  $f^{\text{op}} : \mathcal{G} \rightarrow K_2$ .  $\square$

**Theorem 7.9.** *Let  $\mathcal{G} = (B, \psi, A)$  be a  $d$ -regular undirected tracial quantum graph. The following are equivalent:*

- (1)  $\mathcal{G}$  has a bipartite component.
- (2)  $-d \in \text{spec}(A)$ . If  $d = 0$ , we require that the multiplicity of  $0 \in \text{spec}(A)$  is at least two, i.e.,  $\dim B \geq 2$ .

*Proof.* If  $\dim B = 1$ ,  $\mathcal{G} \rightarrow K_2 \sqcup T_1$  cannot be surjective to  $K_2$ . Hence  $\mathcal{G}$  does not have a bipartite component, and  $-d \in \text{spec}(A)$  does not hold as in the previous proof. If  $d = 0$  and  $\dim B \geq 2$ , then  $d = 0 = -d$  is the multiple root of  $A = 0$  and has a graph homomorphism  $\mathcal{G} \rightarrow K_2 \sqcup T_1$  that is surjective to  $K_2$ , hence  $\mathcal{G}$  has a bipartite component and  $-d \in \text{spec}(A)$ . In the sequel of the proof, we may assume  $d > 0$  and  $\dim B \geq 2$ .

((1)  $\implies$  (2)): We have a unital  $*$ -homomorphism  $f : \mathbb{C}^3 \rightarrow B$  such that  $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \bullet f^\dagger Af = f^\dagger Af$  and  $f$  is injective on  $\mathbb{C}^2 \oplus 0$ . Put  $x_i = f(e_i) \in B$  for  $i = 1, 2, 3$ , which are mutually orthogonal projections satisfying  $x_1 + x_2 + x_3 = 1$  and  $x_1, x_2$  are nonzero. Then the regularity implies

$$Ax_1 + A(1 - x_1) = A1_B = dx_2 + d(1 - x_2).$$

By  $(f^\dagger Af)_{ij} = 3 \langle e_i | f^\dagger Af | e_j \rangle = 3 \langle x_i | Ax_j \rangle$  and  $\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \bullet f^\dagger Af = f^\dagger Af$ ,

it follows that

$$\begin{aligned} \langle 1 - x_1 | Ax_2 \rangle &= \langle 1 - x_2 | Ax_1 \rangle = \langle 1 - x_3 | Ax_3 \rangle = 0; \\ \langle x_1 | Ax_2 \rangle &= \langle x_1 + (1 - x_1) | Ax_2 \rangle = \psi(Ax_2) = d\psi(x_2) \\ &= \overline{\langle x_2 | Ax_1 \rangle} = d\psi(x_1). \end{aligned}$$

Thus  $\psi(x_1) = \psi(x_2)$ , and  $Ax_1 = dx_2 + (d(1 - x_2) - A(1 - x_1))$  gives the orthogonal decomposition of  $Ax_1$  along  $\mathbb{C}x_2 \oplus (x_2)^\perp$ . Then we have

$$\begin{aligned} d^2\psi(x_1) &= \|A\|^2 \|x_1\|_2^2 \geq \|Ax_1\|_2^2 = \|dx_2\|_2^2 + \|d(1 - x_2) - A(1 - x_1)\|_2^2 \\ &= d^2\psi(x_2) + \|d(1 - x_2) - A(1 - x_1)\|_2^2, \end{aligned}$$

hence  $\|d(1 - x_2) - A(1 - x_1)\|_2 = 0$ , i.e.,  $A(1 - x_1) = d(1 - x_2)$  and  $Ax_1 = dx_2$ . By symmetry, we also have  $Ax_2 = dx_1$ . Therefore we obtain

$$A(x_1 - x_2) = -d(x_1 - x_2),$$

which shows  $-d \in \text{spec}(A)$ .

((2)  $\implies$  (1)): By Lemma 2.36, we can take a self-adjoint  $x \in \ker(d \text{id} + A)$ . Consider the spectral projections  $\{p_\lambda | \lambda \in \text{spec}(x)\}$  of

$$x = \sum_{\lambda} \lambda p_\lambda = \sum_{\lambda > 0} \lambda(p_\lambda - p_{-\lambda}); \quad x_+ = \sum_{\lambda > 0} \lambda p_\lambda; \quad x_- = \sum_{\lambda > 0} \lambda p_{-\lambda}.$$

In the same way as the proof of Theorem 7.8, we obtain  $Ax_\pm = dx_{\mp}$  and  $x_+ + x_- \in \ker(d \text{id} - A)$ . Therefore it follows from Lemma 7.6 that  $p_\lambda + p_{-\lambda} \in \ker(d \text{id} - A)$  for all  $\lambda > 0$ . Thus it follows for a fixed  $\lambda > 0$  that

$$Ap_\lambda = dp_\lambda + dp_{-\lambda} - Ap_{-\lambda} \leq dp_\lambda + dp_{-\lambda}. \quad (7.1)$$

Now  $\lambda p_\lambda \leq x_+$  implies

$$Ap_\lambda \leq \lambda^{-1} Ax_+ = \frac{d}{\lambda} x_- = \sum_{\mu > 0} \frac{d\mu}{\lambda} p_{-\mu}. \quad (7.2)$$

By taking the meet of (7.1) and (7.2) in the lattice of self-adjoint elements in the commutative algebra  $C^*(x)$ , we obtain

$$Ap_\lambda \leq (dp_\lambda + dp_{-\lambda}) \wedge \sum_{\mu > 0} \frac{d\mu}{\lambda} p_{-\mu} = dp_{-\lambda}. \quad (7.3)$$

Similarly we have  $Ap_{-\lambda} \leq dp_\lambda$ , i.e.,

$$Ap_\lambda = A(1 - p_{-\lambda}) \geq d(1 - p_\lambda) = dp_{-\lambda}. \quad (7.4)$$

Combining (7.3) and (7.4) we get  $Ap_\lambda = dp_{-\lambda}$  and  $Ap_{-\lambda} = dp_\lambda$ . Hence  $p_\lambda - p_{-\lambda} \in \ker(d\text{id} + A)$  for all  $\lambda > 0$ . Thus we may initially take  $x = x_+ - x_- \in \ker(d\text{id} + A)$  for mutually orthogonal nonzero projections  $x_\pm \in B$  satisfying

$$Ax_\pm = dx_{\mp}.$$

Then we have a \*-homomorphism  $f : \mathbb{C}^2 \oplus \mathbb{C} \rightarrow B$  defined by  $f(e_1) = x_+$ ,  $f(e_2) = x_-$ ,  $f(e_3) = 1 - x_+ - x_-$  that is injective on  $\mathbb{C}^2 \oplus 0$ . It satisfies

$$3 \langle e_i | f^\dagger A f | e_i \rangle = 3 \langle x_\pm | Ax_\pm \rangle = 3d \langle x_\pm | x_{\mp} \rangle = 0 \quad (i = 1, 2);$$

$$3 \langle e_1 | f^\dagger A f | e_2 \rangle = 3 \langle x_+ | Ax_- \rangle = 3d \langle x_+ | x_+ \rangle = 3d\psi(x_+);$$

$$3 \langle e_i | f^\dagger A f | e_3 \rangle = 3 \langle x_\pm | d1 - dx_+ - dx_- \rangle = 0 \quad (i = 1, 2);$$

$$3 \langle e_3 | f^\dagger A f | e_3 \rangle = 3d \langle 1 - x_+ - x_- | 1 - x_+ - x_- \rangle = 3d(1 - 2\psi(x_+)).$$

Thus  $f^\dagger A f = \begin{pmatrix} 0 & 3d\psi(x_+) & 0 \\ 3d\psi(x_+) & 0 & 0 \\ 0 & 0 & 3d(1 - 2\psi(x_+)) \end{pmatrix}$ , which gives a graph homomorphism  $f^{\text{op}} : \mathcal{G} \rightarrow K_2 \sqcup T_1$ .  $\square$

## 8 Two-colorability and bipartiteness

It is known that a classical graph is bipartite if and only if it is two-colorable. We compare the bipartiteness defined in this thesis and the local two-colorability introduced in [10].

### 8.1 $t$ -homomorphism

The gap of bipartiteness and two-colorability arises from the two notions of graph homomorphisms: one is Definition 7.1 and the other is the following  $t$ -homomorphisms:

**Definition 8.1** (Modified generalization of Brannan, Ganesan, Harris [10]). Let  $\mathcal{G}_0 = (B_0, \psi_0, A_0, \mathcal{S}_0), \mathcal{G}_1 = (B_1, \psi_1, A_1, \mathcal{S}_1)$  be quantum graphs with  $\delta_i$ -forms  $\psi_i$  and quantum relations  $\mathcal{S}_i = \text{range}(A_i \bullet \cdot) \subset B(L^2(\mathcal{G}_i))$ . A  $t$ -homomorphism  $(f, \mathcal{A}) : \mathcal{G}_0 \xrightarrow{t} \mathcal{G}_1$  ( $t \in \{loc, q, qa, qc, C^*, alg\}$ ) is consisting of a unital  $*$ -homomorphism  $f : B_1 \rightarrow B_0 \otimes \mathcal{A}$  and a unital  $*$ -algebra  $\mathcal{A}$  satisfying

$$f^\dagger(\mathcal{S}_0 \otimes 1_{\mathcal{A}})f \subset \mathcal{S}_1 \otimes \mathcal{A}, \quad (8.1)$$

where  $f^\dagger \in B(L^2(\mathcal{G}_0), L^2(\mathcal{G}_1)) \otimes \mathcal{A}$  is the adjoint  $(\cdot)^\dagger \otimes (\cdot)^*$  of  $f$  as an operator in  $B(L^2(\mathcal{G}_1), L^2(\mathcal{G}_0)) \otimes \mathcal{A}$ , and

- $\mathcal{A} = \mathbb{C}$  if  $t = loc$  (local, classical);
- $\mathcal{A}$  is finite-dimensional if  $t = q$  (quantum);
- $\mathcal{A} = \mathcal{R}^\omega$  is the ultrapower of the hyperfinite  $II_1$ -factor  $\mathcal{R}$  by a free ultrafilter  $\omega$  on  $\mathbb{N}$  if  $t = qa$  (quantum approximate);
- $\mathcal{A}$  is a tracial  $C^*$ -algebra if  $t = qc$  (quantum commuting);
- $\mathcal{A}$  is a  $C^*$ -algebra if  $t = C^*$ ;
- $\mathcal{A}$  is a unital  $*$ -algebra if  $t = alg$ .

These notions of  $t$  show what kind of quantum correlation is allowed in the corresponding graph homomorphism game.

We say that a  $t$ -homomorphism  $(f, \mathcal{A}) : \mathcal{G}_0 \xrightarrow{t} \mathcal{G}_1$  is:

- (vertex-)surjective if  $f : B_1 \rightarrow B_0 \otimes \mathcal{A}$  is injective.

This definition means that the pushforward of the edges of  $\mathcal{G}_0$  by the mapping  $(f, \mathcal{A})$  are edges of  $\mathcal{G}_1$ .



**Remark 8.2.** For a  $t$ -homomorphism  $(f, \mathcal{A}) : \mathcal{G}_0 \xrightarrow{t} \mathcal{G}_1$ , the best definition of (vertex-)injectivity is not sure. If it is a classical homomorphism between classical graphs, then  $(f, \mathcal{A} = \mathbb{C})$  is injective if and only if  $(\delta_0/\delta_1)f$  is a coisometry  $ff^\dagger = (\delta_1/\delta_0)^2 \text{id}_{B_1} \otimes 1_{\mathcal{A}}$ , so this is a candidate for the definition of injectivity. Another weaker candidate is the injectivity of  $f^\dagger : B_0 \rightarrow B_1 \otimes \mathcal{A}$ .

On the other hand, in classical case  $(f, \mathbb{C})$  is surjective if and only if  $f^\dagger f \geq (\delta_1/\delta_0)^2 \text{id}_{B_0} \otimes 1_{\mathcal{A}}$ , which may be too strong for the definition of surjectivity of general  $(f, \mathcal{A})$ .

Consider a toy model  $f : \mathbb{C}^4 \rightarrow \mathbb{C}^2 \otimes M_2$  of a quantum 4-coloring of 2 vertices  $(f, M_2) : (\mathbb{C}^2, \tau, 0) \xrightarrow{q} K_4$  given by

$$f(e_1) = e_1 \otimes e_{11}; \quad f(e_2) = e_2 \otimes e_{11}; \quad f(e_3) = e_1 \otimes e_{22}; \quad f(e_4) = e_2 \otimes e_{22}.$$

Then coisometry condition  $ff^\dagger = 2 \text{id}_{\mathbb{C}^2} \otimes 1_{M_2}$  holds, hence  $(f, M_2)$  is injective in the strong sense. On the other hand, we have an injective homomorphism  $f$  but  $f^\dagger f = 2[(e_1 + e_2) \otimes e_{11} + (e_3 + e_4) \otimes e_{22}] \not\geq 2 \text{id}_{\mathbb{C}^4} \otimes 1_{M_2}$ , hence  $(f, M_2)$  is surjective only in the weak sense as defined above.

**Notation.** For a quantum graph  $\mathcal{G} = (B, \psi, A)$  and a unital algebra  $\mathcal{A}$ , we abbreviate by  $A \bullet \cdot$  the left Schur product by  $A$  acting on the first tensor component of  $B(L^2(\mathcal{G})) \otimes \mathcal{A}$ .

If we faithfully represent  $\mathcal{A} \subset B(H)$  on a Hilbert space  $H$ , we may regard  $f : B_1 \rightarrow B_0 \otimes \mathcal{A}$  as  $f : L^2(\mathcal{G}_1) \otimes H \rightarrow H \otimes L^2(\mathcal{G}_0) \in B(L^2(\mathcal{G}_1), L^2(\mathcal{G}_0)) \otimes B(H)$ . By this identification, we denote  $f$  in string diagrams by

$$f = \begin{array}{c} H \\ \swarrow \quad \searrow \\ \textcircled{f} \\ \swarrow \quad \searrow \\ B_1 \quad H \end{array},$$

where  $H$  is drawn as oriented strings. Even if  $\mathcal{A}$  is not a  $C^*$ -algebra, such a diagram formally makes sense by thinking of the string of  $H$  as an indicator of the order of multiplication in  $\mathcal{A}$ .

Note that  $f$  is unital; multiplicative;  $*$ -preserving (real) respectively if and only if the following are satisfied:

$$\begin{array}{c} \textcircled{f} \\ \swarrow \quad \searrow \\ \circ \end{array} = \begin{array}{c} \swarrow \quad \searrow \\ \circ \end{array}; \quad \begin{array}{c} \textcircled{f} \\ \swarrow \quad \searrow \\ \textcircled{f} \end{array} = \begin{array}{c} \textcircled{f} \\ \swarrow \quad \searrow \\ \textcircled{f} \end{array}; \quad \begin{array}{c} \textcircled{f^\dagger} \\ \swarrow \quad \searrow \\ \textcircled{f} \end{array} = \begin{array}{c} \textcircled{f} \\ \swarrow \quad \searrow \\ \textcircled{f} \end{array}. \quad (8.2)$$

**Proposition 8.3.** Let  $(f, \mathcal{A}) : \mathcal{G}_0 \xrightarrow{t} \mathcal{G}_1$  be as in Definition 8.1 without assumption (8.1). The following are equivalent:

- (1) The inclusion (8.1):  $f^\dagger(\mathcal{S}_0 \otimes 1_{\mathcal{A}})f \subset \mathcal{S}_1 \otimes \mathcal{A}$ ;
- (2)  $A_1 \bullet (f^\dagger(A_0 \bullet T \otimes 1_{\mathcal{A}})f) = f^\dagger(A_0 \bullet T \otimes 1_{\mathcal{A}})f$  for any  $T \in B(L^2(\mathcal{G}_0))$ ;



Therefore it follows by the realness (8.2) of  $f$  that

$$\text{Diagram with } f, A_0, A_1 = \delta_1^2 \cdot \text{Diagram with } f, A_0$$

((4)  $\implies$  (2)): We can transform the diagrams conversely to go back from (4) to (2).  $\square$

Note that [10] defined the quantum-to-classical  $t$ -homomorphisms by the following conditions instead of (8.1) to omit self-loops in particular for the coloring problem.

$$f^\dagger(\mathcal{S}_0 \cap \mathcal{S}_{T(B_0, \psi_0)}^\perp \otimes 1_{\mathcal{A}})f \subset \mathcal{S}_1 \otimes \mathcal{A}; \tag{8.3}$$

$$f^\dagger(\mathcal{S}_{T(B_0, \psi_0)} \otimes 1_{\mathcal{A}})f \subset \mathcal{S}_{T(B_1, \psi_1)} \otimes \mathcal{A}. \tag{8.4}$$

(8.1) and (8.3) coincide under some assumptions, and as a generalization of [10, Lemma 4.8], the second condition (8.4) is redundant as shown below.

**Lemma 8.4.** *Let  $(f, \mathcal{A}) : \mathcal{G}_0 \xrightarrow{t} \mathcal{G}_1$  be as in Definition 8.1 without assumption (8.1).*

- (1) *The inclusion (8.4) always holds.*
- (2) *(8.1) is equivalent to (8.3) if  $\mathcal{G}_0$  is irreflexive, or if  $\mathcal{G}_0$  has no partial loops and  $\mathcal{G}_1$  is reflexive.*

*Proof.* (1) Recall that the adjacency matrix of the trivial graph  $T(B_i, \psi_i)$  is  $\text{id}_{B_i}$ . Thus (8.4) is equivalent to

$$\text{Diagram with } f, f = \delta_1^2 \cdot \text{Diagram with } f, f$$

This is proved by the multiplicativity (8.2) of  $f$  and Frobenius equality:

$$\text{Diagram with } f, f = \text{Diagram with } f, f \stackrel{(8.2)}{=} \text{Diagram with } f, f$$

$$\stackrel{(\delta_1\text{-form})}{=} \delta_1^2 \cdot \text{Diagram with } f, f \stackrel{(8.2)}{=} \delta_1^2 \cdot \text{Diagram with } f, f$$

(2) (i) If  $\mathcal{G}_0$  is irreflexive, then  $\mathcal{S}_0 \subset \mathcal{S}_{T(B_0, \psi_0)}^\perp = \mathcal{S}_{K(B_0, \psi_0)}$ . Thus (8.3) is exactly equal to (8.1). (ii) Note that (8.1) always implies (8.3) by the trivial inclusion

$$f^\dagger(\mathcal{S}_0 \cap \mathcal{S}_{T(B_0, \psi_0)}^\perp \otimes 1_{\mathcal{A}})f \subset f^\dagger(\mathcal{S}_0 \otimes 1_{\mathcal{A}})f \stackrel{(8.1)}{\subset} \mathcal{S}_1 \otimes \mathcal{A}.$$

If  $\mathcal{G}_1$  is reflexive, then  $\mathcal{S}_{T(B_1, \psi_1)} \subset \mathcal{S}_1$ , and no partial loops means that  $\mathcal{S}_0 = \mathcal{S}_0 \cap \mathcal{S}_{T(B_0, \psi_0)}^\perp \oplus \mathcal{S}_0 \cap \mathcal{S}_{T(B_0, \psi_0)}$  gives an orthogonal decomposition. Thus (8.4) and (8.3) implies

$$\begin{aligned} f^\dagger(\mathcal{S}_0 \otimes 1_{\mathcal{A}})f &\subset f^\dagger((\mathcal{S}_0 \cap \mathcal{S}_{T(B_0, \psi_0)}^\perp \oplus \mathcal{S}_{T(B_0, \psi_0)}) \otimes 1_{\mathcal{A}})f \\ &\stackrel{(8.3)}{\subset} (\mathcal{S}_1 + \mathcal{S}_{T(B_1, \psi_1)}) \otimes \mathcal{A} \stackrel{(8.4)}{=} \mathcal{S}_1 \otimes \mathcal{A}. \end{aligned}$$

□

**Remark 8.5.** For a quantum-to-classical  $t$ -homomorphism  $(f, \mathcal{A}) : \mathcal{G}_0 \xrightarrow{t} \mathcal{G}_1 = (\mathbb{C}^n, \tau, A_1)$ , Proposition 8.3 (4) is equivalent to the existence of projections  $P_1, \dots, P_n \in B_0 \otimes \mathcal{A}$  satisfying  $P_i(\mathcal{S}_0 \otimes \mathcal{A})P_j = 0$  for all  $(i, j)$  with  $\langle e_i | A_1 | e_j \rangle = 0$ . Indeed, RHS–LHS of (4) with input  $e_i \otimes e_j$  yields

$$0 = n^{-1} \begin{array}{c} \begin{array}{ccc} & & A_0 \\ & \nearrow & \downarrow \\ f & & f \\ \downarrow & \searrow & \downarrow \\ e_i & & e_j \\ & \nwarrow & \uparrow \\ & & A_1^c \end{array} \\ \end{array} = f(e_i)(A_0 \otimes 1_{\mathcal{A}})f(e_j)$$

where  $A_1^c = J - A_1$  is the complement of  $A_1$  satisfying  $n \langle e_i | A_1^c | e_j \rangle = 1$ . We may put  $P_i = f(e_i)$  and take Schur product with  $\mathcal{S}_0$  from the right to obtain  $P_i(\mathcal{S}_0 \otimes \mathcal{A})P_j = 0$ . Conversely, if we have  $P_i$ 's, then the desired  $f$  is given by  $f(e_i) = P_i$ .

The notion of local homomorphism is stronger than that of graph homomorphism as follows.

**Proposition 8.6.** *Let  $(f, \mathbb{C}) : \mathcal{G}_0 \xrightarrow{loc} \mathcal{G}_1$  be a loc-homomorphism. Then  $f^{\text{op}} : \mathcal{G}_0 \rightarrow \mathcal{G}_1$  is a graph homomorphism.*

*Proof.* Since  $A_0 \in \mathcal{S}_0$  and  $\mathbb{C}$  is the tensor unit, Proposition 8.3 (2) with  $T = A_0$  shows  $A_1 \bullet (f^\dagger A_0 f) = f^\dagger A_0 f$ . □

The following theorem gives a sufficient condition to make the two notions of homomorphisms coincide.

**Theorem 8.7.** *Let  $\mathcal{G}_j = (B_j, \psi_j, A_j, \mathcal{S}_j)$  for  $j = 0, 1$  be real quantum graphs with  $\delta_j$ -forms  $\psi_j$  and quantum relations  $\mathcal{S}_j = \text{range}(A_j \bullet \cdot) \subset B(L^2(\mathcal{G}_j))$ . Suppose that  $f : B_1 \rightarrow B_0$  is modular invariant  $\sigma_i \circ f = f = f \circ \sigma_i$  and  $\mathcal{G}_1$  is Schur central. Then  $f^{\text{op}} : \mathcal{G}_0 \rightarrow \mathcal{G}_1$  is a graph homomorphism if and only if  $(f, \mathbb{C}) : \mathcal{G}_0 \rightarrow \mathcal{G}_1$  is a loc-homomorphism.*

*Proof.* Proposition 8.6 shows that a local homomorphism is a graph homomorphism. It suffices to show the converse, i.e.,

$$\langle S|f^\dagger T f\rangle_{\Psi_1} = \delta_1^2 \langle 1_{B_1}|S^* \bullet (f^\dagger T f)|1_{B_1}\rangle_{\Psi_1} = \textcircled{S^*} \boxed{f^\dagger T f} = 0 \quad (8.5)$$

holds for any  $T \in S_0$  and  $S \in S_1^\perp$  from the assumption that (8.5) holds for  $T = A_0$ .

Take  $T$  as a normal vector  $\langle T|T\rangle_{\Psi_0} = 1$  in  $S_0$ .

By the following Lemma 8.8, we may assume that  $S \in S_1^\perp$  is a Schur projection because  $\mathcal{G}_1$  is Schur central and so is its complement  $(B_1, \psi_1, J - A_1, S_1^\perp = \text{range}(J - A_1))$ .

**Lemma 8.8.** *Let  $\mathcal{G} = (B, \psi, A, \mathcal{S})$  be a real quantum graph. Then  $\mathcal{G}$  is Schur central if and only if  $\mathcal{S}$  is generated by Schur projections.*

And the modular invariance of  $f$  enables us to eliminate loops in diagrams as follows:

$$\begin{array}{c} \textcircled{f^\dagger} \quad (f: \text{real}) \quad \textcircled{f} \quad (f\sigma_i=f) \quad \textcircled{f} \\ \textcircled{f} \quad (\sigma_{-i}f=f) \quad \textcircled{f} \quad (f: \text{real}) \quad \textcircled{f^\dagger} \end{array} ; \quad (8.6)$$

Now we have

$$\begin{aligned} 0 &= \textcircled{S^*} \boxed{f^\dagger A_0 f} \stackrel{(S^*=S=S \bullet S)}{=} \delta_1^{-2} \textcircled{S^*} \textcircled{S} \boxed{f^\dagger A_0 f} = \delta_1^{-2} \textcircled{S^*} \textcircled{S} \boxed{f^\dagger A_0 f} \\ &\stackrel{(f: \text{hom})}{=} \delta_1^{-2} \textcircled{S^*} \textcircled{S} \textcircled{A_0} \textcircled{f} \textcircled{f} \textcircled{f^\dagger} \textcircled{f^\dagger} = \delta_1^{-2} \textcircled{S} \textcircled{A_0} \textcircled{S^*} \textcircled{f^\dagger} \textcircled{f^\dagger} \textcircled{f} \textcircled{f} \stackrel{(f: \text{real})}{=} \delta_1^{-2} \boxed{f S f^\dagger} \textcircled{A_0} \boxed{f S^* f^\dagger} \end{aligned}$$

$$= \delta_1^{-2} \left( \begin{array}{c} \boxed{fSf^\dagger} \\ \circlearrowleft A_0 \\ \boxed{fS^*f^\dagger} \end{array} \right) \stackrel{(8.6)}{=} \delta_1^{-2} \left( \begin{array}{c} \boxed{fSf^\dagger} \\ \circlearrowleft A_0 \\ \boxed{fS^\dagger f^\dagger} \end{array} \right) \stackrel{(2.16)}{=} \delta_0^2 \delta_1^{-2} \left( \begin{array}{c} \boxed{fSf^\dagger} \\ \boxed{P_{A_0}} \\ \boxed{fS^\dagger f^\dagger} \end{array} \right),$$

where the non-indicated equalities are continuous deformations.

Recall (2.16) that  $P_{A_0} = \delta_0^{-2} \left| \begin{array}{c} \circlearrowleft A_0 \end{array} \right|$  is a projection onto  $\iota(\mathcal{S}_0) \subset B_0 \otimes B_0$ .

Since  $\iota(T) \in \iota(\mathcal{S}_0)$ , the rank one projection  $|\iota(T)\rangle \langle \iota(T)| = \left( \begin{array}{c} \circlearrowleft T \\ \circlearrowleft T^\dagger \end{array} \right)$  is smaller than or equal to  $P_{A_0}$ , hence  $P = P_{A_0} - |\iota(T)\rangle \langle \iota(T)|$  is also a projection. Therefore we obtain

$$0 = \delta_0^2 \delta_1^{-2} \left( \begin{array}{c} \boxed{fSf^\dagger} \circlearrowleft T \\ \boxed{fS^\dagger f^\dagger} \circlearrowleft T^\dagger \end{array} + \begin{array}{c} \boxed{fSf^\dagger} \\ \boxed{P} \\ \boxed{fS^\dagger f^\dagger} \end{array} \right).$$

By the vertical symmetry, each term is nonnegative, hence they must be zero. The first term is what we desired:

$$0 = \left| \begin{array}{c} \boxed{fSf^\dagger} \circlearrowleft T \end{array} \right|^2 \stackrel{(f:\text{real})}{=} \left| \begin{array}{c} \circlearrowleft S \boxed{f^\dagger T f} \end{array} \right|^2 \stackrel{(S:\text{real})}{=} |\langle S | f^\dagger T f \rangle|^2.$$

□

**Theorem 8.9.** *Let  $\mathcal{G}_j = (B_j, \psi_j, A_j, \mathcal{S}_j)$  for  $j = 0, 1$  be real tracial quantum graphs such that  $\mathcal{G}_1$  is Schur central. Then  $f^{\text{op}} : \mathcal{G}_0 \rightarrow \mathcal{G}_1$  is a graph homomorphism if and only if  $(f, \mathbb{C}) : \mathcal{G}_0 \rightarrow \mathcal{G}_1$  is a loc-homomorphism.*

*Proof.* Since each  $\psi_j = \text{Tr}(Q_j \cdot)$  is tracial, the density  $Q_j$  is central and its modular automorphism is  $\sigma_i = Q_j^{-1}(\cdot)Q_j = \text{id}_{B_j}$ . Thus we have  $\sigma_i \circ f = f = f \circ \sigma_i$ . Therefore the statement follows from Theorem 8.7. □

*Proof of Lemma 8.8.* Since the statement depends only on the Schur product structure, it suffices to show for a von Neumann algebra  $\mathcal{M}(= B^{\text{op}} \otimes B)$  and a projection  $p \in \mathcal{M}$  that  $p$  is central if and only if  $p\mathcal{M}$  is linearly generated by projections in weak operator topology (WOT).

Suppose  $p$  is central, then  $p\mathcal{M} = p\mathcal{M}p$  is a WOT-closed subalgebra of  $\mathcal{M}$ . Then we can decompose  $x \in p\mathcal{M}p$  into real and imaginary parts, which have spectral projections in  $p\mathcal{M}p$ . Since  $x$  lies in the WOT-closed linear span of such spectral projections, we are done.

Suppose that  $p\mathcal{M}$  is generated by projections. It follows for any projection  $q \in p\mathcal{M}$  that  $pq = q = q^* = qp$ . Since such projections  $q$  span  $p\mathcal{M}$  in WOT, we have  $px = pxp$  for any  $x \in \mathcal{M}$ , and  $px^* = px^*p$  as well. Thus we get  $px = xp$ , i.e.,  $p$  is central.  $\square$

## 8.2 $t$ -2 colorability compared with bipartiteness

**Definition 8.10** ([10]). Let  $t \in \{loc, q, qa, qc, C^*, alg\}$  and  $c \in \mathbb{Z}_{>0}$ . A quantum graph  $\mathcal{G}$  is  $t$ - $c$  colorable if there exists a  $t$ -homomorphism  $\mathcal{G} \rightarrow K_c$ , which is called a  $t$ - $c$  coloring of  $\mathcal{G}$ . The  $t$ -chromatic number of  $\mathcal{G}$  is defined by  $\chi_t(\mathcal{G}) = \inf\{c \in \mathbb{Z}_{>0} \mid \mathcal{G} : t\text{-}c \text{ colorable}\}$ .

Note that a  $t$ - $c$  coloring need not be a surjective  $t$ -homomorphism. Surjectivity means that it uses all the  $c$  colors.

**Remark 8.11.** By the obvious inclusion of the classes of algebras,  $c$ -colorability has the following implication:  $loc \Rightarrow q \Rightarrow qa \Rightarrow qc \Rightarrow C^* \Rightarrow alg$ , and hence the chromatic numbers satisfy

$$\chi_{loc} \geq \chi_q \geq \chi_{qa} \geq \chi_{qc} \geq \chi_{C^*} \geq \chi_{alg}.$$

**Proposition 8.12.** Let  $\mathcal{G} = (B, \psi, A)$  be an  $alg$ -2 colorable real quantum graph. Then  $\mathcal{G}$  has a symmetric spectrum  $\text{spec } A = -\text{spec } A$ . Moreover, if it is  $q$ -2 colorable, then the symmetry of the spectrum holds with its multiplicity.

*Proof.* If  $A = 0$ , the statement is trivial. So we may assume  $A \neq 0$ . Let  $(f, \mathcal{A}) : \mathcal{G} \rightarrow K_2 = (\mathbb{C}^2, \tau, A_{K_2}, \mathcal{S}_{K_2})$  be an  $alg$ -homomorphism. In this case  $(f, \mathcal{A})$  is automatically surjective, i.e.,  $f : \mathbb{C}^2 \rightarrow B \otimes \mathcal{A}$  is injective. Indeed if  $f$  is not injective, then we may assume  $f(e_1) = 1_B \otimes 1_{\mathcal{A}}$  and  $f(e_2) = 0$  without loss of generality. But this implies for  $e_1 e_1^\dagger \in \mathcal{S}_{K_2}^\perp$  that  $\langle e_1 e_1^\dagger \mid f^\dagger(A \otimes 1_{\mathcal{A}})f \rangle_{\text{Tr}} = \langle e_1 \mid f^\dagger(A \otimes 1_{\mathcal{A}})f \mid e_1 \rangle_\tau = \langle 1 \mid A \mid 1 \rangle_\psi 1_{\mathcal{A}} \neq 0$  by Lemma 2.35, which contradicts that  $(f, \mathcal{A})$  is an  $alg$ -homomorphism (Proposition 8.3 (3)).

Now we have nonzero projections  $P_j = \lambda(f(e_j)) \in B(L^2(\mathcal{G})) \otimes \mathcal{A}$ , where  $\lambda$  denotes the left multiplication, satisfying  $P_j(A \otimes 1_{\mathcal{A}})P_j = 0$  for each  $j = 1, 2$ . Then we have

$$A \otimes 1_{\mathcal{A}} = P_1(A \otimes 1_{\mathcal{A}})P_2 + P_2(A \otimes 1_{\mathcal{A}})P_1.$$

and hence

$$\begin{aligned} (A \otimes 1_{\mathcal{A}})(P_1 - P_2) &= P_2(A \otimes 1_{\mathcal{A}})P_1 - P_1(A \otimes 1_{\mathcal{A}})P_2 \\ &= (P_2 - P_1)(A \otimes 1_{\mathcal{A}}), \\ ((\alpha \text{id} + A) \otimes 1_{\mathcal{A}})(P_1 - P_2) &= (P_1 - P_2)((\alpha \text{id} - A) \otimes 1_{\mathcal{A}}) \end{aligned}$$

It follows for  $\alpha \in \text{spec } A$  and  $v \in \ker(\alpha \text{id}_B - A)$  that  $(P_1 - P_2)v \in \ker(\alpha \text{id}_B + A) \otimes \mathcal{A}$ . Indeed  $v$  satisfies

$$((\alpha \text{id} + A) \otimes 1_{\mathcal{A}})(P_1 - P_2)v = (P_1 - P_2)((\alpha \text{id} - A) \otimes 1_{\mathcal{A}})v = 0.$$

For a generalized eigenvector  $v \in \ker(\alpha \text{id}_B - A)^k$  for some positive integer  $k$ , we similarly have  $(P_1 - P_2)v \in \ker(\alpha \text{id}_B + A)^k \otimes \mathcal{A}$  by

$$((\alpha \text{id} + A)^k \otimes 1_{\mathcal{A}})(P_1 - P_2)v = (P_1 - P_2)((\alpha \text{id} - A)^k \otimes 1_{\mathcal{A}})v = 0.$$

Therefore  $-\alpha \in \text{spec } A$ , i.e.,  $\mathcal{G}$  has a symmetric spectrum.

If  $(f, \mathcal{A})$  is a  $q$ -2 coloring, then  $\mathcal{A} \subset M_n = B(\mathbb{C}^n)$  for some positive integer  $n$ . Thus  $P_1 - P_2$  restricts to linear isomorphisms between generalized eigenspaces  $\ker(\alpha \text{id}_B - A)^{\dim B} \otimes \mathbb{C}^n \cong \ker(\alpha \text{id}_B + A)^{\dim B} \otimes \mathbb{C}^n$ , hence the multiplicities coincide as  $\dim \ker(\alpha \text{id}_B - A)^{\dim B} = \dim \ker(\alpha \text{id}_B + A)^{\dim B}$ .  $\square$

**Theorem 8.13.** *Let  $\mathcal{G} = (B, \psi, A)$  be a real tracial quantum graph. Then  $\mathcal{G}$  is bipartite if and only if it is  $loc$ -2 colorable.*

*Proof.* By Theorem 8.9, the existence of a graph homomorphism  $\mathcal{G} \rightarrow K_2$  is equivalent to the existence of a  $loc$ -homomorphism  $\mathcal{G} \rightarrow K_2$  because these are tracial real quantum graphs and the classical  $K_2$  is Schur central. Thus  $\mathcal{G}$  is bipartite if and only if it is  $loc$ -2 colorable.  $\square$

**Corollary 8.14.** *Let  $\mathcal{G} = (B, \psi, A)$  be a connected  $d$ -regular undirected tracial quantum graph. The following are equivalent:*

- (1)  $\mathcal{G}$  is  $loc$ -2 colorable;
- (2)  $\mathcal{G}$  is  $alg$ -2 colorable;
- (3)  $\mathcal{G}$  has a symmetric spectrum;
- (4)  $-d \in \text{spec}(A)$ . If  $d = 0$ , we require  $\dim B \geq 2$ ;
- (5)  $\mathcal{G}$  is bipartite.

*In this case, the symmetry of the spectrum in (3) holds with multiplicity.*

*Proof.* ((1)  $\implies$  (2)): Obvious by definition.

((2)  $\implies$  (3)): The symmetry follows from Proposition 8.12. In particular, if we assume (1), the symmetry holds with multiplicity.

((3)  $\implies$  (4)): Since  $\mathcal{G}$  is  $d$ -regular, the symmetry of spectrum shows  $-d \in \text{spec } A$ .

((4)  $\implies$  (5)): This is shown by Theorem 7.8 as we assumed that  $\mathcal{G}$  is connected.

((5)  $\implies$  (1)): This is the direct consequence of Theorem 8.13.  $\square$

In particular, this means that all kinds of  $t$ -2 colorability are mutually equivalent for connected regular undirected tracial quantum graphs.



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