Logical Aspects of Probability and Quantum Computation

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Submitted in Partial Fulfilment of the Requirements
For the Degree of Doctor of Philosophy
University College London
UCL

I, Octavio Baltasar Zapata Fonseca confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the thesis.

Abstract

Most of the work presented in this document can be read as a sequel to previous work of the author and collaborators, which has been published and appears in [DSZ16, DSZ17, ABdSZ17]. In [ABdSZ17], the mathematical description of quantum homomorphisms of graphs and more generally of relational structures, using the language of category theory is given. In particular, we introduced the concept of 'quantum' monad. In this thesis we show that the quantum monad fits nicely into the categorical framework of *effectus* theory, developed by Jacobs et al. [Jac15, CJWW15]. Effectus theory is an emergent field in categorical logic aiming to describe logic and probability, from the point of view of classical and quantum computation. The main contribution in the first part of this document prove that the Kleisli category of the quantum monad on relational structures is an effectus. The second part is rather different. There, distinct facets of the equivalence relation on graphs called *cospectrality* are described: algebraic, combinatorial and logical relations are presented as sufficient conditions on graphs for having the same spectrum (*i.e.* being 'cospectral'). Other equivalence of graphs (called *fractional* isomorphism) is also related using some 'game' comonads from Abramsky et al. [ADW17, Sha17, AS18]. We also describe a sufficient condition for a pair of graphs to be cospectral using the quantum monad: two Kleisli morphisms (going in opposite directions) between them satisfying certain compatibility requirement.

Impact Statement

This thesis follows the tradition of using category theory to combine concepts across disciplines that are not yet related, with the hope of provide sensible definitions at a formal level, and then use them to single out fundamental aspects along with potential new applications. The work presented in this thesis could be put to a beneficial use inside academia. The main focus is on the flow of ideas between logic and computation, on the one side, and the foundations of quantum and probabilistic reasoning , on the other. We emphasise the logical and structural aspects of this connection, since this gives a more specific focus, and also because we see many very exciting possibilities for progress and increasing interactions between the various scientific communities involved. Therefore, the benefits of this document could be on the computer science field of semantics of quantum computation. These benefits could be brought about through increasing the interaction of researchers within this very active field, by the use of a conceptual framework developed for embracing the common ground of ideas. In general, this is what category-theoretic methods have brought within pure mathematics and logic, so it makes sense to keep using them in more applied areas of mathematics and logic in computer science as *e.g.* probability, statistics, and artificial intelligence. This however, only starts to be seen, for instance in categorical foundations of probabilistic and quantum computation, as briefly expounded within this document.

Acknowledgements

This research has been financially supported by the Mexican government through the National Council of Science and Technology (CONACyT).

The author would like to thank Samson Abramsky, Anuj Dawar, Carlos Gershenson, Robin Hirsch, Bart Jacobs, Aleks Kissinger, Phokion Kolaitis, Marco Larrea, Ricardo Mansilla, Sandra Palau, Matteo Sammartino, Simone Severini, Alexandra Silva, Nadish de Silva, Rui Soares Barbosa and Fabio Zanasi for their patience and guidance during this mathematics (never-ending) learning process. Also thanks to the places and institutions in which I have had some thoughts related to this work: University College London, University of Cambridge, Simons Institute for the Theory of Computing, University of Oxford, Lorentz Center, University of Leeds, and Centro de Ciencias de la Complejidad.

This thesis is dedicated with all my heart to my parents, Lilia Fonseca and German Zapata, and my brother Leonardo, for everything they have given me, and also for what they haven't.

Contents

Chapter 1

Introduction

Over the past decades, starting with the work of Moggi [Mog89, Mog91], monads have been widely used to provide a categorical semantics of computation. In this framework, data types are identified with objects $A, B, \ldots$ of a given category $\mathbf{C}$, and programs of type B taking parameters of type A with morphisms $A \to TB$ in $\mathbf{C}$. The unary type-constructor T is interpreted as the functor part of a monad defined on $\mathbf{C}$, whose monadic structure allows programs to be composed and thus form a category indeed (the so-called Kleisli category $\mathcal{K}\ell(T)$). By changing the choice of T one obtains different notions of computation such as partiality, non-determinism, side-effects, exceptions, inputs and outputs, etc. For a historical overview of monads within mathematics and logic in computer science, we refer the interested reader to the monograph by Manes [Man03].

In the present document, we explore several aspects of probability and quantum computation by defining suitable monads on distinct concrete categories (*e.g.* on sets, graphs, or more generally, relational structures). Morphisms in the corresponding Kleisli categories of these monads represent some kind of probabilistic or quantum processes between objects of the underlying categories. Specifically, we shall be interested in the categorical/logical structure of these

Kleisli morphisms. This view naturally yields a modular way to reason about the logic of probability and computation, from classical to quantum.

Building on the work of Giry [Gir82], and inspired by algebraic methods in program semantics [Koz79, JP89, DDLP06, VW06, TKP09, Pan09], the study of various 'probability' monads has evolved and became part of a new branch of categorical logic called effectus theory. The main goal of effectus theory is to describe the essentials of quantum computation and logic using the language of category theory. This description includes probabilistic and classical logic and computation as special cases. Various publications have promoted the theory, see *e.g.* [Jac10, Jac11, Jac13, Fon13, Jac15, CJWW15, Jac16, JZ16, CJ17a, CJ17b, ABdSZ17, Jac18b, Jac18c, JZ18, Jac18a]. The present work is a contribution to this subject: it shows that the *quantum* monad of [ABdSZ17] fits nicely into this effect-theoretic framework.

An effectus is a rather convenient environment for reasoning about the logic of probability and quantum computation, categorically. More concretely, it is a category with finite coproducts $(+, 0)$ and a final object 1 satisfying two pullback conditions, and one joint monicity requirement (see Definition 2.3.1). The central feature of an effectus $\mathbf{B}$ is that its maps of type $A \to 1 + 1$ form an effect module, *i.e.* $\mathbf{B}(A, 1 + 1) \in \mathbf{EMod}$ for any $A \in \mathbf{B}$; these maps are called predicates and they are thought as the logical abstraction of characteristic functions. This approach emphasises a more 'quantitative' interpretation of predicates as characteristic maps, suitable for quantum and probabilistic *reasoning*. The logic of this predicates is called effect logic [Jac13]. The word 'effect' suggests emphasis in the observer's effect after a measurement procedure has been performed. In quantum computation, one can even make use of these effects to show advantages in tasks which require processing information efficiently, such as constraint satisfaction problems via non-local games [CMN^{+}07, Rob, MR14, CM14, MR16, ABdSZ17, AMR^{+}18].

To put things into context, we start in Chapter 2 reviewing standard framework in effectus theory, describing the mathematical structures of effect algebras, effect modules, and effectuses in general. The main original work presented, in Chapter 3 of this document, consists of introducing the quantum monad on relational structures, which we claim fits into the framework of 'probabilistic' effectuses. We summarise and extend previous work done and published in [ABdSZ17]. Specifically, we show that the Kleisli category of the quantum monad is an effectus (see Theorem 3.3.1). We also explore the notions of states and predicates, validity and conditioning in $\mathcal{K}\ell(\mathcal{Q}_d)$. Supplementary material on the quantum monad is contained in the Appendix A. All of these correspond to this first part of the thesis.

Part two is rather different. It is a summary of various results published by the author and collaborators in [DSZ16, DSZ17]. The relationship with the material in the first part is minimal. Chapter 4 is about graphs and several equivalence relations defined on them, coarser than graph isomorphism, and in relation to *cospectrality*: the equivalence relation on graphs defined by having the same multiset of (adjacency matrix) eigenvalues. The concept of 'game' comonads, introduced by Abramsky et al. [ADW17, Sha17, AS18], is used in Chapter 5 to characterise as coKleisli isomorphisms, in particular, two of the relaxations of graph isomorphism described in the previous chapter. These two relaxations are related to both cospectrality and *quantum* graph isomorphism. Quantum isomorphisms emerge from two maps in the Kleisly category of the quantum monad of part one satisfying certain pairing requirement (see Theorem 5.3.2). An attempt to describe graph spectra, monadically, can be founded in the Appendix B. We finish this document with some concluding remarks and future work in Chapter 6.

Chapter 2

Preliminaries

Prior working knowledge on basic concepts from (fibred) category theory, linear algebra, and first-order logic shall be assumed and used without being formally introduced. The standard references shall be [Jac99, Awo10, Lei14]. The following presentation is standard in the literature of effectus theory. We shall review only the parts that are needed in our exposition about the Kleisli category of the quantum monad, later in Chapter 3. For a more detailed account, see for instance [Jac11, Jac13, Jac15, CJWW15]. Here we shall define effect algebras, effect modules and effectuses. We also review basic definitions about graphs and (binary) relations.

2.1 Effect Algebras

The concept of effect algebras is build on top of the concept of a partial commutative monoid. The prime example of a partial commutative monoid is the real unit interval $[0, 1]$.

Definition 2.1.1. A *partial commutative monoid* consists of a set E with a distinguished element $0 \in E$, and a partial function $\ovee\colon E \times E \rightharpoonup E$ for which $x \perp y$

denotes $x \ovee y$ is defined, satisfying:

(1) $x \perp y \quad \Rightarrow \quad y \perp x \;\wedge\; x \ovee y = y \ovee x$

(2) $y \perp z \;\wedge\; x \perp (y \ovee z) \quad \Rightarrow \quad x \perp y \;\wedge\; (x \ovee y) \perp z \;\wedge\; x \ovee (y \ovee z) = (x \ovee y) \ovee z$

(3) $0 \perp x \;\wedge\; 0 \ovee x = x$

The notation $x \perp y$ for saying $x \ovee y \in E$ is defined can also be read as x and y are 'orthogonal' or 'independent'. Axiom (1) is commutativity of $\ovee$, (2) associativity, and (3) zero element. The partial commutative operation $\ovee$ on $[0,1]$ is given by addition $x \ovee y := x + y$ defined only when the sum $x + y$ is less or equal than 1. So, in this case $x \perp y$ denotes $x + y \leq 1$.

Definition 2.1.2. An *effect algebra* is a partial commutative monoid $(E, 0, \ovee)$ with a unary operation $(-)^{\perp} \colon E \to E$ satisfying the following axioms:

(1) $\exists! x^{\perp} \in E$ such that $x \ovee x^{\perp} = 1$, where $1 := 0^{\perp}$

(2) $x \perp 1 \quad \Rightarrow \quad x = 0$

A morphism $E \to D$ of effect algebras is defined as a function $f \colon E \to D$ satisfying the following axioms:

(1) $f(1) = 1$

(2) $x \perp y \quad \Rightarrow \quad f(x) \perp f(y) \;\wedge\; f(x \ovee y) = f(x) \ovee f(y)$

Effect algebras form a category denoted by **EA**. Indeed, the real unit interval $[0,1] \in \mathbf{EA}$ with $x^{\perp} := 1 - x$ and $x \ovee y := x + y$ if $x + y \leq 1$ is an effect algebra.

2.2 Effect Modules

Monoids in the category of effect algebras are called effect monoids. (Monoids in the category of commutative rings are called semirings.) Effect monoids form a category denoted by $\mathbf{Mon}(\mathbf{EA})$. The usual multiplication of real numbers turns the unit interval $[0,1] \in \mathbf{Mon}(\mathbf{EA})$ into an effect monoid.

Definition 2.2.1. An *effect module* is an effect algebra $E \in \mathbf{EA}$ along with a function $\alpha\colon M \times E \to E$, for some effect monoid $M \in \mathbf{Mon}(\mathbf{EA})$, satisfying the following axioms:

(1) $\alpha(1,1) = 1$

(2) $\alpha(r,-)\colon M \to M$ and $\alpha(-,x)\colon M \to E$ are morphisms in $\mathbf{EA}$

The action of α can be thought as a scalar multiplication. A map of effect modules is a map of the underlying effect algebras that commutes with scalar multiplication. There is a category $\mathbf{EMod}_M$ of effect modules over M, for any effect monoid $M \in \mathbf{Mon}(\mathbf{EA})$. Fuzzy predicates $X \to [0,1]$ on a set X form an effect module, *i.e.* $[0,1]^X \in \mathbf{EMod}_{[0,1]}$.

2.3 Effectuses

Effectus theory is an emergent field in categorical logic aiming to describe logic and probability, from the point of view of classical and quantum computation.

The category $\mathbf{Set}$ of sets and functions has finite coproducts $(+,0)$ and a terminal object $1 \in \mathbf{Set}$. The disjoint union $+$ of $X, Y \in \mathbf{Set}$ is the set defined as $X + Y := \{(x,0) \mid x \in X\} \cup \{(1,y) \mid y \in Y\}$ with coprojections $X \overset{\kappa_1}{\to} X + Y \overset{\kappa_2}{\leftarrow}$

Y, and cotupling $[p,q]\colon X+Y \to Z$ for any pair of maps $X \xrightarrow{p} Z \xleftarrow{q} Y$ given by:

$$[p,q](v) := \begin{cases} p(v) & \text{if } v \in X \\ q(v) & \text{if } v \in Y \end{cases}$$

for all $v \in X+Y$. The empty set $0 := \emptyset \in \mathbf{Set}$ is the initial object, and any choice of a singleton set $1 := \{*\}$ is terminal in $\mathbf{Set}$. The unique function $!_X\colon X \to 1$ is given by $x \mapsto *$ for each $x \in X$. Given functions $f\colon A \to B$ and $g\colon X \to Y$ then $f+g\colon A+X \to B+Y$ is defined as $f+g := [\kappa_1 \circ f, \kappa_2 \circ g]$.

Definition 2.3.1. An *effectus* $\mathbf{B}$ is category with finite coproducts $(+,0)$ and a terminal object $1 \in \mathbf{B}$, where the following commutative squares are pullbacks:

$$\begin{array}{ccc} X+Y & \xrightarrow{!_X+\mathrm{id}_Y} & 1+Y \\ {\scriptstyle \mathrm{id}_X+!_Y}\downarrow & & \downarrow{\scriptstyle \mathrm{id}_1+!_Y} \\ X+1 & \xrightarrow[!_X+\mathrm{id}_1]{} & 1+1 \end{array} \qquad\qquad \begin{array}{ccc} X & \xrightarrow{!_X} & 1 \\ {\scriptstyle \kappa_1}\downarrow & & \downarrow{\scriptstyle \kappa_1} \\ X+Y & \xrightarrow[!_X+!_Y]{} & 1+1 \end{array}$$

for all $X, Y \in \mathbf{B}$ and the following maps in $\mathbf{B}$ are jointly monic:

$$(1+1)+1 \overset{\rhd_1 := [[\kappa_1,\kappa_2],\kappa_2]}{\underset{\rhd_2 := [[\kappa_2,\kappa_1],\kappa_2]}{\rightrightarrows}} 1+1$$

Joint monicity of $\rhd_1, \rhd_2$ means that given f, g functions: $\rhd_1 \circ f = \rhd_1 \circ g$ and $\rhd_2 \circ f = \rhd_2 \circ g$ implies $f = g$.

The category $\mathbf{Set}$ is the effectus used for modelling classical (deterministic, Boolean) computations. More exactly, we have the following result.

Proposition 2.3.1. *The category* $\mathbf{Set}$ *is an effectus.*

Proof. We know how pullbacks are constructed in $\mathbf{Set}$. For the first pullback condition from Definition 2.3.1, let P be the set of pairs $(x,y) \in (X+1) \times (1+Y)$

such that $(! + \mathrm{id})(x) = (\mathrm{id}+!)(y)$. Note that we have:

$$(X+1) \times (1+Y) \cong (X \times 1) + (1 \times 1) + (X \times Y) + (1 \times Y)$$

Let $X + 1 = X + \{1\}$ and $1 + Y = \{0\} + Y$. By cases:

(1) $(x, y) \in X \times \{0\}$ implies $(x, y) = (x, 0)$, and so $(! + \mathrm{id})(x) = 0 = (\mathrm{id}+!)(0)$ for all $x \in X$, thus $X \times 1 \subseteq P$;

(2) $(x, y) \in \{1\} \times \{0\}$ implies $(! + \mathrm{id})(1) = 1 \neq 0 = (\mathrm{id}+!)(0)$, so $1 \times 1 \not\subseteq P$;

(3) $(x, y) \in X \times Y$ implies $(! + \mathrm{id})(x) \neq (\mathrm{id}+!)(y)$, so $X \times Y \not\subseteq P$;

(4) $(x, y) \in \{1\} \times Y$ implies $(x, y) = (1, y)$, and so $(! + \mathrm{id})(1) = 1 = (\mathrm{id}+!)(y)$ for all $y \in Y$, thus $1 \times Y \subseteq P$.

Hence, the pullback is indeed given by $(X \times 1) + (1 \times Y) \cong X + Y$.

For the second pullback condition from Definition 2.3.1, take $1 = \{0\}$ and consider the set of pairs $(w, 0) \in (X + Y) \times 1$ such that $(!+!)(w) = \kappa_1(0)$. Note that $(X + Y) \times 1 \cong (X \times 1) + (Y \times 1)$. By cases:

(1) if $(w, 0) \in X \times 1$ then $(!+!)(w) = 0 = \kappa_1(0)$ for all $w \in X$;

(2) if $(w, 0) \in Y \times 1$ then $(!+!)(w) = 1 \neq 0 = \kappa_1(0)$ for all $w \in Y$.

Thus the pullback is indeed given by $X \times 1 \cong X$.

For the joint monicity requirement from Definitions 2.3.1, we consider sets $1 + 1 + 1 \cong \{a, b, c\}$ and $1 + 1 \cong \{0, 1\}$, and functions $\succ_1, \succ_2 \colon 3 \rightrightarrows 2$ defined as:

$$\succ_1(a) = 0 \qquad \succ_1(b) = \succ_1(c) = 1 \qquad\qquad \succ_2(a) = \succ_2(c) = 1 \qquad \succ_2(b) = 0$$

Further assume we have functions $f, g \colon X \rightrightarrows 3$ such that:

$$\succ_1 \circ f = \succ_1 \circ g \qquad\qquad \succ_2 \circ f = \succ_2 \circ g$$

We need to show that $f = g$. Suppose that $f \neq g$. Then $f(x) \neq g(x)$ for some $x \in X$. Assuming the existence of such x, we arrive to the following contradictions:

- $f(x) = a \Rightarrow g(x) \in \{b, c\} \Rightarrow \rightarrowtail_1(f(x)) \neq \rightarrowtail_1(g(x))$
- $f(x) = b \Rightarrow g(x) \in \{a, c\} \Rightarrow \rightarrowtail_2(f(x)) \neq \rightarrowtail_2(g(x))$
- $f(x) = c \Rightarrow g(x) \in \{a, b\} \Rightarrow \rightarrowtail_1(f(x)) \neq \rightarrowtail_1(g(x))$ if $g(x) = a$, or $\rightarrowtail_2(f(x)) \neq \rightarrowtail_2(g(x))$ if $g(x) = b$

Hence it must be the case that $f = g$, and so $\rightarrowtail_1$ and $\rightarrowtail_2$ are jointly monic. □

2.4 Discrete Probabilities

Effectuses are intended to serve also as categorical models for probabilistic (and quantum) logic and computation. To talk about discrete probabilities (categorically) one uses the discrete distribution monad $\mathcal{D}_M$ defined on **Set**, for any effect monoid $M \in \mathbf{Mon}(\mathbf{EA})$ as follows. For any set X, the set $\mathcal{D}_M(X)$ consists of all finite convex combinations of elements from X with 'mixing probabilities' from M, *i.e.* finite formal sums $m_1|x_1\rangle + \cdots + m_r|x_r\rangle \in \mathcal{D}_M(X)$ where $x_i \in X$, $m_i \in M$ and $m_1 \ovee \cdots \ovee m_r = 1$. An element $\omega \in \mathcal{D}_M(X)$ is called a state/distribution on X, and can also be thought as a function $\omega \colon X \to M$ with finite and orthogonal support $\mathrm{supp}(\omega) := \{x \in X \mid \omega(x) \neq 0\}$, satisfying $\bigovee_{x \in X} \omega(x) = 1$. If $\mathrm{supp}(\omega) = \{x_1, \ldots, x_r\}$ then the assignment $\omega(x_i) \mapsto m_i$ gives the bijective correspondence between these two equivalent representations (*i.e.* as convex-sums, or as mixing-functions) of states. States on X can be coarse-grained along a map $f \colon X \to Y$ to get states on Y: for any state $\omega \in \mathcal{D}_M(X)$ there is a state $\mathcal{D}_M(f)(\omega) \in \mathcal{D}_M(Y)$, given by $\mathcal{D}_M(f)(\omega)(y) := \bigovee_{x \in f^{-1}(y)} \omega(x)$.

Now we describe the monadic structure of $\mathcal{D}_M$. The unit $\eta_X \colon X \to \mathcal{D}_M(X)$ is the Dirac delta distribution, *i.e.* $\eta_X(x)(x') = 1$ if $x = x'$ and $\eta_X(x)(x') = 0$ if $x \neq x'$. The multiplication $\mu_X \colon \mathcal{D}^2_M(X) \to \mathcal{D}_M(X)$ is given by the expectation-value of evaluation functions $\omega \mapsto \omega(x)$ with respect to some $\Omega \in \mathcal{D}^2_M(X)$, *i.e.* $\mu_X(\Omega)(x) := \bigovee_{\omega \in \mathcal{D}_M(X)} \Omega(\omega) \cdot \omega(x)$. So there is a ($M$-valued, discrete) distribution monad $\mathcal{D}_M = (\mathcal{D}_M, \eta, \mu)$ on **Set** for each effect monoid $M \in \mathbf{Mon}(\mathbf{EA})$.

The Kleisli category $\mathcal{K}\ell(\mathcal{D}_M)$ of the distribution monad $\mathcal{D}_M$ on **Set** has sets as objects, and morphisms $X \to Y$ in $\mathcal{K}\ell(\mathcal{D}_M)$ are precisely functions of type $X \to \mathcal{D}_M(Y)$ in **Set**. For every $X \in \mathbf{Set}$, the identity map $X \to X$ in $\mathcal{K}\ell(\mathcal{D}_M)$ is given by the unit $\eta_X \colon X \to \mathcal{D}_M(X)$. One can define the Kleisli extension $c_* \colon \mathcal{D}_M(X) \to \mathcal{D}_M(Y)$ of a Kleisli map $c \colon X \to \mathcal{D}_M(Y)$ as $c_* := \mu_Y \circ \mathcal{D}_M(c)$. More concretely, this is $c_*(\omega)(y) = \bigovee_{x \in X} \omega(x) \cdot c(x)(y)$ for all $\omega \in \mathcal{D}_M(X)$ and $y \in Y$. Composition of Kleisli maps $c \colon X \to \mathcal{D}_M(Y)$ and $d \colon Y \to \mathcal{D}_M(Z)$, is given using Klesli extension (to simplify notation) as:

$$X \xrightarrow[= \mu_Z \circ \mathcal{D}_M(d) \circ c]{d_* \circ c} \mathcal{D}_M(Z)$$

Remark 2.4.1. For any set function $f \colon X \to Y$, one can define a Kleisli map:

$$X \xrightarrow[= \mathcal{D}_M(f) \circ \eta_X]{\hat{f} := \eta_Y \circ f} \mathcal{D}_M(Y)$$

given by naturality of η.

Thus, the category $\mathcal{K}\ell(\mathcal{D}_M)$ has finite coproducts $(0, +)$ given by the empty set $0 := \varnothing \in \mathbf{Set}$, and disjoint union $X_1 + X_2$ with coprojections:

$$X_i \xrightarrow[= \mathcal{D}_M(\kappa_i) \circ \eta_{X_i}]{\hat{\kappa}_i := \eta_{X_1 + X_2} \circ \kappa_i} \mathcal{D}_M(X_1 + X_2)$$

for $i = 1, 2$. The following result is well-known, see *e.g.* [Jac11, Proposition 6.4].

Lemma 2.4.1. *The distribution monad $\mathcal{D}_M$ is affine, i.e. $\mathcal{D}_M(1) \cong 1$, for any effect monoid $M \in \mathbf{Mon}(\mathbf{EA})$. Moreover, $\mathcal{D}_M(2) \cong M$.*

Proof. An element $\omega \in \mathcal{D}_M(1)$ can be regarded as a function $\omega\colon 1 \to M$ such that $\bigovee_{x\in\{1\}} \omega(x) = 1$. Therefore, it must be the case that $\omega(1) = 1$. Thus $\mathcal{D}_M(1) \cong 1$. Now, an M-valued distribution over a 2-element set consists of a choice of an element $m \in M$, which in turn immediately determines a choice of $m^\perp \in M$ such that $m \ovee m^\perp = 1 \in M$. Hence $\mathcal{D}_M(2) \cong M$. □

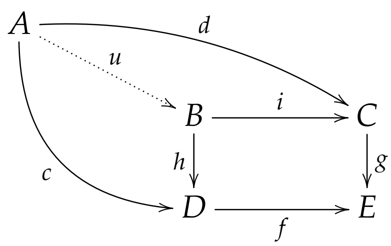
By Lemma 2.4.1 above, any choice of a singleton set $1 \in \mathbf{Set}$ is a terminal object in $\mathcal{K}\ell(\mathcal{D}_M)$ so we have unique arrows:

$$X \xrightarrow[= \mathcal{D}_M(!_X)\circ\eta_X]{\hat{!}_X := \eta_1 \circ !_X} \mathcal{D}_M(1)$$

for any $X \in \mathbf{Set}$. Since $1 \cong \mathcal{D}_M(1)$, the unit $\eta_1\colon 1 \to \mathcal{D}_M(1)$ and the identity function $\mathrm{id}_1\colon 1 \to 1$ are equal $\eta_1 = \mathrm{id}_1$. Therefore, we have $\hat{!}_X = !_X$ for all $X \in \mathbf{Set}$. So $\mathcal{K}\ell(\mathcal{D}_M)$ has finite coproducts and a terminal object.

Now, we would like to have the two pullbacks from Definition 2.3.1 instantiated in $\mathcal{K}\ell(\mathcal{D}_M)$. Let's describe this situation in general first.

Remark 2.4.2. Assume we have the following commutative diagram:



where all the arrows live in $\mathcal{K}\ell(\mathcal{D}_M)$, and the dashed arrow means that u is uniquely defined. That is, we have a function $u\colon A \to \mathcal{D}_M(B)$ which is determined in a unique way given Kleisli maps:

$$c\colon A \to \mathcal{D}_M(D) \qquad f\colon D \to \mathcal{D}_M(E) \qquad h\colon B \to \mathcal{D}_M(D)$$
$$d\colon A \to \mathcal{D}_M(C) \qquad g\colon C \to \mathcal{D}_M(E) \qquad i\colon B \to \mathcal{D}_M(C)$$

satisfying the following four equations:

$$h_* \circ u = c \tag{2.1}$$
$$i_* \circ u = d \tag{2.2}$$
$$f_* \circ c = g_* \circ d \tag{2.3}$$
$$f_* \circ h = g_* \circ i \tag{2.4}$$

In that case, we have that B is the pullback of g along f in $\mathcal{K}\ell(\mathcal{D}_M)$.

Proposition 2.4.1. *Let $M \in \mathbf{Mon}(\mathbf{EA})$ be an effect monoid. The Kleisli category $\mathcal{K}\ell(\mathcal{D}_M)$ of the distribution monad $\mathcal{D}_M$ on sets is an effectus.*

Proof. We need to check two pullback conditions and one joint monicity requirement for the Kleisli category $\mathcal{K}\ell(\mathcal{D}_M)$. We start with the first pullback from Definition 2.3.1. We assume to have the following Kleisli maps:

$$c\colon A \to \mathcal{D}_M(X+1) \qquad f\colon X+1 \to \mathcal{D}_M(1+1) \qquad h\colon X+Y \to \mathcal{D}_M(X+1)$$
$$d\colon A \to \mathcal{D}_M(1+Y) \qquad g\colon 1+Y \to \mathcal{D}_M(1+1) \qquad i\colon X+Y \to \mathcal{D}_M(1+Y)$$

where:

$$f := \mathcal{D}_M(!_X + \mathrm{id}_1) \circ \eta_{X+1} \qquad h := \mathcal{D}_M(\mathrm{id}_X + !_Y) \circ \eta_{X+Y}$$
$$g := \mathcal{D}_M(\mathrm{id}_1 + !_Y) \circ \eta_{1+Y} \qquad i := \mathcal{D}_M(!_X + \mathrm{id}_Y) \circ \eta_{X+Y}$$

By definition of Kleisli extension we have:

$$\begin{aligned} f_* &= \mu_{1+1} \circ \mathcal{D}_M(f) \\ &= \mu_{1+1} \circ \mathcal{D}_M(\mathcal{D}_M(!_X + \mathrm{id}_1) \circ \eta_{X+1}) \\ &\overset{\star}{=} \mu_{1+1} \circ \mathcal{D}_M(\eta_{1+1} \circ (!_X + \mathrm{id}_1)) \\ &= \mu_{1+1} \circ \mathcal{D}_M(\eta_{1+1}) \circ \mathcal{D}_M(!_X + \mathrm{id}_1) \\ &= \mathcal{D}_M(!_X + \mathrm{id}_1) \end{aligned}$$

where the marked equality $\overset{\star}{=}$ follows from naturality of η, and the last one from the axioms of monads. Similarly, we have:

$$\begin{aligned} g_* &= \mathcal{D}_M(\mathrm{id}_1 + !_Y) \\ h_* &= \mathcal{D}_M(\mathrm{id}_X + !_Y) \\ i_* &= \mathcal{D}_M(!_X + \mathrm{id}_Y) \end{aligned}$$

Therefore, equation (2.4) above holds:

$$\begin{aligned} f_* \circ h &= \mathcal{D}_M(!_X + \mathrm{id}_1) \circ h \\ &= \mathcal{D}_M(!_X + \mathrm{id}_1) \circ \mathcal{D}_M(\mathrm{id}_X + !_Y) \circ \eta_{X+Y} \\ &= \mathcal{D}_M((!_X + \mathrm{id}_1) \circ (\mathrm{id}_X + !_Y)) \circ \eta_{X+Y} \\ &\overset{\star}{=} \mathcal{D}_M((\mathrm{id}_1 + !_Y) \circ (!_X + \mathrm{id}_Y)) \circ \eta_{X+Y} \\ &= \mathcal{D}_M(\mathrm{id}_1 + !_Y) \circ \mathcal{D}_M(!_X + \mathrm{id}_Y) \circ \eta_{X+Y} \\ &= g_* \circ i \end{aligned}$$

where the marked equality $\overset{\star}{=}$ follows from the fact that both squares in the definition of effectus (see Definition 2.3.1) commute in every category with finite coproducts and a terminal object.

Let $X+1 = X+\{1\}$ and $1+Y = \{0\}+Y$. Further suppose the Kleisli maps $c\colon A \to \mathcal{D}_M(X+\{1\})$ and $d\colon A \to \mathcal{D}_M(\{0\}+Y)$ satisfy equation (2.3) above. More concretely, suppose:

$$\mathcal{D}(!+\mathrm{id})(c(a)) = \mathcal{D}(\mathrm{id}+!)(d(a)) \quad \in \quad \mathcal{D}_M(\{0\}+\{1\}) \tag{2.5}$$

for all $a \in A$. Specifically, this equation (2.5) expanded and evaluated says that:

$$\begin{aligned} \mathcal{D}(!+\mathrm{id})(c(a))(0) &\overset{(2.5)}{=} \mathcal{D}(\mathrm{id}+!)(d(a))(0) \\ &= \bigovee_{y\in(\mathrm{id}+!)^{-1}(0)} d(a)(y) \\ &= d(a)(0) \quad \in \quad M \end{aligned} \tag{2.6}$$

$$\begin{aligned} \mathcal{D}(!+\mathrm{id})(c(a))(1) &= \bigovee_{x\in(!+\mathrm{id})^{-1}(1)} c(a)(x) \\ &= c(a)(1) \quad \in \quad M \end{aligned} \tag{2.7}$$

Thus:

$$d(a)(0) \ovee c(a)(1) = 1 \in M \tag{2.8}$$

Let $u\colon A \to \mathcal{D}_M(X+Y)$ be the Kleisli map defined as $u(a)(x) := c(a)(x) \in M$

for all $x \in X$ and $u(a)(y) := d(a)(y) \in M$ for all $y \in Y$. We have:

$$
\begin{aligned}
\bigovee_{x\in X} u(a)(x) \ovee \bigovee_{y\in Y} u(a)(y) &\overset{\text{def}}{=} \bigovee_{x\in X} c(a)(x) \ovee \bigovee_{y\in Y} d(a)(y) \\
&= \bigovee_{!(x)=0} c(a)(x) \ovee \bigovee_{!(y)=1} d(a)(y) \\
&= \mathcal{D}(!+\mathrm{id})(c(a))(0) \ovee \mathcal{D}(!+\mathrm{id})(c(a))(1) \\
&\overset{\star}{=} d(a)(0) \ovee c(a)(1) \\
&= 1
\end{aligned}
$$

where the marked equality $\overset{\star}{=}$ follows from (2.6) and (2.7), and the last equality from (2.8). Hence u is well-defined. We still need to check (2.1) and (2.2) above, which in this case amounts to show that:

$$
\mathcal{D}(\mathrm{id}+!) \circ u = c
$$

$$
\mathcal{D}(!+\mathrm{id}) \circ u = d
$$

For all $a \in A$, we have indeed:

$$
\begin{aligned}
\mathcal{D}(\mathrm{id}+!)(u(a))(x) &= \bigovee_{x' \in (\mathrm{id}+!)^{-1}(x)} u(a)(x') \\
&= u(a)(x) \\
&\overset{\text{def}}{=} c(a)(x) \\
\mathcal{D}(\mathrm{id}+!)(u(a))(1) &= \bigovee_{y \in (\mathrm{id}+!)^{-1}(1)} u(a)(y) \\
&= \bigovee_{y\in Y} u(a)(y) \\
&\overset{\text{def}}{=} \bigovee_{y\in Y} d(a)(y) \\
&= c(a)(1)
\end{aligned}
$$

$$
\begin{aligned}
\mathcal{D}(!+\mathrm{id})(u(a))(y) &= \bigovee_{y' \in (!+\mathrm{id})^{-1}(y)} u(a)(y') \\
&= u(a)(y) \\
&\stackrel{\text{def}}{=} d(a)(y) \\
\mathcal{D}(!+\mathrm{id})(u(a))(0) &= \bigovee_{x \in (!+\mathrm{id})^{-1}(0)} u(a)(x) \\
&= \bigovee_{x \in X} u(a)(x) \\
&\stackrel{\text{def}}{=} \bigovee_{x \in X} c(a)(x) \\
&= d(a)(0).
\end{aligned}
$$

By definition, $u\colon A \to \mathcal{D}_M(X+Y)$ is the unique Kleisli map satisfying the needed requirements. This completes the proof of the first pullback condition for $\mathcal{K}\ell(\mathcal{D}_M)$.

For the second pullback from Definition 2.3.1, let $1 := \{0\}$ and $1 := \{1\}$ be two distinct (choices of) singleton sets, and $\theta = 1|0\rangle \in \mathcal{D}_M(1)$ where $\mathcal{D}_M(1) \cong \{\theta\}$ and $1 \in M$ is a (Dirac) distribution on the first singleton $\{0\}$ defined above. Consider Kleisli maps $!\colon A \to \{\theta\}$ and $c\colon A \to \mathcal{D}_M(X+Y)$ such that:

$$
\mathcal{D}(!+!) \circ c = \mathcal{D}(\kappa_1) \circ ! \tag{2.9}
$$

Since $c(a) = \sum_x m_x|x\rangle + \sum_y m_y|y\rangle \in \mathcal{D}_M(X+Y)$ with $\bigovee_x m_x \ovee \bigovee_y m_y = 1 \in M$ for all $a \in A$, we have that the left-hand side of equation (2.9) expands to:

$$
\mathcal{D}(!+!)(c(a)) = \sum_x m_x|0\rangle + \sum_y m_y|1\rangle
$$

The right-hand side of equation (2.9)expands to:

$$
\begin{aligned}
\mathcal{D}(\kappa_1)(!(a)) &= \mathcal{D}(\kappa_1)(\theta) \\
&= 1|\kappa_1(0)\rangle \\
&= 1|0\rangle
\end{aligned}
$$

Hence $\bigovee_x m_x = 1$, and so $c(a) \in \mathcal{D}_M(X)$. Let $u\colon A \to \mathcal{D}_M(X)$ be defined as $u(a)(x) := c(a)(x)$. By definition, the Kleisli map $u\colon A \to \mathcal{D}_M(X)$ is the unique arrow satisfying the needed requirements.

Now we prove that the maps $\succ_1, \succ_2\colon (1+1)+1 \rightrightarrows 1+1$ in are jointly monic in $\mathcal{K}\ell(\mathcal{D}_M)$. This part is taken exactly from [Jac15, Example 4.7]. Let $\sigma, \tau \in \mathcal{D}_M(3)$ be distributions such that

$$
\begin{aligned}
\mathcal{D}(\succ_1)(\sigma) &= \mathcal{D}(\succ_1)(\tau) \\
\mathcal{D}(\succ_2)(\sigma) &= \mathcal{D}(\succ_2)(\tau)
\end{aligned}
\tag{2.10}
$$

in $\mathcal{D}_M(2)$. Assume $3 = \{a, b, c\}$ and $2 = \{0, 1\}$. We have the following convex combinations for σ in $\mathcal{D}_M(2)$:

$$
\begin{aligned}
\mathcal{D}(\succ_1)(\sigma) &= \sigma(a)|0\rangle + (\sigma(b) + \sigma(c))|1\rangle \\
\mathcal{D}(\succ_2)(\sigma) &= \sigma(b)|0\rangle + (\sigma(a) + \sigma(b))|1\rangle
\end{aligned}
$$

Similarly for τ:

$$
\begin{aligned}
\mathcal{D}(\succ_1)(\tau) &= \tau(a)|0\rangle + (\tau(b) + \tau(c))|1\rangle \\
\mathcal{D}(\succ_2)(\tau) &= \tau(b)|0\rangle + (\tau(a) + \tau(b))|1\rangle
\end{aligned}
$$

Hence, by the first equation in (2.10), we have $\sigma(a) = \tau(a)$. Similarly, by the second equation in (2.10), we have $\sigma(b) = \tau(b)$. We still need to show that

$\sigma(c) = \tau(c)$. Since $\sigma(a) \oslash \sigma(b) \oslash \sigma(c) = 1 = \tau(a) \oslash \tau(b) \oslash \tau(c)$, then:

$$\begin{aligned}\sigma(c) &= (\sigma(a) \oslash \sigma(b))^{\perp} \\ &= (\tau(a) \oslash \tau(b))^{\perp} \\ &= \tau(c)\end{aligned}$$

This completes the proof. □

2.5 Graphs and Relations

To begin our formal discussion about another 'probabilistic' monad in the next chapter, we shall consider graphs as they are rather generic objects.

Definition 2.5.1. A *graph* G consists of a set of vertices $V(G)$, together with a set of edges $E(G) \subseteq V(G) \times V(G)$ which are pairs of adjacent vertices.

By definition $E(G)$ is a binary relation on the vertex set $V(G)$. We shall write $v \sim v'$ to denote a pair of adjacent vertices $v, v' \in V(G)$, *i.e.* a pair $(v, v') \in V(G) \times V(G)$ in the edge/adjacency relation $(v, v') \in E(G)$. A morphism $G \to H$ of graphs is given by a function $f \colon V(G) \to V(H)$ between vertices preserving edge adjacency: if $v \sim v'$ in G then $f(v) \sim f(v')$ in H. Morphisms of graphs are also known as *graph homomorphisms*. Graphs and their homomorphisms form a category denoted by **Gph**.

Remark 2.5.1. Essentially, the category **Gph** defined as above is the category **Rel** of binary relations on sets: there is a category **Rel** whose objects are pairs (A, R) where $R \subseteq A \times A$ is a (binary) relation on $A \in \mathbf{Set}$, and morphisms $(A, R) \to (B, S)$ are functions $f \colon A \to B$ between the underlying sets such that $(a, a') \in R$ implies $(f(a), f(a')) \in S$ for all $a, a' \in A$ (see [Jac99, Chapter 0]).

Hence, we have **Gph** $\cong$ **Rel** by definition. Recall that $\mathbf{Sub}(\mathbf{Set})$ is the category with pairs (A, X) where $X \subseteq A$ is subset of a set $A \in \mathbf{Set}$ as objects, and functions $f\colon A \to B$ satisfying $a \in X$ implies $f(a) \in Y \subseteq B$ for each $a \in A$ as morphisms. The forgetful functor $\mathbf{Gph} \to \mathbf{Set}$ which maps a graph to its vertex set $G \mapsto V(G)$ is a bifibration obtained, by taking the ordinary pullback of categories (*i.e.* pullback in the category **Cat** of small categories and functors), from the subsets fibration $\mathbf{Sub}(\mathbf{Set}) \to \mathbf{Set}$ defined by $(A, X) \mapsto A$, as follows:

$$\begin{array}{ccc} \mathbf{Gph} & \longrightarrow & \mathbf{Sub}(\mathbf{Set}) \\ \downarrow & \lrcorner & \downarrow \\ \mathbf{Set} & \xrightarrow[A \mapsto A \times A]{} & \mathbf{Set} \end{array}$$

Actually, more can be said about the bifibration $\mathbf{Gph} \to \mathbf{Set}$. For instance, it preserves finite products and coproducts (see [Jac99, Example 9.2.5 (ii)]).

Remark 2.5.2. From now on, throughout this document, we use the word graph to refer to *simple*, *irreflexive* and *undirected* graphs always, unless otherwise is explicitly stated. Simple means that there is at most one edge between pairs of vertices. Irreflexive means that $E(G)$ is not a reflexive relation, *i.e.* $v \not\sim v$ for all $v \in V(G)$. Undirected means that $E(G)$ is a symmetric relation, *i.e.* $v \sim v'$ if and only if $v' \sim v$. However, for the sake of convenience, the category **Gph** shall include all type of graphs in the sense of Definition 2.5.1.

There is a category **Pre** of preordered sets with monotone functions. A preorder is a reflexive and transitive binary relation. Preordered sets are sets carrying a preorder.

Definition 2.5.2. A *preordered monoid* $\mathbb{E} = (E, \sqsubseteq, *, \cdot)$ consists of a preordered set $(E, \sqsubseteq) \in \mathbf{Pre}$ with a distinguished element $* \in E$, together with a monotone function $\cdot \colon (E, \sqsubseteq) \times (E, \sqsubseteq) \to (E, \sqsubseteq)$ satisfying the axioms of monoids:

$$\begin{array}{ccc} 1 \times E & \xrightarrow{e \times \mathrm{id}} & E \times E \\ & \searrow^{\lambda} & \downarrow{\scriptstyle \cdot} \\ & & E \end{array} \qquad \begin{array}{ccc} E \times 1 & \xrightarrow{\mathrm{id} \times e} & E \times E \\ & \searrow^{\rho} & \downarrow{\scriptstyle \cdot} \\ & & E \end{array} \qquad \begin{array}{ccc} E \times E \times E & \xrightarrow{\mathrm{id} \times \cdot} & E \times E \\ {\scriptstyle \cdot \times \mathrm{id}} \downarrow & & \downarrow{\scriptstyle \cdot} \\ E \times E & \xrightarrow[\cdot]{} & E \end{array}$$

where $1 = \{*\}$ is a (choice of a) one-element set, and λ and ρ are bijections given by $\lambda(*, e) := e$ and $\rho(e, *) := e$ for all $e \in E$.

Preordered monoids are monoids in the cateogry of preordered sets **Pre**. Preordered monoids form a category **Mon**(**Pre**). Graded monads on an arbitrary category **C** can be described as preordered monoids in the (functor) category $[\mathbf{C}, \mathbf{C}]$ of endofunctors $\mathbf{C} \to \mathbf{C}$ and natural transformations between them. The natural numbers $\mathbb{N}$ with $1 \in \mathbb{N}$ as the distinguished element is a preordered monoid, and is in fact the one we use for grading the quantum monad [ABdSZ17].

Chapter 3

The Quantum Monad on Relational Structures

Measurement is a central aspect in any frequentist interpretation of probability. Quantum theory is a physical theory of measurements in the sense that it provides a framework to build models for predicting the probability distributions of observable properties (aka 'observables'). Physical indeed because the probabilities given by the distributions are interpreted as statistical frequencies of observables, after a measurement procedure has been performed repeatedly for a sufficient number of times. A good mathematical introduction to quantum theory (with foundational aspects) can be founded in [Ish01].

In quantum computation, one uses the mathematical representation of quantum systems and measurements for processing information more efficiently, like finding solutions to systems of polynomial equations for which it is known there are no classical solutions, as for instance in proving existence of *e.g.* non-classical 'quantum' perfect strategies for non-local games [CMN$^+$07, Rob, MR14, CM14, MR16, ABdSZ17, AMR$^+$18].

3.1 Quantum Graph Homomorphisms

The language of graphs is simple, yet powerful enough to talk about key aspects of logic and computation (see Remark 2.5.2). For instance, consider the following game involving a given pair of graphs G and H, played by Alice and Bob cooperating against a Verifier. Their goal is to establish the existence of a graph homomorphism from G to H. The game is 'non-local' which means that Alice and Bob are not allowed to communicate during the game, however they are allowed to agree on a strategy before the game has started. In each round Verifier sends to Alice and Bob vertices $v_1, v_2 \in V(G)$, respectively; in response they produce outputs $w_1, w_2 \in V(H)$. They win the round if the following conditions hold:

$$v_1 = v_2 \Rightarrow w_1 = w_2 \qquad \text{and} \qquad v_1 \sim v_2 \Rightarrow w_1 \sim w_2$$

If there is indeed a graph homomorphism $G \to H$, then Alice and Bob can win any round of the game described above by using such homomorphism as strategy for responding accordingly. Conversely, they can win any round with certainty only when there is a graph homomorphism $G \to H$. A strategy for Alice and Bob in which they win with probability 1 is called a *perfect strategy*. Hence, the existence of a perfect strategy is equivalent to the existence of a graph homomorphism. Using quantum resources in the form of a maximally entangled bipartite state, where Alice and Bob can each perform measurements on their part, there are perfect strategies in cases where no classical homomorphism exists.

We write $M_d(\mathbb{C})$ for the set of all $d \times d$ matrices with complex entries ($d \in \mathbb{N}$). Also, we write $1 \in M_d(\mathbb{C})$ for the $d \times d$ identity matrix. Let $E \in M_n(\mathbb{C})$ and $F \in M_m(\mathbb{C})$ be two complex square matrices of possibly different size.

Their *tensor product* is defined as $E \otimes F := (e_{ij}F) \in M_{nm}(\mathbb{C})$ if $E = (e_{ij})$ with $i, j \in \{1, \ldots, n\}$.

Definition 3.1.1. A *quantum perfect strategy* for the homomorphism game from G to H consists of a complex unitary vector $\psi \in \mathbb{C}^{d_A} \otimes \mathbb{C}^{d_B}$ for some $d_A, d_B \in \mathbb{N}$ finite, and families $(E_{vw})_{w \in V(H)}$ and $(F_{vw})_{w \in V(H)}$ of $d_A \times d_A$ and $d_B \times d_B$ complex matrices for all $v \in V(G)$, satisfying:

(1) $\sum_{w \in V(H)} E_{vw} = 1 \in M_{d_A}(\mathbb{C})$ and $\sum_{w \in V(H)} F_{vw} = 1 \in M_{d_B}(\mathbb{C})$;

(2) $w \neq w' \quad \Rightarrow \quad \psi^*(E_{xy} \otimes F_{vw'})\psi = 0$;

(3) $v \sim v' \wedge w \not\sim w' \quad \Rightarrow \quad \psi^*(E_{vw} \otimes F_{v'w'})\psi = 0$.

This characterisation of quantum perfect strategies eliminates the two-person aspect of the game and the shared state, leaving a 'matrix-valued relation' as the witness for existence of a quantum perfect strategy. It also gives rise to the notion of 'quantum' graph homomorphism. This concept was introduced in [Rob], as a generalisation of the notion of quantum chromatic number from [CMN$^+$07]. Analogous results for constraint systems are proved in [MR14, CM14, MR16, ABdSZ17, AMR$^+$18].

Definition 3.1.2. A *quantum graph homomorphism* from G to H is given by an indexed family $(E_{vw})_{v \in V(G), w \in V(H)}$ of $d \times d$ complex matrices ($E_{vw} \in M_d(\mathbb{C})$), for some $d \in \mathbb{N}$, such that:

(1) $E_{vw}^* = E_{vw}^2 = E_{vw}$ for all $v \in V(G)$ and $w \in V(H)$;

(2) $\sum_{w \in V(H)} E_{vw} = 1 \in M_d(\mathbb{C})$ for all $v \in V(G)$;

(3) $(v = v' \wedge w \neq w') \vee (v \sim v' \wedge w \not\sim w') \quad \Rightarrow \quad E_{vw}E_{v'w'} = 0$.

An important further step is taken in [Rob]: a construction $G \mapsto \mathsf{M}G$ on graphs is introduced, such that the existence of a quantum graph homomorphism from G to H is equivalent to the existence of a graph homomorphism of type $G \to \mathsf{M}H$. This construction is called the *measurement graph*, and it turns out to be a graded monad on the category of graphs. Hence the Kleisli maps of this monad are exactly the 'quantum' maps between graphs of [Rob, MR14, MR16, AMR$^+$18].

3.2 The Quantum Monad

A simple undirected graph G is a relational structure with a single, binary irreflexive and symmetric relation $E(G)$ that we have been written as $\sim$ in infix notation. The objects of the category **Gph** (as in Definition 2.5.1) are sets together with a binary relation. Relational structures are even more general.

Definition 3.2.1. A *relational structure* $\mathscr{A}$ consists of a set A together with an indexed family $R(\mathscr{A}) = (R_i^{\mathscr{A}})_{i \in I}$ of relations $R_i^{\mathscr{A}} \subseteq A^{k_i}$ with $I \in \mathbf{Set}$, and $k_i \in \mathbb{N}$ for all $i \in I$.

A map of relational structures $\mathscr{A} \to \mathscr{B}$ is a function $f\colon A \to B$ between the underlying sets, preserving all relations: $(x_1, \ldots, x_k) \in R^{\mathscr{A}} \Rightarrow (f(x_1), \ldots, f(x_k)) \in R^{\mathscr{B}}$ for all $(x_1, \ldots, x_k) \in A^k$ and all $R \in R(\mathscr{A})$ with arity $k \in \mathbb{N}$. In fact, there is a category of relational structures that we denote by **RStr**. This category **RStr** has a relationship with the category **Rel** of binary relations defined in Section 2.5. By definition, **Rel** $\cong$ **Gph** is a (full) subcategory of **RStr**.

Remark 3.2.1. For the sake of simplicity (wrt. notation), we shall assume that all the relational structures have only one relation of a fixed arity $k \in \mathbb{N}$, *i.e.* $R(\mathscr{A}) = \{R^{\mathscr{A}}\}$ and $R^{\mathscr{A}} \subseteq A^k$ for all $\mathscr{A} \in \mathbf{RStr}$. That is, the category **RStr** is obtained from the fibration $\mathbf{Sub}(\mathbf{Set}) \to \mathbf{Set}$ of subsets by taking the pullback:

$$\begin{array}{ccc} \mathbf{RStr} & \longrightarrow & \mathbf{Sub}(\mathbf{Set}) \\ \big\downarrow & \lrcorner & \big\downarrow \\ \mathbf{Set} & \xrightarrow[A \mapsto A \times \cdots \times A]{} & \mathbf{Set} \end{array}$$

Since $\mathbf{RStr} \to \mathbf{Set}$ is obtained from the above change-of-base situation, it is a bifibration by construction. This is indeed very similar to the case of the category **Gph** (see Remark 2.5.1). In particular, $\mathbf{RStr} \to \mathbf{Set}$ is defined by $\mathscr{A} \mapsto A$, and it also preserves finite products and coproducts.

The measurement graph construction from [Rob], which we mentioned in the last paragraph of the previous section, is an instance of the *quantum* monad $\mathcal{Q}_d$ defined on **RStr** instantiated in the category of (simple, undirected) graphs. We write $\mathrm{Proj}(d) \subseteq M_d(\mathbb{C})$ for the set of all $d \times d$ complex matrices that are both self-adjoint and idempotent, *i.e.* $\mathrm{Proj}(d) = \{a \in M_d(\mathbb{C}) \mid a^* = a^2 = a\}$ for all $d \in \mathbb{N}$. The set $\mathrm{Proj}(d)$ of 'projectors' (of dimension $d \in \mathbb{N}$) is an effect monoid with the usual operations of sum and product of matrices, defined partially: $p + q$ is defined only when projectors $p, q \in \mathrm{Proj}(d)$ are orthogonal $p \cdot q = 0$, and $p \cdot q$ only when they commute $p \cdot q = q \cdot p$. That is, for all $d \in \mathbb{N}$ we have $\mathrm{Proj}(d) \in \mathbf{Mon}(\mathbf{EA})$. The functor part of this monad $\mathcal{Q}_d \in \mathbf{Mon}([\mathbf{RStr}, \mathbf{RStr}])$ is defined as follows.

Definition 3.2.2. Let $\mathscr{A} = (A, R^{\mathscr{A}})$ be a relational structure. We define the set of *projection-valued* distributions $\mathcal{Q}_d(A) := \mathcal{D}_M(A)$ on A with $M := \mathrm{Proj}(d)$, where $\mathcal{D}_M$ is the distribution functor/monad (see Section 2.4). The k-ary relation $R^{\mathcal{Q}_d(\mathscr{A})} \subseteq \mathcal{Q}_d(A)^k$ is defined as $(p_1, \ldots, p_k) \in R^{\mathcal{Q}_d(\mathscr{A})}$ if and only if the projection-valued distributions $p_1, \ldots, p_k \in \mathcal{Q}_d(A)$ satisfy the following two conditions: (1) $p_i(x)$ and $p_j(x')$ commute for all $x, x' \in A$, and (2) $(x_1, \ldots, x_k) \notin$

$R^{\mathscr{A}}$ implies $\prod_{i=1}^{k} p_i(x_i) = 0$ for all $(x_1, \ldots, x_k) \in A^k$.

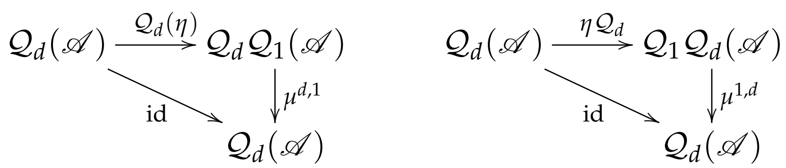
Remark 3.2.2. An element $p \in \mathcal{Q}_d(A)$ is a map $p\colon A \to \mathrm{Proj}(d)$ satisfying $\sum_{x \in A} p(x) = 1$. Note that because of the normalisation condition, all these projectors $p(x)$ resolving the identity 1 are pairwise orthogonal.

This was the definition of the relational structure $\mathcal{Q}_d(\mathscr{A}) = (\mathcal{Q}_d(A), R^{\mathscr{A}}) \in$ **RStr** from [ABdSZ17]. Given a map $f\colon \mathscr{A} \to \mathscr{B}$ of relational structures, we define $\mathcal{Q}_d(f)\colon \mathcal{Q}_d(\mathscr{A}) \to \mathcal{Q}_d(\mathscr{B})$ by coarse-graining $p\colon A \to \mathrm{Proj}(d)$ along f as given by the formula:

$$\mathcal{Q}_d(f)(p)(y) = \sum_{x \in f^{-1}(y)} p(x) \qquad (y \in B)$$

This is a well-defined homomorphism between relational structures, see Proposition A.1.1. This definition preserves composites and identities, so there is a functor $\mathcal{Q}_d\colon \mathbf{RStr} \to \mathbf{RStr}$ for every dimension $d \in \mathbb{N}$ (see Appendix A for more details).

Note that $\mathrm{Proj}(1) = \{0, 1\} \cong 2 = 1 + 1$. We define $\eta\colon \mathscr{A} \to \mathcal{Q}_1(\mathscr{A})$ to be a Dirac delta distribution: $\eta(x)(x') = 1$ if $x = x'$ and $\eta(x)(x') = 0$ if $x \neq x'$. Verification that this is well-defined is straight-forward. For $\mu^{d,d'}\colon \mathcal{Q}_d\mathcal{Q}_{d'}(\mathscr{A}) \to \mathcal{Q}_{dd'}(\mathscr{A})$, let $\mu^{d,d'}(P)(x) = \sum_{p \in \mathcal{Q}_{d'}(A)} P(p) \otimes p(x) \in \mathrm{Proj}(dd')$. Verification that this is well-defined is also straight-forward: one just need to recall that all of our distributions have finite support. These two maps turn out to be components of two natural transformations $\eta\colon 1 \Rightarrow \mathcal{Q}_1$ and $\mu^{d,d'}\colon \mathcal{Q}_d\mathcal{Q}_{d'} \Rightarrow \mathcal{Q}_{dd'}$ satisfying the axioms of graded monads [MPS15]:



$$
\begin{array}{ccc}
\mathcal{Q}_d \mathcal{Q}_{d'} \mathcal{Q}_{d''}(\mathscr{A}) & \xrightarrow{\mathcal{Q}_d(\mu^{d',d''})} & \mathcal{Q}_d \mathcal{Q}_{d'd''}(\mathscr{A}) \\
{\scriptstyle \mu^{d,d'} \mathcal{Q}_{d''}} \big\downarrow & & \big\downarrow {\scriptstyle \mu^{d,d'd''}} \\
\mathcal{Q}_{dd'} \mathcal{Q}_{d''}(\mathscr{A}) & \xrightarrow[\mu^{dd',d''}]{} & \mathcal{Q}_{dd'd''}(\mathscr{A})
\end{array}
$$

The full proof of this fact can be found in [ABdSZ17]. For the sake of completeness, we included the complete details in the Appendix A. We have:

Proposition 3.2.1. $((\mathcal{Q}_d)_{d\in\mathbb{N}}, \eta, (\mu^{d,d'})_{d,d'\in\mathbb{N}})$ *is a graded monad defined on* **RStr**.

Also in [ABdSZ17], we have defined a quantum version of homomorphisms between relational structures, and shown that the Kleisli category of the quantum monad $\mathcal{Q}_d$ is (equivalent to) the category of relational structures with quantum homomorphism between them. Hence, by Theorem 16 from [ABdSZ17], in the case of graphs, we have that the existence of a Kleisli map $G \to \mathcal{Q}_d(H)$ implies the existence of a quantum graph homomorphism $G \to \mathrm{M}H$ in the sense of [Rob, MR14, MR16] (*i.e.* in the sense of Definition 3.1.2 above).

3.3 Quantum Maps of Relational Structures

We have observed that 'quantum' maps $\mathscr{A} \to \mathcal{Q}_d(\mathscr{B})$ between relational structures can be interpreted as projection-valued relations called quantum homomorphisms or, more operationally, as quantum perfect strategies for the nonlocal homomorphism game on relational structures from [ABdSZ17]. In this section we shall prove that the category of relational structures with quantum maps is an effectus. More exactly, we shall see that relational structures with maps $\mathscr{A} \to \mathcal{Q}_d(\mathscr{B})$ form an effectus.

3.3.1 Relational Structures on Sets

Since the functor $\mathbf{RStr} \to \mathbf{Set}$ is a bifibration (see Remark 3.2.1) preserving finite products and coproducts, the category **RStr** of relational structures inherits the finite coproducts $(+, 0)$ and (a choice of) a terminal object 1 from the category **Set** of sets. For instance, given $\mathscr{A}, \mathscr{B} \in \mathbf{RStr}$ relational structures, $\mathscr{A} + \mathscr{B} \in \mathbf{RStr}$ is the relational structure over the set $A + B$ where the k-ary relation $R^{\mathscr{A}+\mathscr{B}}$ is defined as all the tuples $(x_1, \dots, x_k) \in (A + B)^k$ satisfying either $(x_1, \dots, x_k) \in R^{\mathscr{A}}$ or $(x_1, \dots, x_k) \in R^{\mathscr{B}}$. Also, we have the structure $0 \in \mathbf{RStr}$ over the empty set $\emptyset = 0 \in \mathbf{Set}$ with no relations. Further we have a structure $1 \in \mathbf{RStr}$ over some singleton set $1 = \{*\}$ with the universal relation of arity k, *i.e.* one has $R^1 := 1^k = 1 \times \cdots \times 1$.

Like the distribution monad $\mathcal{D}_M$ (see Subsection 2.4), the quantum monad $\mathcal{Q}_d$ is also an affine monad since $\mathcal{Q}_d(1) \cong 1$. In fact, the functor $\mathcal{Q}_d$ is a lift of $\mathcal{D}_M$ along the fibration $\mathbf{RStr} \to \mathbf{Set}$ when $M = \mathrm{Proj}(d)$:

$$\begin{array}{ccc} \mathbf{RStr} & \xrightarrow{\mathcal{Q}_d} & \mathbf{RStr} \\ \downarrow & & \downarrow \\ \mathbf{Set} & \xrightarrow[\mathcal{D}_M]{} & \mathbf{Set} \end{array}$$

That is, $\mathcal{D}_M(A) = \mathcal{Q}_d(A)$ if $M = \mathrm{Proj}(d)$ for any $\mathscr{A} = (A, R^{\mathscr{A}}) \in \mathbf{RStr}$ (see Definition 3.2.2). Hence $\mathcal{K}\ell(\mathcal{Q}_d)$ has a terminal object $1 \cong \mathcal{Q}_d(1) \in \mathcal{K}\ell(\mathcal{Q}_d)$ and finite coproducts (+,0) given by disjoint union $+$ of relational structures and $0 \in \mathcal{K}\ell(\mathcal{Q}_d)$ the empty structure.

Theorem 3.3.1. *The Kleisli category $\mathcal{K}\ell(\mathcal{Q}_d)$ of the quantum monad $\mathcal{Q}_d$ is an effectus.*

Proof. This proof is very similar to the one for the distribution monad in Proposition 2.4.1. We need to check two pullback conditions and one joint monicity requirement for the Kleisli category $\mathcal{K}\ell(\mathcal{Q}_d)$. We start with the first pullback from Definition 2.3.1. Let $A + 1 = A + \{1\}$ and $1 + B = \{0\} + B$ be the underlying sets of relational structures $\mathscr{A} + 1 \in \mathbf{RStr}$ and $1 + \mathscr{B} \in \mathbf{RStr}$. Suppose we have Kleisli maps $f \colon \mathscr{P} \to \mathcal{Q}_d(\mathscr{A} + 1)$ and $h \colon \mathscr{P} \to \mathcal{Q}_d(1 + \mathscr{B})$ which are homomorphisms of relational structures in **RStr**, such that for all $a \in P$:

$$\mathcal{Q}_d(! + \mathrm{id})(f(a)) = \mathcal{Q}_d(\mathrm{id}+!)(h(a)) \quad \in \quad \mathcal{Q}_d(\{0\} + \{1\}) \tag{3.1}$$

Specifically, this equation (3.1) expanded and evaluated says that:

$$\begin{aligned} \mathcal{Q}_d(! + \mathrm{id})(f(a))(0) &\overset{(3.1)}{=} \mathcal{Q}_d(\mathrm{id}+!)(h(a))(0) \\ &= \sum_{y \in (\mathrm{id}+!)^{-1}(0)} h(a)(y) \\ &= h(a)(0) \quad \in \quad \mathrm{Proj(d)} \end{aligned} \tag{3.2}$$

$$\begin{aligned} \mathcal{Q}_d(! + \mathrm{id})(f(a))(1) &= \sum_{x \in (!+\mathrm{id})^{-1}(1)} f(a)(x) \\ &= f(a)(1) \quad \in \quad \mathrm{Proj}(d) \end{aligned} \tag{3.3}$$

Thus:

$$h(a)(0) + f(a)(1) = 1 \in \mathrm{Proj}(d) \tag{3.4}$$

Let $u \colon \mathscr{P} \to \mathcal{Q}_d(\mathscr{A} + \mathscr{B})$ be the Kleisli map defined for each $a \in P$ as $u(a)(x) := f(a)(x) \in \mathrm{Proj}(d)$ for all $x \in A$, and $u(a)(y) := h(a)(y) \in \mathrm{Proj}(d)$ for all $y \in B$. This Kleisli map u is homomorphism by definition, since both f and h are. Hence, we have:

$$\begin{aligned}
\sum_{x\in A} u(a)(x) + \sum_{y\in B} u(a)(y) &\stackrel{\text{def}}{=} \sum_{x\in A} f(a)(x) + \sum_{y\in B} h(a)(y) \\
&= \sum_{!(x)=0} f(a)(x) + \sum_{!(y)=1} h(a)(y) \\
&= \mathcal{Q}_d(!+\text{id})(f(a))(0) + \mathcal{Q}_d(!+\text{id})(f(a))(1) \\
&\stackrel{\star}{=} h(a)(0) + f(a)(1) \\
&=1
\end{aligned}$$

where the marked equality $\stackrel{\star}{=}$ follows from (3.2) and (3.3), and the last equality from (3.4). Hence u is well-defined. We still do need to check that:

$$\begin{aligned}
\mathcal{Q}_d(\text{id}+!) \circ u &= f \\
\mathcal{Q}_d(!+\text{id}) \circ u &= h
\end{aligned} \tag{3.5}$$

For all $a \in P$, the two equations (3.5) hold since:

$$\begin{aligned}
\mathcal{Q}_d(\text{id}+!)(u(a))(x) &= \sum_{x'\in(\text{id}+!)^{-1}(x)} u(a)(x') \\
&= u(a)(x) \\
&\stackrel{\text{def}}{=} f(a)(x)
\end{aligned}$$

$$\begin{aligned}
\mathcal{Q}_d(\text{id}+!)(u(a))(1) &= \sum_{y\in(\text{id}+!)^{-1}(1)} u(a)(y) \\
&= \sum_{y\in B} u(a)(y) \\
&\stackrel{\text{def}}{=} \sum_{y\in Y} h(a)(y) \\
&= f(a)(1)
\end{aligned}$$

$$
\begin{aligned}
\mathcal{Q}_d(! + \mathrm{id})(u(a))(y) &= \sum_{y' \in (! + \mathrm{id})^{-1}(y)} u(a)(y') \\
&= u(a)(y) \\
&\stackrel{\text{def}}{=} h(a)(y) \\
\mathcal{Q}_d(! + \mathrm{id})(u(a))(0) &= \sum_{x \in (! + \mathrm{id})^{-1}(0)} u(a)(x) \\
&= \sum_{x \in X} u(a)(x) \\
&\stackrel{\text{def}}{=} \sum_{x \in X} f(a)(x) \\
&= h(a)(0).
\end{aligned}
$$

By definition, $u \colon \mathscr{P} \to \mathcal{Q}_d(\mathscr{A} + \mathscr{B})$ is the unique homomorphism satisfying equations (3.5). This completes the proof of the first pullback condition for $\mathcal{K}\ell(\mathcal{Q}_d)$.

For the second pullback from Definition 2.3.1, let $1 := \{0\}$ and $1 := \{1\}$ be two distinct (choices of) singleton sets, and $\rho = 1|0\rangle \in \mathcal{Q}_d(1) \cong \{\rho\}$ with $1 \in \mathrm{Proj}(d)$ a (Dirac) distribution on the first singleton. Consider Kleisli maps $! \colon \mathscr{P} \to \{\rho\}$ and $f \colon \mathscr{P} \to \mathcal{Q}_d(\mathscr{A} + \mathscr{B})$, which are homomorphisms of relational structures in **RStr** such that:

$$
\mathcal{Q}_d(!+!) \circ f = \mathcal{Q}_d(\kappa_1) \circ \, ! \tag{3.6}
$$

Since $f(a) = \sum_x p_x|x\rangle + \sum_y p_y|y\rangle \in \mathcal{Q}_d(A + B)$ with $\sum_x p_x + \sum_y p_y = 1 \in \mathrm{Proj}(d)$ for all $a \in P$, we have that the left-hand side of equation (3.6) expands to:

$$
\mathcal{Q}_d(!+!)(f(a)) = \sum_x p_x|0\rangle + \sum_y p_y|1\rangle
$$

The right-hand side of equation (3.6)expands to:

$$\begin{aligned}\mathcal{Q}_d(\kappa_1)(!(a)) &= \mathcal{Q}_d(\kappa_1)(\rho)\\ &= 1|\kappa_1(0)\rangle\\ &= 1|0\rangle\end{aligned}$$

Hence $\sum_x p_x = 1$, and so $f(a) \in \mathcal{Q}_d(A)$. Let $u \colon \mathscr{P} \to \mathcal{Q}_d(\mathscr{A})$ be defined as $u(a)(x) := f(a)(x)$. Once again, here we have that $u \colon \mathscr{P} \to \mathcal{Q}_d(\mathscr{A})$ is homomorphism by definition since f is homomorphism by assumption. Therefore, the Kleisli map u is the unique homomorphism of relational structures satisfying the needed requiremnts.

Now we prove that the maps $\succ_1, \succ_2 \colon (1+1)+1 \rightrightarrows 1+1$ in are jointly monic in $\mathcal{K}\ell(\mathcal{Q}_d)$. This part is (again) taken exactly from [Jac15, Example 4.7]. Let $\sigma, \tau \in \mathcal{Q}_d(3)$ be distributions such that

$$\begin{aligned}\mathcal{Q}_d(\succ_1)(\sigma) &= \mathcal{Q}_d(\succ_1)(\tau)\\ \mathcal{Q}_d(\succ_2)(\sigma) &= \mathcal{Q}_d(\succ_2)(\tau)\end{aligned} \tag{3.7}$$

in $\mathcal{Q}_d(2)$. Assume $3 = \{a, b, c\}$ and $2 = \{0, 1\}$. We have the following convex combinations for σ in $\mathcal{Q}_d(2)$:

$$\begin{aligned}\mathcal{Q}_d(\succ_1)(\sigma) &= \sigma(a)|0\rangle + (\sigma(b) + \sigma(c))|1\rangle\\ \mathcal{Q}_d(\succ_2)(\sigma) &= \sigma(b)|0\rangle + (\sigma(a) + \sigma(b))|1\rangle\end{aligned}$$

Similarly for τ:

$$\begin{aligned}\mathcal{Q}_d(\succ_1)(\tau) &= \tau(a)|0\rangle + (\tau(b) + \tau(c))|1\rangle\\ \mathcal{Q}_d(\succ_2)(\tau) &= \tau(b)|0\rangle + (\tau(a) + \tau(b))|1\rangle\end{aligned}$$

Hence, by the first equation in (3.7), we have $\sigma(a) = \tau(a)$. Similarly, by the second equation in (3.7), we have $\sigma(b) = \tau(b)$. We still need to show that $\sigma(c) = \tau(c)$. Since $\sigma(a) + \sigma(b) + \sigma(c) = 1 = \tau(a) + \tau(b) + \tau(c)$, then:

$$\begin{aligned} \sigma(c) &= 1 - \sigma(a) - \sigma(b) \\ &= 1 - \tau(a) - \tau(b) \\ &= \tau(c) \end{aligned}$$

This completes the proof. □

3.3.2 States and Predicates, Validity and Channels

Essential aspects of the semantics of programs like state and predicate transformers are core parts of the internal logic of an effectus. Speaking intuitively, states are used for representing a state of affairs and predicates for representing evidence (classically, in the form of events). In the effectus obtained by taking the Kleisli category of the quantum monad $\mathcal{K}\ell(\mathcal{Q}_d)$, states are quantum measurments and predicates are 'quantum' events represented by assignments of orthogonal subspaces to possible outcomes. We shall start describing what is the situation with respect to states and predicates in general for an arbitrary effectus $\mathbf{B}$. A *state* on $X \in \mathbf{B}$ is a morphism in $\mathbf{B}$ with type $1 \to X$. A *predicate* on X is a morphism in $\mathbf{B}$ with type $X \to 1 + 1$. There is an adjunction:

$$\begin{array}{ccc} \mathrm{Pred}(\mathbf{B})^{\mathrm{op}} & \underset{\longleftarrow}{\overset{\longrightarrow}{\top}} & \mathrm{Stat}(\mathbf{B}) \\ & \nwarrow \quad \nearrow & \\ & \mathbf{B} & \end{array}$$

where $\mathbf{B} \to \mathrm{Stat}(\mathbf{B})$ and $\mathbf{B} \to \mathrm{Pred}(\mathbf{B})^{\mathrm{op}}$ are the functors defined on objects as $\mathrm{Stat}(X) := \mathbf{B}(1, X)$ and $\mathrm{Pred}(X) := \mathbf{B}(X, 1+1)$ for any $X \in \mathbf{B}$; the action of these functors on a given morphism $f\colon X \to Y$ in $\mathbf{B}$ produce morphisms $\mathrm{Stat}(f)\colon \mathrm{Stat}(X) \to \mathrm{Stat}(Y)$ and $\mathrm{Pred}(f)\colon \mathrm{Pred}(Y) \to \mathrm{Pred}(X)$ called *state* and *predicate transformer* defined as $\mathrm{Stat}(f)(\omega) := f \circ \omega$ and $\mathrm{Pred}(f)(q) := q \circ f$, for any $\omega \in \mathrm{Stat}(X)$ and $q \in \mathrm{Pred}(Y)$. The following notation is standard in the field:

$$f \gg \omega := \mathrm{Stat}(f)(\omega) \in \mathrm{Stat}(Y) \qquad\qquad f \ll q := \mathrm{Pred}(f)(q) \in \mathrm{Pred}(X)$$

With this terminology and notation, we have that state transformer acts forwardly while predicate transformer acts backwardly. Given a state $\omega \in \mathrm{Stat}(X)$ and a predicate $p \in \mathrm{Pred}(X)$ on the same object $X \in \mathbf{B}$, the *validity* $\omega \models p$ of p in ω is defined to be the morphism $p \circ \omega \in \mathbf{B}(1, 1+1)$. Morphisms in $\mathbf{B}(1, 1+1)$ are called *scalars*. Hence, validity is a scalar representing the degree of certainty of some evidence in the current state of affairs.

The effectus $\mathcal{K}\ell(\mathcal{Q}_d)$ has relational structures as objects and homomorphisms of type $\mathscr{A} \to \mathcal{Q}_d(\mathscr{B})$ as morphisms. At the level of sets, states of $\mathcal{K}\ell(\mathcal{Q}_d)$ are quantum measurements (*i.e.* projection valued distributions) and since $\mathcal{Q}_d(2) \cong \mathrm{Proj}(d)$, predicates are assignments of projectors. We can think about $\mathrm{Proj}(d)$ as a relational structure of projectors with a k-ary relation $R^{\mathrm{Proj}(d)}$ given by $(p_1, \ldots, p_k) \in R^{\mathrm{Proj}(d)}$ if and only if $p_i \cdot p_j = p_j \cdot p_i$ for all $i, j = 1, \ldots, k$.

Proposition 3.3.1. *Let $\mathscr{A} = (A, R^{\mathscr{A}}) \in$ **RStr** be a relational structure. Then:*

- *a* state *on $\mathscr{A}$ is a quantum (projective) measurement $p \in \mathcal{Q}_d(\mathscr{A})$ on the underlying set A;*
- *a* predicate *$f\colon \mathscr{A} \to \mathrm{Proj}(d)$ is an assignment of projectors $f\colon A \to \mathrm{Proj}(d)$ such that points appearing in some tuple in the relation $R^{\mathscr{A}}$ get assigned commuting projectors, i.e. projectors $f(x_i), f(x_j) \in \mathrm{Proj}(d)$ commute if there exists $\alpha \in A^k$ such that $\alpha = (x_1, \ldots, x_i, \ldots, x_j, \ldots, x_k)$ and $\alpha \in R^{\mathscr{A}}$.*

Given a state and a predicate we can always compute their validity, or expected value, of the predicate in the state.

Proposition 3.3.2. *Let $p \in \mathcal{Q}_d(\mathscr{A})$ be a state and $f\colon \mathscr{A} \to \mathrm{Proj}(d')$ be a predicate. The* validity $p \models f \in \mathrm{Proj}(dd')$ *of the predicate f in the measurement p is the projector given by Kleisli composition $f_* \circ p$:*

$$p \models f := \sum_{x \in A} p(x) \otimes f(x)$$

The concept of 'channel' is central in the logical essentials of effect-theoretic reasoning and its applications, see *e.g.* [CJ17a, JZ18, Jac18b]. Formally, a *channel* is just a morphism in some effectus. For the category **Set**, channels are functions. For discrete probabilities $\mathcal{K}\ell(\mathcal{D}_M)$, channels are conditional probability distributions $X \to \mathcal{D}_M(Y)$. Finally, for quantum probabilities $\mathcal{K}\ell(\mathcal{Q}_d)$, channels are quantum homomorphisms of relational structures $\mathscr{A} \to \mathcal{Q}_d(\mathscr{B})$.

Chapter 4

Graph Spectra

The algebraic theory of graphs that we shall describe in this part is concerned with properties of certain type of matrices which are naturally associated with graphs. Specifically, we shall focus on the adjacency matrix. In particular, we look at the spectra of adjacency matrices and the equivalence relation on graphs called cospectrality defined by having the same spectrum. From the algebraic perspective, the spectrum of a graph is relevant because it is an invariant of the isomorphism class of the graph. We begin describing other algebraic and combinatorial invariant of graphs that does have an exact logical characterisation. With graph spectra, in contrast, we only know a logical equivalence sufficient for cospectrality but not necessary.

4.1 The Adjacency Matrix

The most natural way to assign an algebraic object to a graph is defining a matrix. A good treatment of algebraic graph theory can be founded in the book of Godsil and Royle [GR13].

Definition 4.1.1. The *adjacency matrix* $A(G)$ of a graph G is the integer matrix with rows and columns indexed by the vertices of G, such that the uv-entry of $A(G)$ is equal to the number of edges from u to v for all $u, v \in V(G)$.

Since we are working with simple and undirected graphs (see Remark 2.5.2), adjacency matrices are symmetric binary matrices with all diagonal entries equal to zero. Permutation matrices are binary matrices with a unique one per row and per column.

Definition 4.1.2. Two graphs G and H are isomorphic $G \cong H$ if there is a permutation matrix P such that $A(G)P = PA(H)$.

4.2 Equitable Partitions

A *partition* of a set X is a collection of mutually disjoint subsets of X called cells, such that the union of all cells is the set X. Given $\pi = \{C_1, \ldots, C_r\}$ and $\pi' = \{C'_1, \ldots, C'_{r'}\}$ partitions of X with $r' \leq r$, we say that π is a *refinement* of π' if there is a surjection $\sigma\colon \{1, \ldots, r\} \to \{1, \ldots, r'\}$ such that $C_i \subseteq C'_{\sigma(i)}$ for all $i \in \{1, \ldots, r\}$. Partitions of a set form a poset by refinement: $\pi \leq \pi'$ iff π is a refinement of π' which can also be read as π' is *coarser* than π.

Definition 4.2.1. A partition π of the vertex set $V(G)$ of a graph G with cells $C_1, \ldots, C_r$ is *equitable* if the number of neighbours in C_i of a vertex u in C_j is a constant $b_{ij} \in \mathbb{N}$ for all $u \in C_j$ and $i, j \in \{1, \ldots, r\}$.

Every graph has an equitable partition, namely the one where each cell consists of a singleton set containing one of the vertices of the graph. If G is a regular graph of degree $d \in \mathbb{N}$ (*i.e.* all vertices have exactly d neighbours), then a partition of $V(G)$ consisting of a unique cell with all vertices included is an equitable partition. A result in fractional graph theory guarantees that any graph

G has a unique coarsest equitable partition which we shall denote by $\pi(G)$, see *e.g.* [SU11, Theorem 6.3.2].

Computing the coarsest equitable partition $\pi(G)$ of G can be done efficiently (quasilinear time), with an algorithm called *colour refinement* (see *e.g.* [AKRV15]): first, all vertices are in the same cell/colour; then, vertices $u, v \in V(G)$ get different colours (*i.e.* we add a cell to the partition) if there is a cell $C \in \pi(G)$ such that u and v have different numbers of neighbours in C; this process is repeated until the number of colours/cells stops increasing. Every pair of isomorphic graphs have a common coarsest equitable partition. Hence, if two graphs have different coarsest equitable partitions then it must be the case that they are not isomorphic. Thus, colour refinement is a test for *non-isomorphism*. However, two regular graphs of the same degree and the same number of vertices (see *e.g.* Figure (4.1) below) have the same coarsest equitable partition.

In a branch of modern mathematical logic called model theory one is usually concerned with *models*, or mathematical structures (for instance, relational structures from Definition 3.2.1), and the sets of sentences (aka theories) in certain formal language, as *e.g.* in finite-variable fragments of first-order logic, that are true for them.

Definition 4.2.2. Two graphs G and H are *elementary L-equivalent* $G \equiv_L H$ with respect to some fragment L of first-order logic if G and H satisfy the same set of first-order sentences in L.

Let C^k be the k-variable fragment of first-order logic, boosted with *counting* quantifiers. A counting quantifier is of the form $\exists^n$ for some $n \in \mathbb{N}$, and its semantics is such that $\exists^n x\ \varphi(x)$ is true in a structure/model if there are at least n elements which can be substituted for x to make $\varphi(x)$ true. The following is a well-known result in descriptive complexity theory, see *e.g.* [IL90].

Theorem 4.2.1 (Immerman-Lander)**.** *Two graphs G and H are indistinguishable by colour refinement* $\pi(G) = \pi(H)$ *if and only if they are* C^2*-equivalent* $G \equiv_{C^2} H$.

4.3 Fractional Isomorphism

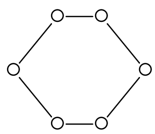
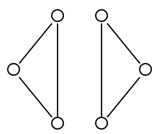
Doubly stochastic matrices are square matrices with entries from $[0,1]$ for which the sum of each row and each column is equal to 1. There are two reasons why this type of matrices are of interest to us: (1) any permutation matrix is doubly stochastic (and isomorphism is always implemented by a permutation, see Definition 4.1.2); and (2) the set of all doubly stochastic matrices of a fixed size forms a convex set. In fact, points (1) and (2) are formally related. Let $\Pi_n := \{P \in M_n(\mathbb{R}) \mid P \text{ permutation}\}$ and $\Delta_n := \{D \in M_n(\mathbb{R}) \mid D \text{ doubly stochastic}\}$ be the sets of all permutation and doubly stochastic matrices of size $n \in \mathbb{N}$, respectively. Then $\mathcal{D}(\Pi_n) \cong \Delta_n$. The proof of this statement is called the Birkhoff–von Neumann theorem. It says that every doubly stochastic matrix is a convex combination of permutation matrices.

Definition 4.3.1. Two graphs G and H are *fractionally isomorphic* $G \cong_f H$ if there is a doubly stochastic matrix D such that $A(G)D = DA(H)$.

Surely, isomorphic graphs are fractional isomorphic:

$$G \cong H \qquad \Rightarrow \qquad G \cong_f H$$

The converse is not true and here is a counterexample:

G  $\cong_f$ H  (4.1)

Actually, fractional isomorphic graphs have the same number of vertices, number of edges, degree sequence, and maximum eigenvalue. The two graphs G and H in (4.1) are, in particular, both regular of degree 2 with 6 vertices each. Therefore, the doubly stochastic matrix $D := \frac{1}{6}J$ where J is the 6×6 all-ones matrix gives us the fractional isomorphism: $A(G)D = \frac{2}{6}J = DA(H)$ but of course $G \ncong H$. The main result of [SU11, Chapter 6] is the following:

Theorem 4.3.1. *Two graphs G and H are fractionally isomorphic $G \cong_f H$ if and only if they have a common coarsest equitable partition $\pi(G) = \pi(H)$.*

4.4 Cospectrality

The coarsest equitable partition aka colour refinement is a combinatorial graph invariant. Indeed, colour refinement is also algebraic since not being distinguished by it is equivalent to fractional isomorphism. Now we shall describe another graph invariant with both combinatorial and algebraic interpretations, starting with the algebraic one. Once again, we turn to the adjacency matrix. The difference (in spirit, at least) is that now we look within and not in relation to another matrices. Thus the algebraic invariant we study by looking closer to the adjacency matrix is its (multiset of) eigenvalues, or its spectrum.

Definition 4.4.1. The *spectrum* $\mathrm{sp}(G)$ of a graph G is the multiset of zeros of the characteristic polynomial $\phi(A(G),\theta) := \det(1 - \theta A(G))$, where 1 denotes the identity matrix.

The elements of $\mathrm{sp}(G)$ are called the *eigenvalues* of G. The adjacency matrices of (simple undirected) graphs have real eigenvalues. It is convenient to think about the adjacency matrix $A := A(G)$ as a linear operator $A\colon \mathbb{R}^{V(G)} \to \mathbb{R}^{V(G)}$

defined for any map $f\colon V(G) \to \mathbb{R}$ and any vertex $u \in V(G)$ by:

$$A(f)(u) := \sum_{v \in V(G)} A_{uv} \cdot f(v)$$

where

$$A_{uv} := \begin{cases} 1 & \text{if } u \sim v \\ 0 & \text{if } u \not\sim v \end{cases}$$

for all $v \in V(G)$. Hence, we have:

$$A(f)(u) = \sum_{u \sim v} f(v)$$

Definition 4.4.2. An *eigenvector* f_θ of a graph G with eigenvalue $\theta \in \mathrm{sp}(G)$ and adjacency matrix $A(G) = A\colon \mathbb{R}^{V(G)} \to \mathbb{R}^{V(G)}$ is a function in $f_\theta \in \mathbb{R}^{V(G)}$ such that $A(f_\theta) = \theta f_\theta$.

Now we are ready to talk about the spectral decomposition of (the adjacency matrix of) a graph G. Let $\mathrm{ev}(G) = \{\theta \in \mathbb{R} \mid \exists f \in \mathbb{R}^{V(G)}.\ A(f) = \theta f\}$ be the set of eigenvalues of $A = A(G)$. Note that $\mathrm{ev}(G)$ is a set while $\mathrm{sp}(G)$ is a multiset, so it is not always the case that $\mathrm{ev}(G) = \mathrm{sp}(G)$. Let $E_\theta\colon \mathbb{R}^{V(G)} \to \mathbb{R}^{V(G)}$ be the orthogonal projection onto the eigenspace of $\theta \in \mathrm{ev}(G)$. The E_θ are also known as *principal idempotents* or *projectors*, as they satisfy the following three equations:

$$\begin{aligned} E_\theta^2 &= E_\theta \qquad (\theta \in \mathrm{ev}(G)) \\ E_\theta \cdot E_\tau &= 0 \qquad (\theta \neq \tau) \\ \sum_{\theta \in \mathrm{ev}(G)} E_\theta &= 1 \end{aligned}$$

Definition 4.4.3. The *spectral decomposition* of a graph G is the spectral decomposition of its adjacency matrix:

$$A(G) = \sum_{\theta \in \mathrm{ev}(G)} \theta E_\theta$$

Orthogonal matrices are square matrices whose rows and columns are orthonormal vectors. By definition, permutation matrices are orthogonal. The relevance of orthogonal matrices here is that they preserve the spectral decomposition.

Definition 4.4.4. Two graphs G and H are *cospectral* $G \cong_{sp} H$ if there is an orthogonal matrix Q such that $A(G)Q = QA(H)$, or equivalently if $\mathrm{sp}(G) = \mathrm{sp}(H)$.

4.5 Closed Walks

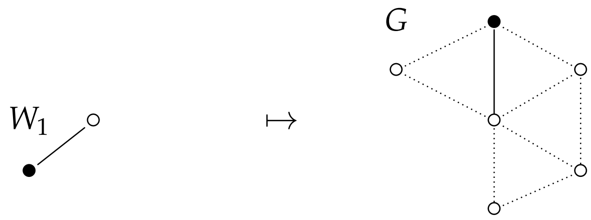
Useful information can be obtained about the internal structure of a graph by looking at its spectrum. Specifically, we get the total number of closed walks of each length in the graph.

Definition 4.5.1. For each $k \in \mathbb{N}$, let W_k be the graph with vertex set $V(W_k) = \{v_0, \ldots, v_k\}$ and edge set $E(W_k) = \{(v_0, v_1), \ldots, (v_{k-1}, v_k)\}$. The *number of walks* $w(G,k) \in \mathbb{N}$ of length k in a graph G is the number of graph homomorphisms $W_k \to G$, *i.e.*

$$w(G,k) := |\mathbf{Gph}(W_k, G)|$$

For example, one possible graph homomorphism $W_1 \to G$ for some graph

G could be:



(4.2)

In fact, there are two graph homomorphisms $W_1 \to G$ for each edge in G (one as shown in Figure (4.2) above, and the other defined by mapping the black instead of the white vertex from W_1 to the central vertex of largest degree in G). The image of a given homomorphism $W_k \to G$ is said to be a *walk* of length k in G, so we identify walks in G with homomorphisms of certain type into G. Walks of length 1 are the same thing as traveling along single edges in one direction. Thus $w(G, 1) = 2 \cdot |E(G)|$ for any graph G.

Definition 4.5.2. For each $k \in \mathbb{N}$, let C_k be the graph with vertex set $V(C_k) = \{v_0, \ldots, v_{k-1}\}$ and edge set $E(C_k) = \{(v_0, v_1), \ldots, (v_{k-1}, v_0)\}$. The *number of closed walks* $cw(G, k) \in \mathbb{N}$ of length k in a graph G is the number of graph homomorphisms $C_k \to G$, *i.e.*

$$cw(G, k) := |\mathbf{Gph}(C_k, G)|$$

Since our graphs are not reflexive (see Remark 2.5.2), then $\mathbf{Gph}(C_1, G) = \emptyset$. Therefore, $cw(G, 1) = 0$ for any graph G. The image of a given homomorphism $C_k \to G$, and C_k itself, is called a *cycle* of length k, so we identify cycles in G with homomorphisms of certain type into G. Cycles of length 2 are the same thing as traveling along an edge in one direction and then going back to the vertex where we started. Thus, every edge gives a pair of cycles of length 2. Hence, we have $cw(G, 2) = w(G, 1) = 2 \cdot |E(G)|$.

Actually, for counting the number of cycles there is more that can be said. By definition, the uv-entry of the kth power $A(G)^k$ of the adjacency matrix of a graph G is equal to the number of walks of length k from vertex u to vertex v in G. Therefore, we have $\mathrm{tr}A(G)^k = cw(G,k)$ for each $k \in \mathbb{N}$. Now, by the spectral decomposition $\mathrm{tr}A(G)^k = \mathrm{tr}(\sum_{\theta\in\mathrm{ev}(G)} \theta^k E_\theta^k) = \sum_{\theta\in\mathrm{ev}(G)} \theta^k$ which implies $cw(G,k) = \sum_{\theta\in\mathrm{sp}(G)} \theta^k$. Thus, if we have two graphs G and H cospectral $\mathrm{sp}(G) = \mathrm{sp}(H)$, then both graphs have the same total number of closed walks of every length. The converse holds as well and this is a well-known theorem in spectral graph theory, see *e.g.* [VDH03, Lemma 1].

Theorem 4.5.1. *Two graphs G and H are cospectral $G \cong_{sp} H$ if and only if they have the same number of closed walks $cw(G,k) = cw(H,k)$ for all $k \in \mathbb{N}$.*

This theorem was the motivation to define the following formulas of the counting three-variable fragment C^3 of first-order logic. Given $n \geq 0$ and $k \geq 1$, there is a formula $\mathsf{wlk}_n^k(x,y)$ of C^3 so that for any graph G and vertices $v,u \in V(G)$, we have $G \models \mathsf{wlk}_n^k[v,u]$ iff there are exactly n walks of length k in G that start at v and end at u. We define this formula by induction on k. Note that in the inductive definition, we refer to a formula $\mathsf{wlk}_n^k(z,y)$. This is to be read as the formula $\mathsf{wlk}_n^k(x,y)$ with all occurrences of x and z (free or bound) interchanged. In particular, the free variables of $\mathsf{wlk}_n^k(x,y)$ are exactly x,y and those of $\mathsf{wlk}_n^k(z,y)$ are exactly z,y. For $k=1$, the formulas are defined as follows:

$$\mathsf{wlk}_0^1(x,y) := \neg E(x,y);\ \ \mathsf{wlk}_1^1(x,y) := E(x,y);$$

$$\text{and }\ \mathsf{wlk}_n^1(x,y) := \text{false} \quad \text{for }\ n > 1.$$

For the inductive case, we shall need some notation. A collection $(i_1,n_1),\ldots,(i_r,n_r)$ of pairs of integers with $i_j,n_j \geq 1$ is called an *indexed partition* of n if the $n_1,\ldots,n_r$ are pairwise distinct and $n = \sum_{j=1}^r i_j n_j$. Let N denote the set of all indexed partitions of n and note that this is a finite set. Assuming we have defined the formulas $\mathsf{wlk}_n^k(x,y)$ for all values of $n \geq 0$, we proceed to define them for $k+1$:

$$\mathsf{wlk}_0^{k+1}(x,y) := \forall z(E(x,z) \rightarrow \mathsf{wlk}_0^k(z,y))$$

$$\mathsf{wlk}_n^{k+1}(x,y) := \bigvee_{(i_1,n_1),\ldots,(i_r,n_r)\in N} \Big(\big(\bigwedge_{j=1}^{r} \exists^{=i_j} z \; \mathsf{wlk}_{n_j}^k(z,y) \big) \wedge \exists^d z \; E(x,z) \Big)$$

where $d = \sum_{j=1}^r i_j$. We have used i_j to denote the number of neighbours of x for which there are exactly n_j walks of length k from each of them to y. Note that without allowing counting quantification it would be necessary to use many more distinct variables to rewrite the last formula.

Similarly, we can define the sentence:

$$\mathsf{clw}_n^k := \bigvee_{(i_1,n_1),\ldots,(i_r,n_r)\in N} \Big(\bigwedge_{j=1}^{r} \exists^{=i_j} x \exists y \big(x = y \wedge \mathsf{wlk}_n^k(x,y) \big) \Big)$$

Thus, we have that $G \models \mathsf{clw}_n^k$ if and only if the total number of closed walks of length k in G is exactly n. Hence $G \models \mathsf{clw}_n^k$ if and only if $cw(G,k) = \mathrm{tr} A(G)^k = n$. The following result was inspired on Theorem 4.2.1 and appears published in [DSZ16]. It says that elementary equivalence in C^3 refines cospectrality and cospectrality of complements. Recall that the *complement* of a graph G is the graph $\bar{G}$ with vertex set $V(\bar{G}) = V(G)$ and edge set $E(\bar{G}) = V(G)^2 \setminus E(G)$.

Theorem 4.5.2. *Two graphs G and H are cospectral* $\mathrm{sp}(G) = \mathrm{sp}(H)$ *with cospectral complements* $\mathrm{sp}(\bar{G}) = \mathrm{sp}(\bar{H})$ *if they are C^3-equivalent $G \equiv_{C^3} H$.*

Proof. By contrapositive, let G and H be non-isomorphic graphs such that either $\mathrm{sp}(G) \neq \mathrm{sp}(H)$ or $\mathrm{sp}(\bar{G}) \neq \mathrm{sp}(\bar{H})$. Without loss of generality, suppose there is some $k > 0$ such that $n(k) := cw(G,k) \neq cw(H,k)$. Then $G \models \mathsf{clw}_{n(k)}^k$ and $H \not\models \mathsf{clw}_{n(k)}^k$. Thus $G \not\equiv_{C^3} H$. □

Chapter 5

Game Comonads

Pebble games are certain type of two-person games of perfect information used to study elementary equivalence in various logics with limited access to resources, such as *e.g.* finite number of variables or different kinds of quantifiers. We construct a graph $\mathbb{G}_k(G)$ (with $k \in \mathbb{N}$) that encodes all the possible moves that a player can make in G during a *k-pebble game* played on a pair of graphs G, H when H is left unspecified. In fact, this construction is the functor part of a comonad called the 'pebbling' comonad in [ADW17, Sha17]. The logical equivalence that isomorphism in the coKleisli category of $\mathbb{G}_k$ encodes is elementary equivalence in C^k the k-variable fragment of first-order logic with counting quantifiers.

5.1 Logical Games

Consider the following pebble game played by Spoiler against Duplicator on two given graphs G and H. Each player has initially $k \in \mathbb{N}$ distinct pebbles and their goal would be to either distinguish (Spoiler) or identify (Duplicator) the graphs under consideration. In each round, Duplicator selects a bijection f between $V(G)$ and $V(H)$, and Spoiler places one of his pebbles on a vertex v of G; Duplicator then places her pebble on $f(v)$ and a new round starts. Spoiler wins the game if, after some round, the partial map $v \mapsto f(v)$ defined on vertices carrying a pebble is not an isomorphism between the induced subgraphs.

The pebble game defined above is called the *k-bijective game*, and it is used to characterise the expressive power of k-variable first-order logic with counting quantifiers C^k.

Theorem 5.1.1 ([Hel96]). *Duplicator has a winning strategy in the k-bijective game for graphs G, H if and only if $G \equiv_{C^k} H$ for each $k \in \mathbb{N}$.*

Therefore, two graphs G and H have the same coarsest equitable partition $\pi(G) = \pi(H)$ if Duplicator has a winning strategy in the 2-bijective game played on them $G \equiv_{C^2} H$ (see Theorem 4.2.1). Similarly, G and H have the same number of closed walks $cw(G,k) = cw(H,k)$ and so their complements $cw(\bar{G},k) = cw(\bar{H},k)$ for all $k \in \mathbb{N}$, if Duplicator has a winning strategy in the 3-bijective game played on them $G \equiv_{C^3} H$. This is because G and H are cospectral $\mathrm{sp}(G) = \mathrm{sp}(H)$ with cospectral complements $\mathrm{sp}(\bar{G}) = \mathrm{sp}(\bar{H})$ if $G \equiv_{C^3} H$ (see Theorem 4.5.2).

Now consider the slightly different pebble game called *existential k-pebble game* for some $k \in \mathbb{N}$, again played by Spoiler versus Duplicator on a pair of graphs G, H and defined as follows: each round consists of Spoiler placing one of his k pebbles on a vertex v of G; in response, Duplicator places one of her k pebbles on a vertex w of H. The winning condition for this game is that Spoiler wins if after some round, the partial map $v \mapsto w$ defined on pebbled vertices only, fails to be a homomorphism of the induced subgraphs. In contrast with the k-bijective game, here the first move in each round is made by Spoiler rather than Duplicator, no bijection is explicitly involved and so, the winning condition is stated in terms of homomorphisms rather than isomorphisms. The logical equivalence that this existential k-pebble game characterise is elementary equivalence in the k-variable existential positive fragment $\exists^+ L^k$ of first-order logic ($k \in \mathbb{N}$). Positive means that no universal quantifiers or negations are allowed.

Theorem 5.1.2 ([Lib13])**.** *Duplicator has a winning strategy in the existential k-pebble game for graphs G, H if and only if $G \equiv_{\exists^+ L^k} H$ for each $k \in \mathbb{N}$.*

5.2 The Pebbling Comonad on Graphs

There has been recent formulations of game-theoretic concepts in terms of category theory [ADW17, Sha17, AS18]. Specifically, winning strategies of Duplicator in the existential k-pebble game for graphs G, H can be formalised as coKleisli morphisms $\mathbb{G}_k(G) \to H$ for a commonad $(\mathbb{G}_k, \varepsilon, \delta)$ called the *pebbling* comonad. Recall that **Gph** denotes the category of (all) graphs and homomorphisms between them (see Remark 2.5.1). Let $\mathbb{G}_k \colon \mathbf{Gph} \to \mathbf{Gph}$ be the functor defined on objects as follows. For any $G \in \mathbf{Gph}$, let $\mathbb{G}_k(G)$ be the graph with vertex set:

$$V(\mathbb{G}_k(G)) := \bigcup_{r \in \mathbb{N}} \{[(p_1, v_1), \ldots, (p_r, v_r)] \mid \forall i \leq r.\ p_i \in \{1, \ldots, k\},\ v_i \in V(G)\}$$

For any $s, s' \in V(\mathbb{G}_k(G))$, let $(s, s') \in E(\mathbb{G}_k(G))$ if and only if (1) either $s \sqsubseteq s'$ or $s' \sqsubseteq s$, where $s \sqsubseteq s'$ if and only if there exists $t \in V(\mathbb{G}_k(G))$ such that $st = s'$; (2) the last p_i in s is not in t, where $st = s'$ if $s \sqsubseteq s'$ and similarly for the case when $s' \sqsubseteq s$; (3) $\varepsilon_G(s)$ and $\varepsilon_G(s')$ are adjacent in G, where the map $\varepsilon_G \colon V(\mathbb{G}_k(G)) \to V(G)$ is defined by $[(p_1, v_1), \ldots, (p_n, v_r)] \mapsto v_r$.

Given a graph homomorphism $f \colon G \to H$, let $\mathbb{G}_k(f) \colon \mathbb{G}_k(G) \to \mathbb{G}_k(H)$ be the map defined on tuples of pairs by:

$$[(p_1, v_1), \ldots, (p_n, v_r)] \mapsto [(p_1, f(v_1)), \ldots, (p_n, f(v_r))]$$

Indeed, the map ε_G defined above is the counit of the pebbling comonad. For the comultiplication, let $\delta_G \colon \mathbb{G}_k(G) \to \mathbb{G}_k\mathbb{G}_k(G)$ be defined by:

$$[(p_1, v_1), \ldots, (p_n, v_r)] \mapsto [(p_1, s_1), \ldots (p_r, s_r)]$$

where $s_i := [(p_1, v_1), \ldots, (p_i, v_i)]$ for $i \in \{1, \ldots, r\}$ with $r \in \mathbb{N}$.

In [ADW17], it was shown that these data satisfy the required properties to form a comonad $(\mathbb{G}_k, \varepsilon, \delta)$ for each $k \in \mathbb{N}$. The graph $\mathbb{G}_k(G)$ precisely captures all the moves Spoiler can make during the existential k-pebble game when playing on a given pair of finite graphs G, H. By specialising Theorem 13 in [ADW17] from finite relational structures to the particular case of finite graphs we obtain the following:

Theorem 5.2.1. *Duplicator has a winning strategy in the existential k-pebble game for finite graphs G, H if and only if there is a coKleisli map $\mathbb{G}_k(G) \to H$.*

Again by specialising to finite graphs Theorem 18 from [ADW17], we have the following result:

Theorem 5.2.2. *Two finite graphs G and H are isomorphic in $\mathrm{co}\mathcal{K}\ell(\mathbb{G}_k)$ if and only if $G \equiv^{C^k} H$.*

Finally, the next result is a consequence of Theorem 4.5.2, combined with Theorem 5.2.2. It provides yet another necessary condition for cospectrality.

Corollary 5.2.1. *Two finite graphs G and H are cospectral with cospectral complements if they are isomorphic in the coKleisli category $\mathrm{co}\mathcal{K}\ell(\mathbb{G}_3)$ of the pebbling comonad $\mathbb{G}_3$.*

5.3 Quantum Isomorphisms

Collecting results from previous sections, we have that fractional isomorphism is equivalent to isomorphism in $\mathrm{co}\mathcal{K}\ell(\mathbb{G}_2)$. Also we saw that cospectrality is refined by isomorphism in $\mathrm{co}\mathcal{K}\ell(\mathbb{G}_3)$. In this last section, we shall see two more relaxations of graph isomorphism that are related.

For any graph G, let $\mathrm{rel}\colon V(G)^2 \to \{0,1,2\}$ be the function defined for all $v, v' \in V(G)$ by:

$$\mathrm{rel}(v,v') := \begin{cases} 0 & \text{if} \quad v = v' \\ 1 & \text{if} \quad v \sim v' \\ 2 & \text{if} \quad v \neq v' \quad \& \quad v \not\sim v' \end{cases}$$

Recall that a real square matrix $M \in M_d(\mathbb{R})$ is *positive semidefinite* if it is symmetric and $x^T M x \geq 0$ for all x.

Definition 5.3.1. Two graphs G and H are *doubly nonnegative* isomorphic $G \cong_{dn} H$ if there is a positive semidefinite matrix M with rows and columns indexed by $V(G) \times V(H)$, which is also entrywise nonnegative and satisfies the following:

(1) $\sum_{w,w' \in V(H)} M_{vw,v'w'} = 1$ for all $v, v' \in V(G)$;

(2) $\sum_{v,v' \in V(G)} M_{vw,v'w'} = 1$ for all $w, w' \in V(H)$;

(3) $M_{vw,v'w'} = 0$ if $\mathrm{rel}(v,v') \neq \mathrm{rel}(w,w')$.

In an unpublished manuscript available online [MRV18], Mančinska et al. have shown that doubly nonnegative graph isomorphism coincides with C^3-equivalence. We can immediately derive the following:

Theorem 5.3.1. *Two graphs G and H are isomorphic in* $\mathrm{co}\mathcal{K}\ell(\mathbb{G}_3)$ *if and only if they are doubly nonnegative isomorphic* $G \cong_{dn} H$.

It is also known that cospectrality is refined by *quantum* graph isomorphism, as defined in [AMR+18].

Definition 5.3.2. Two graphs G and H are *quantumly* isomorphic $G \cong_q H$ if there are projectors $E_{vw} \in \mathrm{Proj}(d)$ for some $d \in \mathbb{N}$, $v \in V(G)$ and $w \in V(H)$ satisfying the following:

(1) $\sum_{w \in V(H)} E_{vw} = 1$ for all $v \in V(G)$;

(2) $\sum_{v \in V(G)} E_{vw} = 1$ for all $w \in V(H)$;

(3) $E_{vw} \cdot E_{v'w'} = 0$ if $\mathrm{rel}(v, v') \neq \mathrm{rel}(w, w')$.

We think the following fact is relevant as well:

Theorem 5.3.2. *Let $f\colon G \to \mathcal{Q}_d(H)$ and $g\colon H \to \mathcal{Q}_d(G)$ be graph homomorphisms for some $d \in \mathbb{N}$, such that $f(v)(w) = g(w)(v)$ for all $v \in V(G)$ and $w \in V(H)$. Then, f and g give rise to a quantum isomorphism $G \cong_q H$ between graphs G and H.*

Proof. Let us define the projectors $E_{vw} := f(v)(w) = g(w)(v)$ for $v \in V(G)$ and $w \in V(H)$. The claim is that $(E_{vw})_{v,w}$ is a quantum isomorphism. We already know that for all $v \in V(G)$ and $w \in V(H)$, we have:

$$\sum_{w' \in V(H)} f(v)(w') = \sum_{v' \in V(G)} g(w)(v') = 1$$

We shall prove that for all pairs of vertices $v, v' \in V(G)$ and $w, w' \in V(H)$, if $\mathrm{rel}(v, v') \neq \mathrm{rel}(w, w')$ then $E_{vw} \cdot E_{v'w'} = 0$.

By cases, suppose $\mathrm{rel}(v, v') = 0$; if $\mathrm{rel}(w, w') = 1$, *i.e.* $w \sim w'$ then $g(w) \sim g(w')$, because $v \not\sim v'$ since $v = v'$, so $g(w)(v) \cdot g(w')(v') = E_{vw} \cdot E_{v'w'} = 0$; if

$\mathrm{rel}(w, w') = 2$, then $f(v)(w) \cdot f(v')(w') = E_{vw} \cdot E_{v'w'} = 0$ because $f(v) = f(v')$. Now suppose $\mathrm{rel}(v, v') = 1$; if $\mathrm{rel}(w, w') = 0$ or $\mathrm{rel}(w, w') = 2$, then $w \not\sim w'$ so $f(v)(w) \cdot f(v')(w') = 0$ since $f(v) \sim f(v')$. Finally, suppose $\mathrm{rel}(v, v') = 2$; if $\mathrm{rel}(w, w') = 0$ then $g(w) = g(w')$ so $g(w)(v) \cdot g(w')(v') = 0$; if $\mathrm{rel}(w, w') = 1$ then $g(w) \sim g(w')$, and so $g(w)(v) \cdot g(w')(v') = 0$. This completes the proof. □

Chapter 6

Conclusions

With the intention to place this thesis in a wider context and to mention its significance as a whole, here we provide a general overview of the work presented in this document. First of all we see that indeed it is a mixture of two distinct parts:

- **Part I:** *Quantum Probability and Logic*
- **Part II:** *Descriptive Complexity and Finite Model Theory*

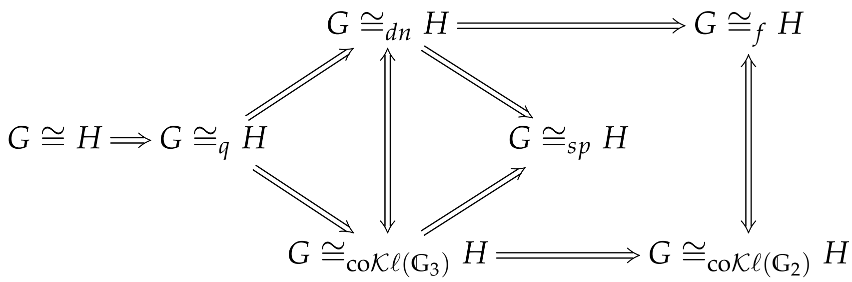
So the purpose has admittedly been to combine ideas and concepts across two different general situations in a coherent manner. Below we provide an outlook.

Quantum Probability and Logic

The first part of this document consists of Chapters 2 and 3. This part has expounded details regarding quantum and probabilistic reasoning via the notion of *effectus* from categorical logic [Jac15]. The exposition has build on previous work [ABdSZ17] about the logical and categorical structure of quantum solutions to constraint systems via the quantum monad $\mathcal{Q}_d$. Here it has been shown that the Kleisli category $\mathcal{K}\ell(\mathcal{Q}_d)$ of the quantum monad forms an effectus. States are quantum measurements (*i.e.* projection-valued distributions) and predicates are assignments of d-dimensional projections to elements. In case of having relations and not just sets, predicates must assign commuting projections to elements in some tuple in some relation. Essential aspects of the semantics of programs like validity and channels which are core parts of the internal logic of an effectus were also described, instantiated in the effectus $\mathcal{K}\ell(\mathcal{Q}_d)$. Details regarding the quantum monad $\mathcal{Q}_d$ are presented in Appendix A.

Descriptive Complexity and Finite Model Theory

The second part of the thesis was concerned with the descriptive complexity of graph spectra. This second part consists of Chapters 4 and 5. We presented formal connections between finite model theory and descriptive complexity, on one side, and probability and quantum computation, on the other. For doing this we used certain 'game' comonads $\mathbb{G}_k$ from [ADW17, Sha17, AS18]. Specifically, we considered coKleisli maps $\mathbb{G}_k(G) \to H$ which corresponds to strategies for combinatorial games encoding the notion of elementary equivalence in first-order logic with k variables called *k-pebble* games. Unfortunately, the natural attempt to provide with formal semantics to arrows of type $\mathbb{G}_k(G) \to \mathcal{Q}_d(H)$, as a notion of *quantum* strategies for k-pebble games, has not been expanded here because of the failure to provide a distributive law between the comonad $\mathbb{G}_k$ and the monad $\mathcal{Q}_d$. However, some other investigation of the author and collaborators found that if G and H are graphs isomorphic in the coKleisli category co$\mathcal{K}\ell(\mathbb{G}_k)$ of the comonad $\mathbb{G}_k$ for $k = 3$, then the (adjacency matrices of the) graphs G and H are cospectral $G \cong_{sp} H$, *i.e.* G and H have the same spectrum [DSZ16, DSZ17]. We contrasted this fact against the existence of an exact logical characterisation for isomorphism in co$\mathcal{K}\ell(\mathbb{G}_k)$ with $k = 2$, in terms of an algebraic and combinatorial graph invariant called *fractional* isomorphism (fractionally isomorphic graphs are precisely those graphs that are not distinguished by their coarsest equitable partition). We have summarised the whole second part of this document in the following picture:



Other Directions

One direction of research that we would like to pursue is to describe in more detail the effect logic of the Kleisli category of the quantum monad $\mathcal{Q}_d$ with respect to other effectuses coming also from 'probability' monads, as for instance wrt. the Giry monad, the Kantorovich monad, the Radon monad and the expectation monad (see *e.g.* [Jac18c]). Future work could also include to study the categorical formulation of Bayesian networks given in [Fon13], and try using the quantum monad in the places where the Giry monad is used. Another direction would be to look at a categorical description of various stochastic processes and their applications in *e.g.* statistics and machine learning, with the same idea of 'quantisation' via the quantum monad. Another possible line of work could be to study more deeply the monad $\mathbb{S}$ on graphs defined in Appendix B, since it captures the spectral information of a graph G by arranging in the form of a graph $\mathbb{S}(G)$ all the closed walks of each length in G.

Appendix A

Quantum Monads

Here we reproduce the details of the proof of Proposition 3.2.1, which can also be founded in [ABdSZ17]. For simplicity let us assume that all the relational structures have only one relation of a fixed arity k, *i.e.* $R(\mathscr{A}) = \{R^{\mathscr{A}}\}$ and $R^{\mathscr{A}} \subseteq A^k$ for all $\mathscr{A} \in \mathbf{RStr}$. That is, the category $\mathbf{RStr}$ is obtained from the fibration $\mathbf{Sub}(\mathbf{Set}) \to \mathbf{Set}$ of subsets by taking the pullback:

$$
\begin{array}{ccc}
\mathbf{RStr} & \longrightarrow & \mathbf{Sub}(\mathbf{Set}) \\
\big\downarrow \lrcorner & & \big\downarrow \\
\mathbf{Set} & \xrightarrow[A \,\mapsto\, A \times \cdots \times A]{} & \mathbf{Set}
\end{array}
$$

A.1 Functor Part

The next three results show that indeed, for any $d \in \mathbb{N}$, we have a functor $\mathcal{Q}_d \colon \mathbf{RStr} \to \mathbf{RStr}$ giving a relational structure $\mathcal{Q}_d(\mathscr{A})$ whose underlying set is the convex set $\mathcal{Q}_d(A)$ of all formal orthogonal convex combinations $\sum_x p_x |x\rangle \in \mathcal{Q}_d(A)$ of elements in $x \in A$, for each $\mathscr{A} \in \mathbf{RStr}$, with probabilities/scalars $p_x \in \text{Proj}(d)$ from the set of projections into a d-dimensional complex space, satisfying $\sum_x p_x = 1 \in \text{Proj}(d)$. Such formal convex combinations can also be regarded as projection-valued distributions (aka projection-valued measures PVMs) which are the mathematical description of sharp observables in quantum theory, see *e.g.* [HZ11, Definition 3.27]. The relation $R^{\mathcal{Q}_d(\mathscr{A})} \subseteq \mathcal{Q}_d(A)^k$ is defined as follows: given $p_1, \ldots, p_k \in \mathcal{Q}_d(A)$, we have $(p_1, \ldots, p_k) \in R^{\mathcal{Q}_d(\mathscr{A})}$ if and only if (1) the p_i's pairwise commute, *i.e.* for all $x, x' \in A$ we have $p_i(x) \cdot p_j(x') = p_j(x') \cdot p_i(x)$, and (2) for all $x_1, \ldots, x_k \in A$ if $(x_1, \ldots, x_k) \notin R^{\mathscr{A}}$ then $\prod_{i=1}^k p_i(x_i) = 0$. Again, from a homomorphism $f\colon \mathscr{A} \to \mathscr{B}$ of relational structures, we define a map $\mathcal{Q}_d(f)\colon \mathcal{Q}_d(\mathscr{A}) \to \mathcal{Q}_d(\mathscr{B})$ as $\mathcal{Q}_d(f)(p)(y) := \sum_{x \in f^{-1}(y)} p(x)$ for all $p \in \mathcal{Q}_d(A)$ and $y \in B$.

Proposition A.1.1. *For any homomorphism $f\colon \mathscr{A} \to \mathscr{B}$ of relational structures with $d \in \mathbb{N}$, the map $\mathcal{Q}_d(f)\colon \mathcal{Q}_d(\mathscr{A}) \to \mathcal{Q}_d(\mathscr{B})$ is a homomorphismof relational srtructures.*

Proof. Fix $d \in \mathbb{N}$ and take $p_1, \ldots, p_k \in \mathcal{Q}_d(A)$ such that $(p_1, \ldots, p_k) \in R^{\mathcal{Q}_d(\mathscr{A})}$. Given $y_1, \ldots, y_k \in B$ with $(y_1, \ldots, y_k) \notin R^{\mathcal{Q}_d(\mathscr{B})}$, we have $\prod_{i=1}^k p_i(x_i) = 0$ for all $x_i \in f^{-1}(y_i)$. Hence

$$\begin{aligned}\prod_{i=1}^{k} \mathcal{Q}_d(f)(p_i)(y_i) &= \prod_{i=1}^{k} \sum_{x_i \in f^{-1}(y_i)} p_i(x_i) \\ &= \sum_{x_i \in f^{-1}(y_i)} \prod_{i=1}^{k} p_i(x_i) = 0\end{aligned}$$

and so $(\mathcal{Q}_d(f)(p_1), \ldots, \mathcal{Q}_d(f)(p_k)) \in R^{\mathcal{Q}_d(\mathscr{B})}$. $\square$

Proposition A.1.2. *Let $f\colon \mathscr{A} \to \mathscr{B}$ and $g\colon \mathscr{B} \to \mathscr{C}$ be homomorphisms of relational structures. Then $\mathcal{Q}_d(g) \circ \mathcal{Q}_d(f) = \mathcal{Q}_d(g \circ f)$ for all $d \in \mathbb{N}$.*

Proof. Fix $d \in \mathbb{N}$. Let $p \in \mathcal{Q}_d(A)$ and $z \in C$. The claim is that the following equation holds:

$$\mathcal{Q}_d(g) \circ \mathcal{Q}_d(f)(p)(z) = \mathcal{Q}_d(g \circ f)(p)(z)$$

The proof of the above equation is the following calculation:

$$\begin{aligned}
\mathcal{Q}_d(g) \circ \mathcal{Q}_d(f)(p)(z) &= \sum_{y \in g^{-1}(z)} \mathcal{Q}_d(f)(p)(y) \\
&= \sum_{y \in g^{-1}(z)} \sum_{x \in f^{-1}(y)} p(x) \\
&= \sum_{x \in (g \circ f)^{-1}(z)} p(x) \\
&= \mathcal{Q}_d(g \circ f)(p)(z)
\end{aligned}$$

□

Proposition A.1.3. *Let $\mathscr{A} \in$ **RStr** be a relational structure. Then $\mathcal{Q}_d(\mathrm{id}_{\mathscr{A}}) = \mathrm{id}_{\mathcal{Q}_d(\mathscr{A})}$ for all $d \in \mathbb{N}$.*

Proof. Let $p \in \mathcal{Q}_d(A)$ for some $d \in \mathbb{N}$, and $x \in A$. Then, we have:

$$\begin{aligned}
\mathcal{Q}_d(\mathrm{id}_{\mathscr{A}})(p)(x) &= \sum_{x' = x} p(x') \\
&= p(x) \\
&= \mathrm{id}_{\mathcal{Q}_d(\mathscr{A})}(p)(x)
\end{aligned}$$

□

A.2 Graded Monad Structure

Now, as mentioned already in Section 3.2, let $\eta_{\mathscr{A}} \colon \mathscr{A} \to \mathcal{Q}_1(\mathscr{A})$ be defined by

$$\eta_{\mathscr{A}}(x)(x') := \begin{cases} 1 & \text{if} \quad x = x' \\ 0 & \text{if} \quad x \neq x' \end{cases}$$

and $\mu^{d,d'}_{\mathscr{A}} \colon \mathcal{Q}_d \mathcal{Q}_{d'}(\mathscr{A}) \to \mathcal{Q}_{dd'}(\mathscr{A})$ be defined by

$$\mu^{d,d'}_{\mathscr{A}}(P)(x) := \sum_{p \in \mathcal{Q}_{d'}(A)} P(p) \otimes p(x).$$

Proposition A.2.1. *For any $\mathscr{A} \in$ **RStr**, the maps $\eta_{\mathscr{A}} \colon \mathscr{A} \to \mathcal{Q}_1(\mathscr{A})$ and $\mu_{\mathscr{A}} \colon \mathcal{Q}_d \mathcal{Q}_{d'}(\mathscr{A}) \to \mathcal{Q}_{dd'}(\mathscr{A})$ are homomorphism of relational structures.*

Proof. Let $x_1, \ldots, x_k \in A$ such that $(x_1, \ldots, x_k) \in R^{\mathscr{A}}$. Consider $x'_1, \ldots, x'_k \in A$ such that $(x'_1, \ldots, x'_k) \notin R^{\mathscr{A}}$. We need to show that the following equation holds:

$$\prod_{i=1}^{k} \eta_{\mathscr{A}}(x_i)(x'_i) = 0 \tag{A.1}$$

But $\prod_{i=1}^{k} \eta_{\mathscr{A}}(x_i)(x'_i) \neq 0$ if and only if $x_i = x'_i$ for all $i = 1, \ldots, k$, and so the only case when equation (A.1) does not hold is when $(x_1, \ldots, x_k) = (x'_1, \ldots, x'_k)$ and by assumption this is not the case since one tuple is in the relation and the other is not. Hence $(\eta_{\mathscr{A}}(x_1), \ldots, \eta_{\mathscr{A}}(x_k)) \in R^{\mathcal{Q}_1(\mathscr{A})}$.

Now, suppose we have $P_1, \ldots, P_k \in \mathcal{Q}_d \mathcal{Q}_{d'}(A)$ such that $(P_1, \ldots, P_k) \in R^{\mathcal{Q}_d \mathcal{Q}_{d'}(\mathscr{A})}$. Consider $x_1, \ldots, x_k \in A$ such that $(x_1, \ldots, x_k) \notin R^{\mathscr{A}}$. We need to show that the following equation holds:

$$\prod_{i=1}^{k} \mu^{d,d'}_{\mathscr{A}}(P_i)(x_i) = 0$$

The proof of the equation above is the following calculation:

$$
\begin{aligned}
\prod_{i=1}^{k} \mu_{\mathscr{A}}^{d,d'}(P_i)(x_i) &= \prod_{i=1}^{k} \sum_{p_i \in \mathcal{Q}_{d'}(A)} P_i(p_i) \otimes p_i(x_i) \\
&= \sum_{p_i \in \mathcal{Q}_{d'}(A)} \prod_{i=1}^{k} P_i(p_i) \otimes p_i(x_i) \\
&= \sum_{p_i \in \mathcal{Q}_{d'}(A)} \prod_{i=1}^{k} P_i(p_i) \otimes \prod_{i=1}^{k} p_i(x_i) \\
&= 0
\end{aligned}
$$

where the last equality holds because our assumptions imply $\prod_{i=1}^{k} p_i(x_i) = 0$. ☐

Proposition A.2.2. *Let $f \colon \mathscr{A} \to \mathscr{B}$ be a homomorphism of relational structures. Then the following diagram commutes:*

$$
\begin{array}{ccc}
\mathscr{A} & \xrightarrow{\quad f \quad} & \mathscr{B} \\
\downarrow{\scriptstyle \eta_{\mathscr{A}}} & & \downarrow{\scriptstyle \eta_{\mathscr{B}}} \\
\mathcal{Q}_1(\mathscr{A}) & \xrightarrow[\mathcal{Q}_1(f)]{} & \mathcal{Q}_1(\mathscr{B})
\end{array}
$$

Proof. For any $x \in A$ and $y \in B$, the claim is that:

$$
(\mathcal{Q}_1(f) \circ \eta_{\mathscr{A}})(x)(y) = (\eta_{\mathscr{B}} \circ f)(x)(y)
$$

The proof of equation above this is the following calculation:

$$
\begin{aligned}
\mathcal{Q}_1(f)(\eta_{\mathscr{A}}(x))(y) &= \sum_{x' \in f^{-1}(y)} \eta_{\mathscr{A}}(x)(x') \\
&= \sum_{y = f(x')} \eta_{\mathscr{A}}(x)(x') \\
&= \eta_{\mathscr{B}}(f(x))(y).
\end{aligned}
$$

$\square$

Proposition A.2.3. *Let $f\colon \mathscr{A} \to \mathscr{B}$ be a homomorphism between relational structures and $d, d' \in \mathbb{N}$. Then the following diagram commutes:*

$$\begin{array}{ccc} \mathcal{Q}_d\mathcal{Q}_{d'}(\mathscr{A}) & \xrightarrow{\mathcal{Q}_d\mathcal{Q}_{d'}(f)} & \mathcal{Q}_d\mathcal{Q}_{d'}(\mathscr{B}) \\ {\scriptstyle \mu_{\mathscr{A}}^{d,d'}}\downarrow & & \downarrow{\scriptstyle \mu_{\mathscr{B}}^{d,d'}} \\ \mathcal{Q}_{dd'}(\mathscr{A}) & \xrightarrow[\mathcal{Q}_{dd'}(f)]{} & \mathcal{Q}_{dd'}(\mathscr{B}) \end{array}$$

Proof. For any $P \in \mathcal{Q}_d\mathcal{Q}_{d'}(A)$ and $y \in B$, the claim is that the following equation holds:

$$(\mu_{\mathscr{B}}^{d,d'} \circ \mathcal{Q}_d\mathcal{Q}_{d'}(f))(P)(y) = (\mathcal{Q}_{dd'}(f) \circ \mu_{\mathscr{A}}^{d,d'})(P)(y) \tag{A.2}$$

The proof of the equation above is the following calculation:

$$
\begin{aligned}
\mu^{d,d'}_{\mathscr{B}}(\mathcal{Q}_d\mathcal{Q}_{d'}(f))(P)(y) &= \sum_{q \in \mathcal{Q}_{d'}(B)} (\mathcal{Q}_d\mathcal{Q}_{d'}(f)(P))(q) \otimes q(y) \\
&= \sum_{q \in \mathcal{Q}_{d'}(B)} \left(\sum_{\mathcal{Q}_{d'}(f)(p)=q} P(p) \right) \otimes q(y) \\
&= \sum_{q \in \mathcal{Q}_{d'}(B)} \; \sum_{\mathcal{Q}_{d'}(f)(p)=q} P(p) \otimes \mathcal{Q}_{d'}(f)(p)(y) \\
&= \sum_{q \in \mathcal{Q}_{d'}(B)} \; \sum_{\mathcal{Q}_{d'}(f)(p)=q} P(p) \otimes \sum_{f(x)=y} p(x) \\
&= \sum_{q \in \mathcal{Q}_{d'}(B)} \; \sum_{\mathcal{Q}_{d'}(f)(p)=q} \; \sum_{f(x)=y} P(p) \otimes p(x) \\
&= \sum_{p \in \mathcal{Q}_{d'}(A)} \; \sum_{f(x)=y} P(p) \otimes p(x) \\
&= \sum_{f(x)=y} \; \sum_{p \in \mathcal{Q}_{d'}(A)} P(p) \otimes p(x) \\
&= \sum_{f(x)=y} \mu^{d,d'}_{\mathscr{A}}(P)(x) \\
&= \mathcal{Q}_{dd'}(f)(\mu^{d,d'}_{\mathscr{A}}(P))(y).
\end{aligned}
$$

□

Hence $\eta\colon 1_{\mathbf{RStr}} \Rightarrow \mathcal{Q}_1$ is a natural transformation, and for all $d, d' \in \mathbb{N}$ we have a natural transformation $\mu^{d,d'}\colon \mathcal{Q}_d\mathcal{Q}_{d'} \Rightarrow \mathcal{Q}_{dd'}$.

Lemma A.2.1. *Let $\mathscr{A} \in \mathbf{RStr}$ be a relational structure and $d \in \mathbb{N}$. Then the following diagrams commute:*

$$
\begin{array}{ccc}
\mathcal{Q}_d(\mathscr{A}) & \xrightarrow{\mathcal{Q}_d(\eta_{\mathscr{A}})} & \mathcal{Q}_d\mathcal{Q}_1(\mathscr{A}) \\
& \searrow^{\mathrm{id}_{\mathcal{Q}_d(\mathscr{A})}} & \downarrow \mu^{d,1}_{\mathscr{A}} \\
& & \mathcal{Q}_d(\mathscr{A})
\end{array}
\qquad\qquad
\begin{array}{ccc}
\mathcal{Q}_d(\mathscr{A}) & \xrightarrow{\eta_{\mathcal{Q}_d(\mathscr{A})}} & \mathcal{Q}_1\mathcal{Q}_d(\mathscr{A}) \\
& \searrow^{\mathrm{id}_{\mathcal{Q}_d(\mathscr{A})}} & \downarrow \mu^{1,d}_{\mathscr{A}} \\
& & \mathcal{Q}_d(\mathscr{A})
\end{array}
$$

Proof. Take $p \in \mathcal{Q}_d(A)$ and $x \in A$. Recall $\mathrm{Proj}(d) = \{0, 1\}$ when $d = 1$. Commutativity of the left-hand side triangle above is the following calculation:

$$\begin{aligned}
\mu_{\mathscr{A}}^{d,1}(\mathcal{Q}_d(\eta_{\mathscr{A}})(p))(x) &= \sum_{p' \in \mathcal{Q}_1(A)} \mathcal{Q}_d(\eta_{\mathscr{A}})(p)(p') \otimes p'(x) \\
&= \sum_{p' \in \mathcal{Q}_1(A)} \sum_{\eta_G(x') = p'} p(x') \otimes p'(x) \\
&= \sum_{x' \in A} p(x') \otimes \eta_{\mathscr{A}}(x')(x) \\
&= p(x)
\end{aligned}$$

The right-hand side triangle above commutes, since:

$$\begin{aligned}
\mu_{\mathscr{A}}^{1,d}(\eta_{\mathcal{Q}_d(\mathscr{A})}(p))(x) &= \sum_{p' \in \mathcal{Q}_d(A)} \eta_{\mathcal{Q}_d(\mathscr{A})}(p)(p') \otimes p'(x) \\
&= p(x)
\end{aligned}$$

□

Lemma A.2.2. *Let $\mathscr{A} \in$ **RStr** be a relational structure and $a, b, c \in \mathbb{N}$. Then the following diagram commutes:*

$$\begin{array}{ccc}
\mathcal{Q}_a\mathcal{Q}_b\mathcal{Q}_c(\mathscr{A}) & \xrightarrow{\mathcal{Q}_a(\mu_{\mathscr{A}}^{b,c})} & \mathcal{Q}_a\mathcal{Q}_{bc}(\mathscr{A}) \\
{\scriptstyle \mu_{\mathcal{Q}_c(\mathscr{A})}^{a,b}} \downarrow & & \downarrow {\scriptstyle \mu_{\mathscr{A}}^{a,bc}} \\
\mathcal{Q}_{ab}\mathcal{Q}_c(\mathscr{A}) & \xrightarrow[\mu_{\mathscr{A}}^{ab,c}]{} & \mathcal{Q}_{abc}(\mathscr{A})
\end{array}$$

Proof. Let $P \in \mathcal{Q}_a\mathcal{Q}_b\mathcal{Q}_c(A)$ and $x \in A$. The claim is that the following equation holds:

$$(\mu_{\mathscr{A}}^{a,bc} \circ \mathcal{Q}_a(\mu_{\mathscr{A}}^{b,c}))(P)(x) = (\mu_{\mathscr{A}}^{ab,c} \circ \mu_{\mathcal{Q}_c(\mathscr{A})}^{a,b})(P)(x) \tag{A.3}$$

The left-hand side of equation (A.3) expands to:

$$
\begin{aligned}
\mu_{\mathscr{A}}^{a,bc}(\mathcal{Q}_a(\mu_{\mathscr{A}}^{b,c})(P))(x) &= \sum_{q\in\mathcal{Q}_{bc}(A)} \Big(\mathcal{Q}_a(\mu_{\mathscr{A}}^{b,c})(P)(q)\Big) \otimes q(x) \\
&= \sum_{q\in\mathcal{Q}_{bc}(A)} \sum_{\mu_{\mathscr{A}}^{b,c}(q')=q} P(q') \otimes q(x) \\
&= \sum_{q\in\mathcal{Q}_{bc}(A)} \sum_{\mu_{\mathscr{A}}^{b,c}(q')=q} P(q') \otimes \mu_{\mathscr{A}}^{b,c}(q')(x) \\
&= \sum_{q\in\mathcal{Q}_{bc}(A)} \sum_{\mu_{\mathscr{A}}^{b,c}(q')=q} \sum_{p\in\mathcal{Q}_c(A)} P(q') \otimes q'(p) \otimes p(x) \\
&= \sum_{p'\in\mathcal{Q}_b\mathcal{Q}_c(A)} \sum_{p\in\mathcal{Q}_c(A)} P(p') \otimes p'(p) \otimes p(x)
\end{aligned}
$$

and the right-hand side of (A.3) to:

$$
\begin{aligned}
\mu_{\mathscr{A}}^{ab,c}(\mu_{\mathcal{Q}_c(A)}^{a,b}(P))(x) &= \sum_{p\in\mathcal{Q}_c(A)} \mu_{\mathcal{Q}_c(\mathscr{A})}^{a,b}(P)(p) \otimes p(x) \\
&= \sum_{p\in\mathcal{Q}_c(A)} \sum_{p'\in\mathcal{Q}_b\mathcal{Q}_c(A)} P(p') \otimes p'(p) \otimes p(x).
\end{aligned}
$$

□

Finally, we are ready to prove Proposition 3.2.1 from Section 3:

Proposition 3.2.1. $((\mathcal{Q}_d)_d, \eta, (\mu^{d,d'})_{d,d'})$ is an $\mathbb{N}$-graded monad on **RStr**.

Proof. By Propositions A.1.1, A.1.2, A.1.3, for all $d \in \mathbb{N}$ we have that $\mathcal{Q}_d$ is an endofunctor on **RStr**. By Proposiotions A.2.1, A.2.2 and A.2.3, $\eta\colon 1 \Rightarrow \mathcal{Q}_1$ is a natural transformation, and for all $d, d' \in \mathbb{N}$, we have that $\mu^{d,d'}\colon \mathcal{Q}_d\mathcal{Q}_{d'} \Rightarrow \mathcal{Q}_{dd'}$ is a natural transformation. By Lemmas A.2.1 and A.2.2, we have that η and μ satisfy the axioms for the unit and graded multiplication. □

Appendix B

Graph Spectra Monad

Reflexive graphs were not included in our discussions throughout the course of this thesis. Specifically, they were not referred to when we used the word 'graph' unless otherwise was clearly mentioned. Note, however, that we have been using **Gph** to denote the category whose objects are all graphs in the sense of Definition 2.5.1, *i.e.* including reflexive and directed graphs with multiple edges. Morphisms in **Gph** are edge-preserving functions between the underlying vertex sets. Recall that $C_n \in \mathbf{Gph}$ is the *n-cycle* with:

$$
\begin{aligned}
V(C_n) &= \{v_0, \ldots, v_{n-1}\} \\
E(C_n) &= \{(v_0, v_1), \ldots, (v_{n-1}, v_0)\}
\end{aligned}
$$

for each $n \in \mathbb{N}$. By definition, for all $G \in \mathbf{Gph}$ the number $|\mathbf{Gph}(C_1, G)| \geq 0$ of graph homomorphisms from C_1 to G is equal to the number of vertices in G carrying a loop, *i.e.* vertices $v \in V(G)$ such that $(v, v) \in E(G)$. As previously mentioned in Remark 2.5.2 (and also as noted above), for us graphs don't have loops so this number attains its minimum $|\mathbf{Gph}(C_1, G)| = 0$ when G is a graph.

For any $G \in \mathbf{Gph}$, let $\mathbb{S}(G)$ be defined as:

$$V(\mathbb{S}(G)) := V(G) \cup \sum_{n \in \mathbb{N}} \mathbf{Gph}(C_n, G)$$
$$E(\mathbb{S}(G)) := E(G) \cup \{(\sigma, \sigma') \in V(\mathbb{S}(G))^2 \mid \sigma(v_0) \sim \sigma'(v_0) \text{ in } G\}$$

where the big sum in the vertex set denotes disjoint union of sets of graph homomorphisms of type $C_n \to G$ when n is ranging along the set of natural numbers $\mathbb{N}$. When $G, H \in \mathbf{Gph}$ are finite graphs (*i.e.* irreflexive, simple and undirected) their adjacency matrices have the same spectrum if and only if $V(\mathbb{S}(G)) = V(\mathbb{S}(H))$ (see Theorem 4.5.1).

For any graph homomorphism $f \colon G \to H$, let $\mathbb{S}(f) \colon V(\mathbb{S}(G)) \to V(\mathbb{S}(H))$ be the map defined by $\mathbb{S}(f)(\sigma) := f \circ \sigma \in \mathbf{Gph}(C_n, H) \subseteq V(\mathbb{S}(H))$ for all $\sigma \in \mathbf{Gph}(C_n, G) \subseteq V(\mathbb{S}(G)$ with $n \in \mathbb{N}$, and by $\mathbb{S}(f)(v) := f(v) \in V(H)$ for all $v \in V(G)$. By definition, $\mathbb{S}(f) = f \circ -$ is a graph homomorphism. Given another graph homomorphism $g \colon H \to K$, since $(g \circ f) \circ \sigma = g \circ (f \circ \sigma)$ we have:

$$\begin{array}{ccc} \mathbb{S}(G) & \xrightarrow{\mathbb{S}(f)} & \mathbb{S}(H) \\ & \underset{\mathbb{S}(g \circ f)}{\searrow} & \downarrow{\scriptstyle \mathbb{S}(g)} \\ & & \mathbb{S}(K) \end{array}$$

Hence, we have a functor $\mathbb{S} \colon \mathbf{Gph} \to \mathbf{Gph}$ defined as above.

For every $G \in \mathbf{Gph}$, let $\eta_G \colon V(G) \to V(\mathbb{S}(G))$ be the inclusion map of G into $\mathbb{S}(G)$ defined by $\eta_G(v) := v$ for all $v \in V(G)$. This definition turns $\eta_G \colon G \to \mathbb{S}(G)$ into a (injective) graph homomorphism.

Lemma B.0.1. *Let $f \colon G \to H$ be a graph homomorphism. Then the following diagram* *commutes:*

$$\begin{CD} G @>{f}>> H \\ @V{\eta_G}VV @VV{\eta_H}V \\ \mathbb{S}(G) @>>{\mathbb{S}(f)}> \mathbb{S}(H) \end{CD}$$

Thus $\eta\colon 1 \Rightarrow \mathbb{S}$ *is a natural transformation.*

Proof. For each $v \in V(G)$, traveling along both sides of the square above yields:

$$\begin{aligned} \mathbb{S}(f)(\eta_G)(v) &= \mathbb{S}(f)(v) \\ &= f(v) \\ &= \eta_H(f(v)) \end{aligned}$$

Hence $\mathbb{S}(f) \circ \eta_G = \eta_H \circ f$ indeed. □

Now, let $\varepsilon_G\colon V(\mathbb{S}(G)) \to V(G)$ be the map defined by $\varepsilon_G(\sigma) := \sigma(v_0) \in V(G)$ for all $\sigma \in \mathbf{Gph}(C_n, G)$ with $n \in \mathbb{N}$, and by $\varepsilon_G(v) := v$ for all $v \in V(G)$. Because of the way we defined adjacency in $\mathbb{S}(G)$, we have that $\varepsilon_G\colon \mathbb{S}(G) \to G$ is a graph homomorphism. Finally, we can apply the functor $\mathbb{S}$ to ε_G and obtain a graph homomorphism $\mu_G := \mathbb{S}(\varepsilon_G)\colon \mathbb{S}^2(G) \to \mathbb{S}(G)$. Thus for all $\Sigma \in \mathbf{Gph}(C_n, \mathbb{S}(G))$, $\sigma \in \mathbf{Gph}(C_n, G)$ and $x \in V(C_n)$ with $n \in \mathbb{N}$, and $v \in V(G)$ we have:

$$\begin{aligned} \mu_G(\Sigma)(x) &= \mathbb{S}(\varepsilon_G)(\Sigma)(x) \\ &= \varepsilon_G \circ \Sigma(x) \\ &= \Sigma(x)(v_0) \\ \mu_G(\sigma)(x) &= \sigma(x) \\ \mu_G(v) &= v \end{aligned}$$

Lemma B.0.2. *Let* $f\colon G \to H$ *be a graph homomorphism. Then the following diagram* *commutes:*

$$\begin{array}{ccc} \mathbb{S}^2(G) & \xrightarrow{\mathbb{S}^2(f)} & \mathbb{S}^2(H) \\ \downarrow{\scriptstyle \mu_G} & & \downarrow{\scriptstyle \mu_H} \\ \mathbb{S}(G) & \xrightarrow[\mathbb{S}(f)]{} & \mathbb{S}(H) \end{array}$$

Thus $\mu\colon \mathbb{S}^2 \Rightarrow \mathbb{S}$ *is a natural transformation.*

Proof. Let $\Sigma \in \mathbf{Gph}(C_n, \mathbb{S}(G))$, $\sigma \in \mathbf{Gph}(C_n, G)$ and $x \in V(C_n)$ for some $n \in \mathbb{N}$, and $v \in V(G)$. Then:

$$\begin{aligned}
\mathbb{S}(f)\,(\mu_G(\Sigma))\,(x) &= (f \circ \mu_G(\Sigma))(x) \\
&= f\,(\Sigma(x)(v_0)) \\
&= \mathbb{S}(f)\,(\Sigma(x)(v_0)) \\
&= \mathbb{S}^2(f)(\Sigma)(x)(v_0) \\
&= \mu_H(\mathbb{S}^2(f)(\Sigma))(x) \\
\mathbb{S}(f)(\mu_G(\sigma))(x) &= (f \circ \sigma)(x) \\
&= \mu_H(f \circ \sigma)(x) \\
&= \mu_H(\mathbb{S}(f)(\sigma))(x) \\
&= \mu_H(\mathbb{S}^2(f)(\sigma))(x) \\
\mathbb{S}(f)(\mu_G(v)) &= \mathbb{S}(f)(v) \\
&= f(v) \\
&= \mathbb{S}^2(f)(v) \\
&= \mu_H(\mathbb{S}^2(f)(v))
\end{aligned}$$

Hence $\mathbb{S}(f) \circ \mu_G = \mu_H \circ \mathbb{S}^2(f)$ indeed. □

We have so far an endofunctor $\mathbb{S}\colon \mathbf{Gph} \to \mathbf{Gph}$, and a couple of natural transformations $\eta\colon 1 \Rightarrow \mathbb{S}$ and $\mu\colon \mathbb{S}^2 \Rightarrow \mathbb{S}$ looking very much like a monoid in the category of endofunctors on **Gph** with natural transformations as morphisms.

Theorem B.0.1. *Let $G \in$ **Gph**. Then the following diagrams commute:*

$$
\begin{array}{ccc}
\mathbb{S}(G) & \xrightarrow{\mathbb{S}(\eta_G)} & \mathbb{S}^2(G) \\
& \searrow^{\mathrm{id}} & \downarrow \mu_G \\
& & \mathbb{S}(G)
\end{array}
\qquad
\begin{array}{ccc}
\mathbb{S}(G) & \xrightarrow{\eta_{\mathbb{S}(G)}} & \mathbb{S}^2(G) \\
& \searrow^{\mathrm{id}} & \downarrow \mu_G \\
& & \mathbb{S}(G)
\end{array}
\qquad
\begin{array}{ccc}
\mathbb{S}^3(G) & \xrightarrow{\mathbb{S}(\mu_G)} & \mathbb{S}^2(G) \\
\mu_{\mathbb{S}(G)} \downarrow & & \downarrow \mu_G \\
\mathbb{S}^2(G) & \xrightarrow[\mu_G]{} & \mathbb{S}(G)
\end{array}
$$

Therefore, $(\mathbb{S}, \eta, \mu)$ is a monad on **Gph**.

Proof. Let $\sigma \in \mathbf{Gph}(C_n, G)$ and $x \in C_n$ for some $n \in \mathbb{N}$, and $v \in V(G)$. Commutativity of the first triangle on the left above $\mu_G \circ \mathbb{S}(\eta_G) = \mathrm{id}$ holds:

$$
\begin{aligned}
\mu_G(\mathbb{S}(\eta_G)(\sigma))(x) &= \mathbb{S}(\varepsilon_G)(\mathbb{S}(\eta_G)(\sigma))(x) \\
&= \mathbb{S}(\varepsilon_G)(\eta_G \circ \sigma)(x) \\
&= \varepsilon_G(\eta_G(\sigma(x))) \\
&= \varepsilon_G(\sigma(x)) \\
&= \sigma(x) \\
\mu_G(\mathbb{S}(\eta_G)(v)) &= \mu_G(\eta_G(v)) \\
&= \mu_G(v) \\
&= v
\end{aligned}
$$

Commutativity of the second triangle on the middle above $\mu_G \circ \eta_{\mathbb{S}(G)} = \mathrm{id}$ also holds:

$$
\begin{aligned}
\mu_G(\eta_{\mathbb{S}(G)}(\sigma))(x) &= \mathbb{S}(\varepsilon_G)(\eta_{\mathbb{S}(G)}(\sigma))(x) \\
&= \mathbb{S}(\varepsilon_G)(\sigma)(x) \\
&= \varepsilon_G(\sigma(x)) \\
&= \sigma(x) \\
\mu_G(\eta_{\mathbb{S}(G)}(v)) &= \mu_G(v) \\
&= v
\end{aligned}
$$

Now, let $\hat{\Sigma} \in \mathbf{Gph}(C_n, \mathbb{S}^2(G)) \subseteq V(\mathbb{S}^3(G))$ and $\Sigma \in \mathbf{Gph}(C_n, \mathbb{S}(G)) \subseteq V(\mathbb{S}^2(G))$. Commutativity of the rectangle on the right above $\mu_G \circ \mathbb{S}(\mu_G) = \mu_G \circ \mu_{\mathbb{S}(G)}$ holds as well:

$$
\begin{aligned}
\mu_G(\mathbb{S}(\mu_G)(\hat{\Sigma}))(x) &= \mu_G(\mu_G \circ \hat{\Sigma})(x) \\
&= (\mu_G \circ \hat{\Sigma})(x)(v_0) \\
&= \mu_G(\hat{\Sigma}(x)(v_0)) \\
&= \mu_G(\mu_{\mathbb{S}(G)}(\hat{\Sigma})(x)) \\
\mu_G(\mathbb{S}(\mu_G)(\Sigma))(x) &= \mu_G(\mu_G \circ \Sigma)(x) \\
&= \mu_G \circ \Sigma(x) \\
&= \mu_G(\Sigma)(x) \\
&= \mu_G(\mu_{\mathbb{S}(G)}(\Sigma))(x)
\end{aligned}
$$

$$
\begin{aligned}
\mu_G(\mathbb{S}(\mu_G)(\sigma)(x)) &= \mu_G(\mu_G(\sigma)(x)) \\
&= \mu_G(\sigma(x)) \\
&= \mu_G(\mu_{\mathbb{S}(G)}(\sigma)(x)) \\
\mu_G(\mathbb{S}(\mu_G)(v)) &= \mu_G(\mu_G(v)) \\
&= \mu_G(v) \\
&= \mu_G(\mu_{\mathbb{S}(G)}(v))
\end{aligned}
$$

This completes the proof. □

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