Classical and Quantum Structures in Computation



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A thesis submitted for the degree of

Doctor of Philosophy

Trinity 2018

This thesis is dedicated to my parents Frits and Blanca, who never stopped believing in me and to my husband Heath for making me feel loved and excited about the next chapter of our lives.

Acknowledgements

I have been incredibly lucky to work under the supervision of two outstanding academics, supervisors and mentors, Samson Abramsky and Jamie Vicary, whose work I greatly admire.

My work with Jamie has been a very enjoyable and enriching experience. He introduced me to research five years ago when he supervised my MSc. thesis. Since then, he has helped me to believe in my abilities and to have the courage to explore the unknown. When I hesitantly drew out my incoherent thoughts in our first supervision meeting, his response was: ”Great Linde! You have been doing research!”. Later on, after weeks of hard work had proven our conjectures to be false, he saw it as a sign that the universe is even more interesting than we had thought. His door has always been open and he has been by my side to solve whatever problem has come my way. He has actively sought out opportunities for me to grow and expand my network, giving me the opportunity to teach at Dalhousie University, Halifax, to spend time at the Simon's Institute in Berkeley; and he has connected to some of the superstars of category theory. One rarely comes across a mentor who is as optimistic, inventive, hard-working and upright as Jamie. I could not have wished for a more excellent supervisor.

After the kick-start of my DPhil with Jamie, Samson Abramksy has guided me further towards becoming an independent researcher. I am grateful for his patient support and encouragement. I deeply appreciate the time that he freed up for me alongside his responsibilities as the head of the MSc. program MFoCS and the many other roles he fulfills. With his extensive knowledge of theoretical computer science - which makes him seem like a walking encyclopedia - Samson has been an invaluable guide through the academic literature. Samson has given me all the freedom to go my own way with enough guidance to make my research journey a success. He has never told me what to do. Instead, he patiently reviewed my many drafts and provided me crucial insights through his sharp questions. He has taught me to order my thoughts and to leave no room for ambiguity in my

words. Any feedback from Samson is formulated with the utmost tact and kindness. Most of our discussions ended with the remark ”Well, why don’t you just write what you mean then?”, leaving me with a clear idea of how to proceed.

As my supervisor, Samson seemed to have two goals: to support his students and to have a good time with them. He values the growth and success of his students, without asking for any benefit of his own in return. I personally had a great time, in every meeting, every conversation and every group lunch. It made the 4 years of research some of the best I have had so far.

Michael Shulman has been a third supervisor to me. The little interaction that we had made a huge impact on my development. If he had not shared his intuition about the underlying principles of higher category theory, I would have easily gotten lost in the jungle of abstract definitions. His modesty, sharp mind and clear style of communication has made our collaboration both inspiring and fun.

I have been very fortunate to be part of the Quantum Group at the department of computer science. The welcoming, supportive and fun atmosphere quickly made me feel at home. To a significant extent, I believe this is due to Bob Coecke, who puts his stamp on everything he engages with.

There have been many knowledgeable people in this group who selflessly have gone out of their way to help me get ahead. In particular, I would like to thank Jonathan Barret for carefully reading through my work and highlighting the inaccuracies with his sharp questions; Chris Heunen, for patiently explaining his work on C*-algebras, Rui Soares Barbosa for his critical assessment of my my paper, for sharing his knowledge on contextuality and for exploring new ideas with me. Shane Mansfield has been a mentor to me, who has repeatedly read through my early writings, shared his research ideas and who has continued to offer his thoughts and advice from his new home base in Paris. I have enjoyed talking to Prakash Pangaden about various branches of computing, exploring areas where quantum technology could provide an advantage. I am especially grateful to Matty Hoban, who has helped me greatly to connect abstract mathematical theory to the reality of quantum technology; he has listened to many of my ideas, shared invaluable reflections on my approach and weeded out fruitful directions. He has offered encouragement when it was most needed, by

reminding me that one can only find innovative ideas by leaving the beaten track.

I would like to thank three important people who play a vital role in my life. I am very blessed with my husband Heath Hansen, who has read almost every draft of my thesis with utmost care. Finally, and most importantly, I am very grateful to my parents Frits and Blanca for their unconditional love and faith in me. I hope they know that this achievement is theirs, as much as it is mine.

Abstract

Quantum mechanics exhibits many counter-intuitive features, which challenge our classical understanding of the world. This makes the theory simultaneously difficult to grasp, and a source of great potential for new technologies.

We study various characteristics of classical and quantum mechanics and their respective roles in computation. This is interesting from a philosophical perspective, as it brings us a small step closer to understanding the nature of quantum mechanics. Furthermore, it leads us to discover scenarios where quantum resources provide a genuine advantage over classical resources, as well as more intuitive ways to model quantum protocols.

Firstly, we explore the concept of quantum contextuality, which distinguishes uniquely-quantum experimental outcomes from outcomes that can be realised classically. In pursuit of a universal theory of contextuality, we unify two abstract frameworks: the sheaf-theoretic approach to contextuality by Abramsky and Brandenburger and the equivalence-based approach by Spekkens.

We apply the sheaf-theoretic formalism to the field of communication complexity. We derive a bound on the success probability of a communication complexity protocol, based on the amount of contextuality present in its quantum resource. We provide a set of necessary conditions for distributed functions that allow a contextual advantage.

Secondly, we consider a family of bicategorical models to describe the interaction of classical and quantum information in quantum protocols. We prove that this family is symmetric monoidal, and therefore suitable for describing compound and parallel protocols. This family serves as a mathematical foundation for the planar language for quantum protocols by Vicary. Important examples of this family are the bicategories **2Hilb** and **2Vect**. Additionally, we introduce the structure $2[\mathrm{CP}^*[\mathbf{FHilb}]]$, which contains a symmetric monoidal bicategory of mixed states and completely positive maps. This allows a unified description of quantum teleportation and

classical encryption in a single 2-category, as well as a universal security proof applicable simultaneously to both scenarios.

As part of the process, we develop extensive categorical machinery for constructing symmetric monoidal structures of bicategories, pseudo functors, pseudo transformations and modifications. We consider a method of constructing symmetric monoidal bicategories from symmetric monoidal double categories. We show that this method can be generalised to a functor from the locally cubical bicategory of monoidal double categories to the locally cubical bicategory of monoidal bicategories.

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Chapter 1

Introduction

The way that physicists understand the world has for long been influenced by classical mechanics, also known as 'Newtonian' mechanics. This theory of physics describes the behaviour and attributes of particles, such as their position and momentum. Particles are assumed to have no volume and their position is represented as coordinates in three-dimensional space. Classical mechanics allows one to make predictions about the future state of a particle, or system of particles, as long as one has sufficient knowledge of its attributes. For example, if one knows the position, mass, velocity and force applied to an object, one can predict the object's position and velocity at any future point in time. The theory of classical mechanics assumes that all attributes of a physical system are definite and observable. Uncertainty in classical mechanics, described by probability theory, is always due to a lack of knowledge of the actual attributes. It can, at least in theory, be eliminated by making more accurate measurements. Furthermore, it relies on the assumption that the world is causal, meaning that the events in the present may influence the future, but not vice versa. Finally, forces act only on contiguous objects, a phenomenon known as 'locality'.

Various phenomena, such as black body radiation and the photo-electric effect could not be explained by classical mechanics. This lead to the development of quantum mechanics. The theory of quantum mechanics deviates from classical mechanics in numerous counter-intuitive ways. In most cases, quantum mechanics cannot predict the outcome of an experiment with certainty, it can only predict the probability of various possible outcomes. Furthermore, the statistical behaviour of spatially separated objects can be strongly correlated in remarkable ways. This was famously called "spooky action at a distance" by Albert Einstein, as the correlations are not possible according to the laws of classical mechanics. As a consequence, quantum mechanics was initially regarded as a mathematical tool to make predictions, rather than a description of the physical reality.

In an attempt to explain the mysterious behaviour in quantum mechanics, there was a quest for a suitable 'hidden variable theory'. Such a theory would combine observed attributes, with ones that are not observable, called 'hidden variables'. The hidden variables together with the observable ones should give a full description of the particles, as they really are. Therefore, the hidden variable theory would in principle be sufficient for making predictions with certainty.

However, in 1964 John Bell showed that any such hidden variable theory that explains our experimental observations, cannot be simultaneously local and causal, which means that quantum mechanics is fundamentally different from classical mechanics. The realisation that quantum mechanics cannot be explained in classical terms raises a new question: How can classical phenomena arise in a world that is quantum mechanical at its smallest scale?

In the late 20th century, work by Feynmann and Manin suggested that the peculiar nature of quantum mechanics could be used for computation [Fey82], [Man80]. This motivated the concept of quantum computers.

In this thesis, we study various characteristics of classical and quantum systems. This exploration leads to new insights on the source of computational power of quantum computers. Additionally, we develop a mathematical foundation for an intuitive diagrammatic language of quantum protocols and we make new contributions to the abstract mathematical field of higher category theory.

1.1 Main Results and Outline of the Thesis

This work can be divided into two main parts. In the first part, contained in Chapter 2 and 3, we explore the concept of contextuality and its advantages in communication complexity.

The main results are the following:

- We give a formal account of the equivalence-based formalism for contextuality, containing an explicit list of necessary assumptions.
- We define a categorical isomorphism expressing the relation between the sheaf-theoretic approach and the equivalence-based approach to contextuality.
- We provide a canonical method to detect contextuality for scenarios with preparations and measurements, where factorazibility is justified.
- We formulate a unified notion for one-way communication complexity protocols with classical or quantum resources as constraint satisfaction problems (CSPs).

- We obtain a bound on the success probability of a communication complexity protocol, based on the K-consistency of the CSP and the contextual fraction - a measure for the amount of contextuality of the protocol.

- We give a set of necessary conditions for distributed functions that allow a contextual advantage, based on graph colourings.

The second part of this thesis, contained in Chapter 4 and 5, focuses on modelling the interaction of classical and quantum structures in quantum protocols. We discuss the bicategorical model $2[-]$, which serves as a mathematical basis for an intuitive diagrammatic language for quantum mechanics. We prove that it belongs to a family of models, based on abstract modules and algebras, which has suitable properties for modelling quantum protocols, i.e. being symmetric monoidal. These results are based on a method, developed in this thesis, to construct symmetric monoidal bicategories and higher structures. The abstract result exceeds the presented applications in generality and is applicable to a wide range of questions in mathematics and quantum computing.

The main results are the following:

- We give a definition of braided, sylleptic and symmetric monoidal structures on object and cells of a locally cubical bicategory and prove that such objects and cells form a new locally cubical bicategory.

- We prove that every product-preserving functor of locally cubical bicategories preserves all monoidal structure.

- We show how the assignment $\mathcal{L}$ that lifts double categories to bicategories gives rise to a product-preserving functor of locally cubical bicategories. Hence, it gives rise to a method to construct braided and symmetric monoidal bicategories, pseudo functors, pseudo transformations and modifications.

- We prove that the family $\mathbb{A}lg$ of double categories of algebras, algebra homomorphisms, bimodules and bimodule homomorphisms is symmetric monoidal and contains the required lifting property to give rise to the symmetric monoidal bicategory $\mathcal{L}(\mathbb{A}lg)$ of algebras, bimodules and bimodule homomorphisms.

- As a corollary, we show that the well-known bicategories. **2Hilb** and **2Vect** of finite-dimensional Hilbert spaces and finite-dimensional vector spaces, respectively, are symmetric monoidal.

- We show that this construction gives rise to a functor from the bicategory of monoidal categories to the bicategory of monoidal double categories

- We introduce the bicategory of mixed quantum states as a model for quantum computation, which is symmetric monoidal due to our previous results. This bicategory allows a unified description of quantum teleportation and classical encryption in a single 2-category, as well as a universal security proof applicable simultaneously to both scenarios.

In Chapter 2, we take a step towards a unified notion of contextuality. We explore the approach by Abramsky and Brandenburger, based on sheaf-theory, and the approach by Spekkens, based on statistical equivalences. We discuss which additional assumptions are needed in order to recover traditional examples of contextuality from the equivalence-based approach. By doing so, we clarify the meaning of the contextuality within this framework. We show that the frameworks are equivalent for scenarios with preparations and measurements, whenever factorizability is justified. This connection gives rise to a categorical isomorphism between suitable categories. We combine the advantages of the two approaches to derive a canonical method for detecting contextuality in such settings.

In Chapter 3, we explore contextuality as a resource for communication complexity - the field that studies distributed computation with minimal communication between the different parties. We apply the sheaf-theoretic formalism to questions of communication complexity. This leads to a unified notion for one-way communication complexity protocols with classical or quantum resources and a characterisation of such protocols as constraint satisfaction problems. We derive a bound on the success probability of a communication complexity protocol, based on the K-consistency of the CSP and the contextual fraction - a measure for the amount of contextuality present in the protocol. This bound separates classically simulatable protocols from those where contextuality offers a complexity advantage. Furthermore, we provide a set of necessary conditions for distributed functions that allow a contextual advantage based on graph colourings.

In Chapter 4, we discuss a method to construct symmetric monoidal bicategories. As this is a tedious and laborious exercise in general, we make use of a method to construct such categories from double categories, which are their simpler counterpart. We demonstrate that a similar construction can be used to create symmetric monoidal pseudo functors, pseudo transformations and modifications, and that this construction forms a functor between locally cubical bicategories. These structures represent models for computation and transformations between them. Such transformations are used to show that two models for computation are equivalent, or that one is contained in another. This technical chapter contains background needed for Chapter 5.

In Chapter 5 we build on the main result of Chapter 4 to describe a family of models for quantum computation and transformations between them. This approach captures the interaction of classical and quantum data types and can be used to describe entire protocols, including probabilistic branching due to intermediate measurements. It contains the well-known categories **2Hilb** and **2Vect**, and gives rise to a new model for protocols of mixed states 2[CP*[**FHilb**]]. We prove that the family of models is well-defined and has a symmetric monoidal structure.

1.2 Prerequisites

We use various tools from category theory to describe the specific characteristics of classical and quantum mechanics. Our focus is on the sheaf-theoretic formalism for contextuality and higher categorical models for quantum protocols. We require familiarity with the Hilbert space formalism; a brief overview is provided below. Further details can be found in [NC00, Chapter 2].

1.2.1 The Hilbert Space Formalism of Finite-Dimensional Quantum Mechanics

The Hilbert space formalism is based on linear algebra, which can be described using the Dirac notation for vectors and matrices, specified in the following table.

Notation	Description
z^*	Complex conjugate of the complex number z.
A^*	Complex conjugate of the matrix A.
A^T	Transpose of the matrix A.
$A^\dagger$	Adjoint of the matrix A, $A^\dagger := (A^T)^*$.
$\|\psi\rangle$	Column vector, which is an $n \times 1$ matrix.
$\langle\psi\|$	Row vector, which is the $1 \times n$ matrix corresponding to the adjoint $\|\psi\rangle^\dagger$ of $\|\psi\rangle$.
$\langle\phi\|\psi\rangle$	Matrix product of $\langle\phi\|$ and $\|\psi\rangle$, which defines an inner product of $\|\phi\rangle$ and $\|\psi\rangle$.
$\langle\phi\|A\|\psi\rangle$	Matrix product of $\langle\phi\|$, A and $\|\psi\rangle$, which corresponds to the inner product of $\|\phi\rangle$ and $A\|\psi\rangle$.
$\|\phi\rangle\langle\psi\|$	The matrix arising from the matrix product of $\|\phi\rangle$ and $\langle\psi\|$.
$\|\phi\rangle \otimes \|\psi\rangle$	Tensor product of $\|\phi\rangle$ and $\|\psi\rangle$.
$\|\phi\rangle\|\psi\rangle$	Abbreviated notation for tensor product of $\|\phi\rangle$ and $\|\psi\rangle$.
$\|\phi\psi\rangle$	Abbreviated notation for tensor product of $\|\phi\rangle$ and $\|\psi\rangle$.

Any physical system in quantum mechanics is associated with a Hilbert space, known as the **state space** of the system. The system is completely described by its **state vector**, which is a unit vector $|\psi\rangle$ in the state space. Consequently, any convex

combination $a\,|\phi\rangle + b\,|\psi\rangle$ of two quantum states $|\phi\rangle, |\psi\rangle$ is also a state in quantum theory. Such a state is said to be in a **superposition** of ϕ and ψ. The **evolution** of a system is described by a unitary transformation. For a system that is in state $|\psi\rangle$ at time t_1 and in state $|\psi'\rangle$ at time t_2, the transition from $|\psi\rangle$ to $|\psi'\rangle$ is described by a unitary operator U, satisfying the equation below.

$$|\psi'\rangle = U\,|\psi\rangle$$

A **measurement**, also referred to as a **Positive Operator-Valued Measure (POVM)**, is described by a collection of positive semi-definite operators $\{M_m\}$, indexed by the possible outcomes of the measurement. An operator with corresponding matrix M is **positive semi-definite** when the scalar corresponding to the matrix product $\langle\phi|\,M\,|\phi\rangle$ is bigger than or equal to zero, for every non-zero complex vector $|\phi\rangle$. The operators must satisfy the completeness equation below.

$$\sum_m M_m^\dagger M_m = I$$

Each such set of operators represents an **observable**. This is a variable that can be measured. Each possible outcome value to the observable corresponds to the index of one of the operators. Examples of observables are the position or momentum of a particle. The probability of obtaining outcome m when measuring the state $|\psi\rangle$ with the POVM $\{M_m\}$ is given by the **Born rule**, which states that it equals the scalar below.

$$\langle\psi|M_m^\dagger M_m|\psi\rangle$$

The state of the system after the measurement with outcome m is given below.

$$\frac{M_n\,|\psi\rangle}{\sqrt{\langle\psi|M_m^\dagger M_m|\psi\rangle}}$$

As a special case, we distinguish **projection-valued measurements** (PVMs). These consist of a Hermitian operator M, which has a spectral decomposition

$$M = \sum_m mP_m$$

Here, P_m is the projector onto the eigenspace with eigenvalue m. The probability of obtaining the result m when measuring a state $|\psi\rangle$ with the PVM $M = \sum_m mP_m$ is given below.

$$\langle\psi|P_m|\psi\rangle$$

If the outcome m occurs, the state after measurement is given by the expression below.

$$\frac{P_m |\psi\rangle}{\sqrt{p(m)}}$$

The state space of a composite physical system of states $|\psi_1\rangle, ..., |\psi_n\rangle$ is the tensor product of the state spaces of its respective components

$$H_1 \otimes H_2 \otimes ... \otimes H_n$$

This is also called a **joint state**. We call an n-partite state **entangled** if it cannot be written as a tensor product of n different parts. An example of such a state is the **Bell state**

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

We can measure single components of a joint state. Such a measurement is called a **partial measurement** and corresponds to a set of operators of the form $\{I \otimes M_n\}$ or $\{M_n \otimes I\}$, where I is the identity operator on part of the system.

The Density Matrix Formalism

In reality, it is difficult to completely isolate a quantum system from its environment. Therefore, it is often necessary to take the environment of the system into account. This can be done using *density matrices* to represent states. A **density matrix** is a self-adjoint positive operator ρ on a Hilbert space, such that $\mathrm{Tr}(\rho) = 1$. Evolution of a quantum system is given by a unitary transformation U, which maps the density matrix ρ to $U\rho U^\dagger$. The probability of obtaining outcome m for a measurement $\{M_n\}$ of a density matrix ρ is given below.

$$\mathbb{P}(m) = tr(M_m^\dagger M_m \rho)$$

The resulting state after the measurement is the following.

$$\frac{M_m |\psi_i\rangle}{\sqrt{\langle\psi_i| M_m^\dagger M_m |\psi_i\rangle}}$$

A quantum system A that is part of a bigger system described by the density matrix ρ^{AB} is expressed by the **reduced density matrix**

$$\rho^A = \mathrm{Tr}_B(\rho^{AB}),$$

Here, Tr_B is a map of density operators, called the partial trace. This is defined on states of the form $(|a\rangle\langle a|) \otimes (|b\rangle\langle b|)$ as

$$\mathrm{Tr}_B\Big((|a\rangle\langle a|) \otimes (|b\rangle\langle b|)\Big) := |a\rangle\langle a|\langle b|b\rangle$$

On general density matrices it is the linear expansion

$$\mathrm{Tr}_B\Big(\sum_i p_i |a\rangle\langle a| \otimes |\psi_i\rangle\langle\psi_i|\Big) = \sum_i p_i |a\rangle\langle a|\langle\psi_i|\psi_i\rangle$$

The reduced density matrix captures the measurement statistics of measuring the subsystem, without examining the total system.

A density matrix that can be written as $|\psi\rangle\langle\psi|$ for a single vector $|\psi\rangle$ is called a **pure state**. A density matrix that can only be written as a convex combination of pure states $\sum_i p_i |\psi_i\rangle\langle\psi_i|$ is called a **mixed state**. A state is **maximally mixed** when $\sum_i p_i$ is a uniform distribution and $\{\psi_i\}_i$ is a set of orthonormal states. A mixed state $\sum_i p_i |\psi_i\rangle\langle\psi_i|$ represents a system that is in one of several states $|\psi_i\rangle$, each with probability p_i, respectively. It can arise as a statistical mixture of pure states, or as a subsystem of a bigger quantum system.

Data Types

A **quantum data type** is an n-dimensional Hilbert space. This can be realised by an n-dimensional quantum system. A special case of a quantum data type is a **qubit**, which is a 2-dimensional Hilbert space. A common physical realisation of a qubit is the **spin** of a particle. We write $\{|0\rangle, |1\rangle\}$ as the standard basis for a qubit, where $|0\rangle$ and $|1\rangle$ correspond to the vectors

$$|0\rangle := \begin{pmatrix}1\\0\end{pmatrix} \qquad |1\rangle := \begin{pmatrix}0\\1\end{pmatrix}$$

This basis is called the **computational basis** or Z basis. Other common bases are the X basis $\{|+\rangle, |-\rangle\}$ and the Y basis $\{|+i\rangle, |-i\rangle\}$, defined below.

$$|+\rangle := (|0\rangle + |1\rangle)/\sqrt{2} = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix} \qquad |-\rangle := (|0\rangle - |1\rangle)/\sqrt{2} = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{-1}{\sqrt{2}}\end{pmatrix}$$

$$|+i\rangle := (|0\rangle + i|1\rangle)/\sqrt{2} = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{i}{\sqrt{2}}\end{pmatrix} \qquad |-i\rangle := (|0\rangle - i|1\rangle)/\sqrt{2} = \begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{-i}{\sqrt{2}}\end{pmatrix}$$

Measurements in these respective bases are given by the matrices below.

It is easy to verify that the relations below hold; hence, the different operators do not commute.

Basis	Matrix	Dirac notation	Eigenvectors	Eigenvalues
X	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\|+\rangle\langle+\| - \|-\rangle\langle-\|$	$\begin{matrix}\|+\rangle \\ \|-\rangle\end{matrix}$	$\begin{matrix}1 \\ -1\end{matrix}$
Y	$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$	$\|-i\rangle\langle-i\| + \|i\rangle\langle i\|$	$\begin{matrix}\|-i\rangle \\ \|i\rangle\end{matrix}$	$\begin{matrix}1 \\ -1\end{matrix}$
Z	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$	$\|0\rangle\langle 0\| - \|1\rangle\langle 1\|$	$\begin{matrix}\|0\rangle \\ \|1\rangle\end{matrix}$	$\begin{matrix}1 \\ -1\end{matrix}$

$$XY = iZ \qquad YX = -iZ$$
$$YZ = iX \qquad ZY = -iX$$
$$XZ = iY \qquad ZX = -iY$$

Let α, β be complex numbers, such that $|\alpha|^2 + |\beta|^2 = 1$ and let $\{|b_1\rangle, |b_2\rangle\}$ be a basis for a 2-dimensional Hilbert space. When a qubit is in the state below, we say that it is in the state $|b_1\rangle$ with amplitude α and in state $|b_2\rangle$ with amplitude β.

$$\alpha\,|b_1\rangle + \beta\,|b_2\rangle = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}^T$$

One can check that if we measure in the basis $\{|b_1\rangle, |b_2\rangle\}$, we obtain the state $|b_1\rangle$ with probability $|\alpha|^2$, or the state $|b_2\rangle$ with probability $|\beta|^2$.

A Hilbert space with a basis is isomorphic to $\oplus_{i=1}^{n}\mathbb{C}$, where n is the dimension of the Hilbert space. The decomposition represents a system with n different values, each corresponding to one of the basis elements. We call this a **classical data type**. When n equals two, this is a bit, when n is bigger than two, it is called a **dit**.

1.2.2 Category Theory

We will assume that the reader is familiar with basic concepts of category theory, such as categories, functors, natural transformations, products and equalizers. An overview is provided in [AT10]. Furthermore, we assume familiarity with monoidal categories and bicategories. We provide a brief review below. Further details on these structures and how they are used to describe quantum theory can be found in [HV18].

Bicategories

A **bicategory** consists of the following data:

- A collection of 0-cells or objects **B**

- A category $\mathbf{B}(A, B)$ for each two 0-cells A,B. The objects of this category are called 1-cells and the morphisms are called 2-cells. We call composition in these categories 'tight' composition, depicted with "$\cdot$".
- For each three 0-cells A, B, C, a bifunctor $\otimes : \mathbf{B}(B, C) \times \mathbf{B}(A, B) \to \mathbf{B}(A, C)$. This functor defines 'loose' composition of 1-cells and 2-cells.
- For each 0-cell A, a functor $I_A : 1 \to \mathbf{B}(A, A)$, where 1 is the trivial category. This corresponds to a 1-cell $A \xrightarrow{I_A} A$ called the **unit**.
- For each four 0-cells A, B, C, D, a natural isomorphism, called the **associator**, depicted below.

$$\begin{array}{ccc} \mathbf{B}(C,D) \times \mathbf{B}(B,C) \times \mathbf{B}(A,B) & \xrightarrow{\mathrm{id} \times \otimes} & \mathbf{B}(C,D) \times \mathbf{B}(A,C) \\ \otimes \times \mathrm{id} \downarrow & \Downarrow \alpha & \downarrow \otimes \\ \mathbf{B}(B,D) \times \mathbf{B}(A,B) & \xrightarrow[\otimes]{} & \mathbf{B}(A,D) \end{array}$$

- For each two 0-cells A, B, a natural isomorphisms called the left and right unitor, respectively.

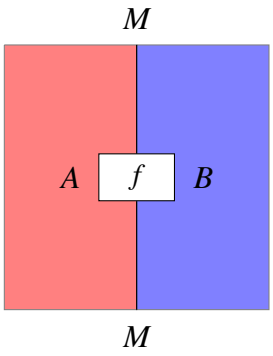
$$\begin{array}{ccc} 1 \times \mathbf{B}(A,B) & & \\ I_B \times \mathrm{id} \downarrow & \cong & \\ & \Downarrow \lambda & \\ \mathbf{B}(B,B) \times \mathbf{B}(A,B) & \xrightarrow[\otimes]{} & \mathbf{B}(A,B) \end{array} \qquad \begin{array}{ccc} \mathbf{B}(A,B) \times 1 & & \\ \mathrm{id} \times I_A \downarrow & \cong & \\ & \Downarrow \rho & \\ \mathbf{B}(A,B) \times \mathbf{B}(A,A) & \xrightarrow[\otimes]{} & \mathbf{B}(A,B) \end{array}$$

This data needs to satisfy the following axioms for all 0-cells A, B and all 1-cells $f, g, h, k \in \mathbf{B}(A, B)$:

$$\begin{array}{ccccc} ((f \otimes g) \otimes h) \otimes k & \xrightarrow{\alpha_{f,g,h} \otimes \mathrm{id}_k} & (f \otimes (g \otimes h)) \otimes k & \xrightarrow{\alpha_{f,g\otimes h,k}} & f \otimes ((g \otimes h) \otimes k) \\ \alpha_{f\otimes g,h,k} \downarrow & & & & \downarrow \mathrm{id}_f \otimes \alpha_{g,h,k} \\ f \otimes (g \otimes (h \otimes k)) & & \xrightarrow{\alpha_{f,g,h\otimes k}} & & (f \otimes g) \otimes (h \otimes k) \end{array} \tag{1.2.1}$$

$$\begin{array}{ccc} (f \otimes I) \otimes g & \xrightarrow{\alpha_{f,I,g}} & f \otimes (I \otimes g) \\ & {\scriptstyle \rho_f \otimes \mathrm{id}_g} \searrow \quad \swarrow {\scriptstyle \mathrm{id}_f \otimes \lambda_g} & \\ & f \otimes g & \end{array} \tag{1.2.2}$$

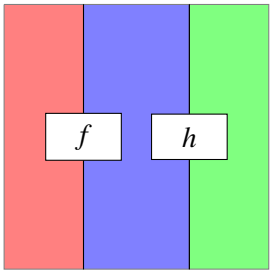
Bicategories can be expressed diagrammatically [BMS13]. In this diagrammatic language, we depict 0-cells as regions, 1-cells (and identity 2-cells) as lines, and 2-cells as boxes between the source 1-cells in the bottom and the target 1-cell on top.



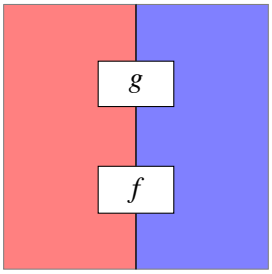
(1.2.3)

Elements of the diagrammatic language can be composed vertically and horizontally. We write tight composition in the vertical direction and loose composition as juxtaposition in the horizontal direction.

Horizontal composition



Vertical composition



This language is sound and complete for bicategories [BMS13, Theorem 1.3], meaning that every statement that can be proven diagrammatically is true for its categorical counterpart and vice versa.

Transformations between bicategories $\mathbf{B}, \mathbf{C}$ are given by *pseudo functors*, which consists of the elements below.

- An assignment on objects $F : A \mapsto FA$

- For each two objects A, B of $\mathbf{B}$, a functor between hom-sets $F_{A,B} : \mathbf{B}(A,B) \to \mathbf{C}(FA, FB)$.

- For each object A and each pair of objects (A, B) of $\mathbf{B}$, natural isomorphisms

$$\begin{array}{ccc} 1 & \xrightarrow{I_A} & \mathbf{B}(A,A) \\ & \Downarrow \phi & \downarrow F_{A,C} \\ 1 & \xrightarrow[I_{FA}]{} & \mathbf{C}(FA,FA) \end{array} \qquad \begin{array}{ccc} \mathbf{B}(B,C) \times \mathbf{B}(A,B) & \xrightarrow{\otimes} & \mathbf{B}(A,C) \\ {\scriptstyle F_{BC} \times F_{AB}} \downarrow & \Downarrow \phi & \downarrow {\scriptstyle F_{A,C}} \\ \mathbf{C}(FB,FC) \times \mathbf{C}(FA,FB) & \xrightarrow[\otimes]{} & \mathbf{C}(FA,FC) \end{array} \tag{1.2.4}$$

  such that the diagrams below commute.

$$\begin{array}{ccccc} (Fh \otimes Fg) \otimes Ff & \xrightarrow{\phi \otimes \mathrm{id}} & F(h \otimes g) \otimes Ff & \xrightarrow{\phi} & (F((h \otimes g) \otimes f) \\ {\scriptstyle \alpha_{Fh,Fg,Ff}} \downarrow & & & & \downarrow {\scriptstyle F\alpha_{h,g,f}} \\ Fh \otimes (Fg \otimes Ff) & \xrightarrow{\mathrm{id} \otimes \phi} & Fh \otimes F(g \otimes f) & \xrightarrow{\phi} & F(h \otimes (g \otimes f)) \end{array} \tag{1.2.5}$$

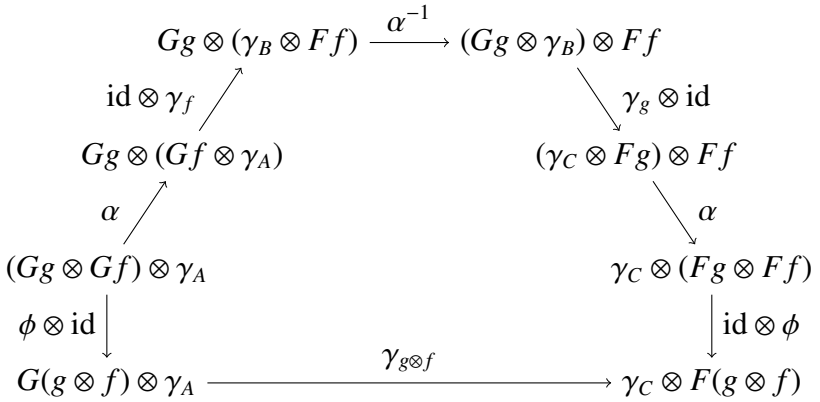
$$\begin{array}{ccc} Ff \otimes I_{FA} & \xrightarrow{\mathrm{id} \otimes \phi} & Ff \otimes FI_A \\ {\scriptstyle \phi} \downarrow & & \downarrow {\scriptstyle \rho} \\ F(f \otimes I_A) & \xrightarrow[F\rho]{} & Ff \end{array} \qquad \begin{array}{ccc} I_{FA} \otimes Ff & \xrightarrow{\phi \otimes \mathrm{id}} & FI_A \otimes Ff \\ {\scriptstyle \phi} \downarrow & & \downarrow {\scriptstyle \lambda} \\ F(I_A \otimes f) & \xrightarrow[F\lambda]{} & \end{array} \tag{1.2.6}$$

If the natural transformations are not isomorphisms, it is called a **lax functor**. If, in addition, they go in the opposite direction, it is called a **colax functor**.

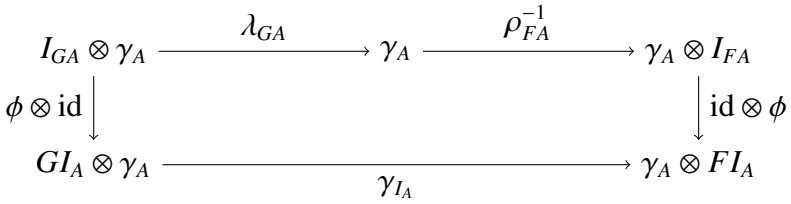
Transformations between pseudo functors $F, G : \mathbf{B} \to \mathbf{C}$ are given by *pseudo natural transformations*, defined below. For this definition, we write $- \otimes f$ and $f \otimes -$ for the functors induced by right- and left composition of f. An **pseudo natural transformation** $\gamma : F \Rightarrow G$ consists of the following data

- For each object A of $\mathbf{B}$, a 1-cell $\gamma_A : FA \to GA$ in $\mathbf{C}$

- For each two objects A, B, a natural isomorphism $\gamma_{A,B} : (- \otimes \gamma_B) \circ F_{A,B} \to (\gamma_A \otimes -) \circ G_{A,B}$, such that the diagrams below commute.



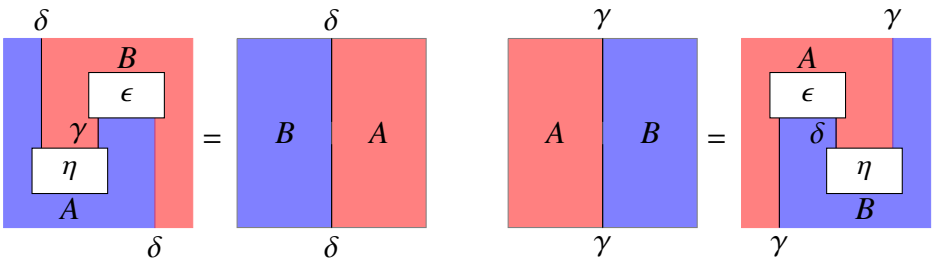
(1.2.7)



(1.2.8)

If the maps $\gamma_{A,B}$ are not isomorphisms, but merely natural transformations, it is an **colax natural transformation**. If, in addition, $\gamma_{A,B}$ goes in the opposite direction for all 1-cells $f : A \to B$, it is a **lax natural transformation**.

As argued in [Gur06], a more appropriate notion of a transformation between pseudo functors is a *pseudo natural adjoint equivalence*. Such a transformation specifies the choice of an inverse equivalence. Its definition makes use of the notion of **adjunction** $\gamma \dashv \delta$ of 1-cells $\gamma : A \to B, \delta : b \to A$. This consists of a pair of 2-cells η, ϵ, such that the equations below hold.

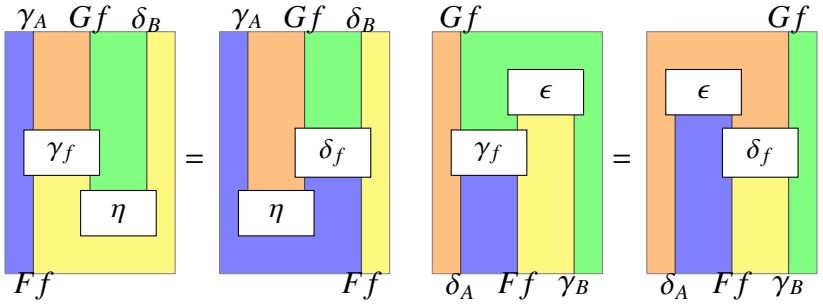


(1.2.9)

A **conjunctional transformation**, $\gamma \prec \delta$ consists of the following data.

- A pair (γ, δ) of colax and lax transformations, respectively.

- For each object A of $\mathbf{B}$, an adjunction $\gamma_A \dashv \delta_A$ in $\mathbf{C}$ such that the diagrams below commute, where we write $\gamma_f : \gamma_B \otimes Ff \to Gf \otimes \gamma_A$ for the 2-cell components of $\gamma_{A,B}$.



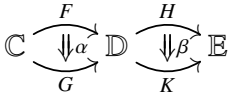
(1.2.10)

If γ and δ are isomorphisms and the adjunctions $\gamma_A \dashv \delta_A$ are adjoint equivalences, it is a **pseudo natural adjoint equivalence**.

When pseudo functors $F, G : \mathbf{B} \to \mathbf{C}$ agree on objects, there is a simpler notion of a transformation, called an *icon*. An **icon** $\alpha : F \Rightarrow G$ is given by a family of 2-cells $\alpha_f : Ff \to Gf$ indexed by the 1-cells of $\mathcal{D}$, which are natural in f and such that for all objects A, B, C and 1-cells $A \xrightarrow{f} B \xrightarrow{g} C$ the following diagrams commute:

$$\begin{array}{ccc} I_{FA} & \xrightarrow{\phi} & FI_A \\ \| & & \downarrow{\scriptstyle \alpha_{I_A}} \\ I_{GA} & \xrightarrow[\phi]{} & GI_A \end{array} \qquad \begin{array}{ccc} F(g)\otimes F(f) & \xrightarrow{\phi} & F(g\otimes f) \\ {\scriptstyle \alpha_g \otimes \alpha_f}\downarrow & & \downarrow{\scriptstyle \alpha_{g\otimes f}} \\ G(g)\otimes G(f) & \xrightarrow[\phi]{} & G(g\otimes f) \end{array} \tag{1.2.11}$$

One can compose the two pseudo natural transformations or icons below. Their composition is given by the **Godement product** $\beta * \alpha$.



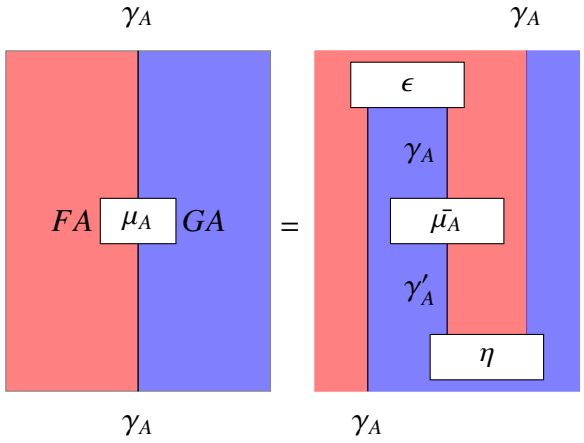
This product has the following components:

$$(\beta * \alpha)_f = \beta_{G(f)} \otimes H(\alpha_f)$$

Let $\gamma, \gamma' : F \Rightarrow G$ be pseudo natural transformations. A **modification** $\mu : \gamma \Rrightarrow \gamma'$ consists of 2-cells $\mu_A : \gamma_A \to \gamma'_A$ for each object A of $\mathbf{B}$, such that the diagram below commutes.

$$\begin{array}{ccc} \gamma_B \otimes F(f) & \xrightarrow{\gamma_f} & G(f) \otimes \gamma_A \\ \Big\downarrow{\scriptstyle \mu_B \otimes \mathrm{id}_{F(f)}} & & \Big\downarrow{\scriptstyle \mathrm{id}_{G(f)} \otimes \mu_A} \\ \gamma'_B \otimes F(f) & \xrightarrow[\gamma'_f]{} & G(f) \otimes \gamma'_A \end{array} \tag{1.2.12}$$

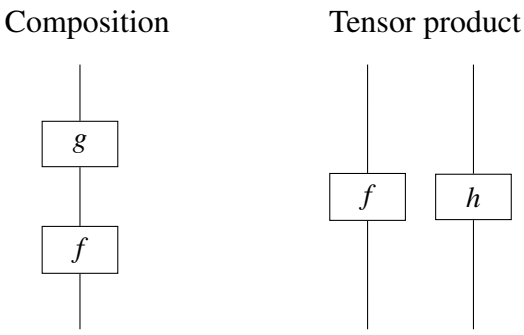
If $\gamma \prec \delta$ and $\gamma' \prec \delta'$ are conjunctional transformations and $\mu : \gamma \Rrightarrow \gamma'$, $\bar{\mu} : \delta \Rrightarrow \delta'$ are modifications, then μ and $\bar{\mu}$ correspond to each other as **mates** with respect to the adjoint equivalences $\gamma_A \dashv \gamma'_A$, $\delta_A \dashv \delta'_A$, if the equation $\mu_A = (\mathrm{id}_{\gamma_A} \otimes \epsilon) \circ (\mathrm{id}_{\gamma_A} \otimes \bar{\mu_A} \otimes \mathrm{id}_{\gamma_A}) \circ (\eta \otimes \mathrm{id}_{\gamma_A})$ depicted below holds.



(1.2.13)

Monoidal Categories

A **monoidal category** is a bicategory with one object. This is a category $\mathbf{C} := \mathbf{B}(*, *)$ equipped with a bifunctor $\otimes : \mathbf{C} \times \mathbf{C} \to \mathbf{C}$, an object I and isomorphisms α, λ, ρ that satisfy axioms 1.2.1 and 1.2.2. An explicit definition can be found in [HV18]. Its corresponding diagrammatic language has trivial regions.



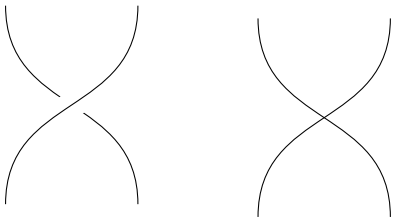
A monoidal category $\mathbf{C}$ is **braided** if it is equipped with a natural isomorphism $\sigma : \otimes \to \otimes$ with components $\sigma_{A,B} : A \otimes B \mapsto B \otimes A$. This natural isomorphism must satisfy the hexagon equations below.

$$\begin{array}{ccccc} (A \otimes B) \otimes C & \xrightarrow{\alpha_{A,B,C}} & A \otimes (B \otimes C) & \xrightarrow{\sigma_{A,B\otimes C}} & (B \otimes C) \otimes A \\ \Big\downarrow{\scriptstyle \sigma_{A,B} \otimes \mathrm{id}_C} & & & & \Big\downarrow{\scriptstyle \alpha_{B\otimes C,A}} \\ (B \otimes A) \otimes C & \xrightarrow{\alpha_{B,A,C}} & B \otimes (A \otimes C) & \xrightarrow{\mathrm{id}_B \otimes \sigma_{A,C}} & B \otimes (C \otimes A) \end{array} \tag{1.2.14}$$

$$\begin{array}{ccccc} A \otimes (B \otimes C) & \xrightarrow{\alpha^{-1}_{A,B,C}} & (A \otimes B) \otimes C & \xrightarrow{\sigma_{A\otimes B,C}} & C \otimes (A \otimes B) \\ \Big\downarrow{\scriptstyle \mathrm{id}_A \otimes \sigma_{B,C}} & & & & \Big\downarrow{\scriptstyle \alpha^{-1}_{C,A,B}} \\ A \otimes (C \otimes B) & \xrightarrow{\alpha^{-1}_{A,C,B}} & (A \otimes C) \otimes B & \xrightarrow{\sigma_{A,C} \otimes \mathrm{id}_B} & (C \otimes A) \otimes B \end{array} \tag{1.2.15}$$

A braided monoidal category is called **symmetric** when $\sigma^{-1} = \sigma$. The braiding is depicted in the diagrammatic language as a crossing of the wires. The symmetry morphism is a symmetrically drawn braiding, as depicted below.

Braiding Symmetry



(1.2.16)

Similarly, one can define a braiding on bicategories. The details can be found in [McC00].

Let $\mathbf{C}$ be a category. A **dagger** $\dagger : \mathbf{C} \to \mathbf{C}$, is a contravariant functor which is the identity on objects such that $\dagger(\dagger(f)) = f$. A **dagger monoidal category** is a monoidal category that is equipped with a dagger $\dagger$, such that the equalities below hold.

$$\begin{aligned} (f \otimes g)^\dagger &= g^\dagger \otimes f^\dagger \\ \alpha^\dagger &= \alpha^{-1} \\ \rho^\dagger &= \rho^{-1} \\ \lambda^\dagger &= \lambda^{-1} \end{aligned}$$

A **dagger braided monoidal category** is a dagger monoidal category with a braiding, such that the equation below holds

$$\sigma^\dagger = \sigma^{-1}$$

1.3 Scientific Background

1.3.1 Quantum Contextuality

In order to understand what causes an advantage of quantum computers, one needs to understand what distinguishes quantum mechanics from classical mechanics. This is not an easy question with a clear-cut answer. One can approach this question operationally, by distinguishing experimental scenarios that are unique to quantum mechanics from those that could arise from classical mechanics based on their outcome statistics. This leads to the notion of contextuality. We give a short introduction to quantum contextuality and its philosophical implications below.

Interpreting the Hilbert Space Formalism for Quantum Mechanics

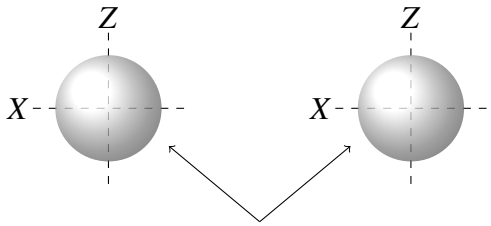
First of all, we should understand what exactly the Hilbert Space Formalism tells us about the nature of the physical world. There are various ways one can regard a theory of physics. One is as a mathematical tool to make predictions. From this point of view, the theory does not need to describe what a physical system is like, it only needs to provide accurate predictions about its observable behaviour. On the contrary, one can require a physical theory to provide a description of the universe as it really is. The accuracy of predictions is a result of the accuracy of the theory as a representation of reality. A theory that satisfies this requirement is called an **ontological theory**. This interpretation of physical theories is called **realism**. Alternatively, one can view a theory of physics as a representation of our knowledge about the physical world. This knowledge may not be accurate or complete. Such a theory is called an **epistemic theory**.

In the theory of quantum mechanics, it is impossible to predict the outcome of a measurement for most - but not all - physical states, with certainty. In the theory, values of a system are not pre-existent, but arise as a result of measurements. Potentially, with the exceptions of those specific properties that *can* be predicted with certainty for a given state. It is therefore difficult to maintain a realist interpretation of quantum mechanics. There are well-known properties of particles that cannot be determined simultaneously. For instance, the position and momentum of a particle, or, as we will discuss below, the spin of a particle with respect to different bases. This indeterminism in quantum mechanics goes against the classic idea that nature exists independently from any observer, and that measurements merely reveal its true values to us. As a consequence, quantum mechanics was suspected to be an epistemic theory. Einstein, Podolsky and Rosen reasoned that if quantum mechanics is a local, ontological physical

theory, it cannot be a complete theory of reality [AE35]. Their argument was made based on the thought experiment described below.

The EPR Thought Experiment

Consider the entangled state $(|01\rangle - |10\rangle)/\sqrt{2}$, shared by two spatially separated parties, Alice and Bob. Let Alice and Bob be given the choice to measure their part of the entangled state in either the X basis, or in the Z basis. The corresponding operators do not commute, which means that if one measures in both bases sequentially, the outcomes differ depending on their order. Suppose that Bob measures in the Z basis. After Bob's measurement, Alice's qubit is either in the state $|1\rangle$ or $|0\rangle$, if Bob's outcome was 1, or -1, respectively. The outcome of a Z measurement can be predicted with certainty if we know that the measured quantum state is in either of these states. Therefore, if we know Bob's outcome, we know the outcome of Alice, if measured in the Z basis, with certainty. However, if Alice measures in the X-basis, she may get any of the two outcomes with equal probability. Now consider what happens if Bob measures his qubit in the X-basis instead. When we write the entangled state $|01\rangle - |10\rangle / \sqrt{2}$ in the basis $\{|+\rangle, |-\rangle\}$, it corresponds to $|+-\rangle - |-+\rangle$. After Bob's measurement, Alice's qubit is either in the state $|-\rangle$, which is the case when Bob's outcome was 1, or in the state $|+\rangle$, which is the case if Bob's outcome was -1. These states determine the outcome of the X measurement for Alice with certainty.



Einstein, Podolsky and Rosen concluded that the quantum mechanical description of Alice's qubit changes in different ways after Bob's measurement. Depending on his choice, either the X-spin or the Z-spin has a definite value. If we assume that quantum mechanics is an ontological theory, this means that these values are predetermined. If, in addition, we assume that quantum mechanics is a local theory - a physical process can only have an instantaneous effect to adjacent physical objects - the predetermined values for the X and Z spin must exist already before Bob's measurement. However, the description of the joint state before the measurement does not contain these predetermined values. One must therefore conclude that if the world is local, quantum

mechanics is not a complete theory of reality. This raises the question whether there exists a more complete local ontological theory of physics that explains the measurement outcomes we obtain in experiments.

Hidden Variable Theories

One can formalize an ontological theory as follows: There is a probability space Λ with measure ρ, representing the real, possibly hidden, values of a physical system. Each measurement has an associated set of values M describing the different possible measurement settings. Each hidden variable $\lambda \in \Lambda$ and each measurement setting $m \in M$ may represent a set of any number of values. The outcome of the measurement A is a function $A : \Lambda \times M \to O$ of the measurement settings and the real values. The probability of obtaining outcome x for measurement setting m is given by the integral below.

$$\int_{\substack{\lambda\in\Lambda:\\ M(\lambda,m)=x}} \rho(\lambda)d\lambda$$

Note that in order to define this integral, one needs to specify a measure space Λ of hidden variables and a measure ρ on Λ. The hidden variable theory should recover the outcome probabilities predicted by quantum mechanics. Let $\{M_x\}$ be the measurement operators defining the measurement with measurement setting m, the following equality must hold.

$$\langle\psi|P_x|\psi\rangle = \int_{\substack{\lambda\in\Lambda:\\ M(\lambda,m)=x}} \rho(\lambda)d\lambda \tag{1.3.1}$$

Let's apply this to the measurement setting above. We write A for the measurement conducted by Alice and B for the measurement conducted by Bob. Furthermore, we write a and b for the X-measurement for Alice and Bob, respectively; and we write a' and b' for the Z-measurement for Alice and Bob, respectively. We know that $A(a,\lambda), A(a',\lambda), B(b,\lambda), B(b',\lambda) \in \{-1, 1\}$. The outcome probabilities and expectation values for the joint measurement (a, b) are given by the probability below.

$$P(a = x, b = y) = \int_{\substack{\lambda\in\Lambda:\\ (A(a,\lambda),B(b,\lambda)=(x,y)}} \rho(\lambda)d\lambda$$

$$\mathbb{E}(a, b) = \int_{\lambda\in\Lambda} \rho(\lambda)A(a,\lambda)B(b,\lambda)d\lambda$$

A **non-local hidden variable theory** would have an additional dependence on the other measurement setting.

$$P(a = x, b = y) = \int\limits_{\substack{\lambda\in\Lambda:\\ (A(a,b,\lambda),B(a,b,\lambda)=(x,y)}} \rho(\lambda)d\lambda$$

$$\mathbb{E}(a,b) = \int\limits_{\lambda\in\Lambda} \rho(\lambda)A(a,b,\lambda)B(a,b,\lambda)d\lambda$$

A weakness in this setup is that it assumes that the measurement outcomes deterministically depend on the hidden variables. It might be true that the universe is inherently indeterministic, in which case we would need a **stochastic hidden variable theory**. In such a theory, the measurement A is a function $A : \Lambda \times M \to D_{\mathbb{R}_+}(O)$ to the set of probability distributions over the outcomes. We call a stochastic hidden variable theory **factorizable** if, for joint measurements AB, the equation below holds.

$$AB(\lambda, a', b') = A(\lambda, a')B(\lambda, b')$$

Factorizability entails that the random variables A and B are independent.

Non-Locality of Quantum Mechanics

It was shown by Bell in [Bel64] that there is a specific scenario in which no deterministic local hidden variable theory can satisfy equation 1.3.1. This was later generalised by Clauser, Horne, Shimony, and Holt, to the **CHSH inequality**, which restricts the expectation values $\mathbb{E}$ of the joint measurements by the equation below [CHSH69].

$$C := \Big|\mathbb{E}(a,b) + \mathbb{E}(a,b') + \mathbb{E}(a',b) - \mathbb{E}(a',b')\Big| \leq 2$$

We derive this equality by the simple equations below. Note that for a non-local hidden variable theory, the 4th equality does not hold.

$$\begin{aligned}
C &:= \Big|\mathbb{E}(a,b) + \mathbb{E}(a,b') + \mathbb{E}(a',b) - \mathbb{E}(a',b')\Big| \\
&= \Big|\int\limits_{\lambda\in\Lambda} A(a,\lambda)B(b,\lambda)\rho(\lambda)d\lambda + \int\limits_{\lambda\in\Lambda} A(a,\lambda)B(b',\lambda)\rho(\lambda)d\lambda + \int\limits_{\lambda\in\Lambda} A(a',\lambda)B(b,\lambda)\rho(\lambda)d\lambda \\
&\quad - \int\limits_{\lambda\in\Lambda} A(a',\lambda)B(b',\lambda)\rho(\lambda)d\lambda\Big| \\
&= \Big|\int\limits_{\lambda\in\Lambda} A(a,\lambda)B(b,\lambda) + A(a,\lambda)B(b',\lambda) + A(a',\lambda)B(b,\lambda) - A(a',\lambda)B(b',\lambda)\rho(\lambda)d\lambda\Big| \\
&= \Big|\int\limits_{\lambda\in\Lambda} A(a,\lambda)\Big[B(b,\lambda) + B(b',\lambda)\Big] + A(a',\lambda)\Big[B(b,\lambda) - B(b',\lambda)\Big]\rho(\lambda)d\lambda\Big| \\
&\leq 2
\end{aligned}$$

For the last inequality, observe that each of the terms $A(a,\lambda), A(a',\lambda), B(b,\lambda)$ and $B(b',\lambda)$ takes the value $+1$ or -1, which means that exactly one of the two expressions $\Big|\Big[B(b,\lambda)+B(b',\lambda)\Big]\Big|$ and $\Big|\Big[B(b,\lambda)-B(b',\lambda)\Big]\Big|$ takes the value 2 and the other takes the value 0. It follows that $A(a,\lambda)\Big[B(b,\lambda)+B(b',\lambda)\Big]+A(a',\lambda)\Big[B(b,\lambda)-B(b',\lambda)\Big]\rho(\lambda)$ is either $+2$ or -2. Integrating over λ yields the inequality, as ρ is a probability measure.

It is easy to verify that quantum mechanics cannot be described by a local hidden variable model. To demonstrate this, consider for instance the Bell state $|00\rangle + |11\rangle \,/\, \sqrt{2}$ and the measurement corresponding to the bases $M^{\phi} := \{cos(\phi)\,|0\rangle + sin(\phi)\,|1\rangle\,,\, sin(\phi)\,|0\rangle - cos(\phi)\,|1\rangle\}$. The first basis element corresponds to the outcome 1 and the second corresponds to the outcome -1. Now we fix the measurements $a = M^{-\pi/16}, a' = M^{-3\pi/16}, b = M^{\pi/16}$ and $b' = M^{3\pi/16}$. Alice can apply the measurement a or a' and Bob apply the measurement b or b'. One can verify that the equations below hold. We will discuss this example further in Chapter 3.

$$\begin{aligned}|\mathbb{E}(a,b)+\mathbb{E}(a,b')+\mathbb{E}(a',b)-\mathbb{E}(a',b')| &= |4(cos^2(\pi/8)-sin^2(\pi/8))| \\ &= 2\sqrt{2} \geq 2.\end{aligned}$$

Since this violates the CHSH inequality, it follows that no local hidden variable theory can reproduce this experiment. Therefore, it is impossible to replicate the laws of quantum mechanics in terms of a local hidden variable theory.

It was shown by Fine that Bell's initial definition of a deterministic hidden variable model is sufficient, even if we do not assume that the universe is deterministic. In [Fin82], he proved that the statements below are equivalent for any Bell-experiment E. This is any experiment where two parties have a choice of 2 dichotomic measurements each. Later, Fine's theorem was generalised by Abramsky and Brandenburger in [AB11b]. Their theorem states that the following statements are equivalent for general experiments:

- There is a deterministic hidden variable theory for E
- There is a factorizable stochastic hidden variable theory for E
- There is a joint probability distribution for all the observables in E

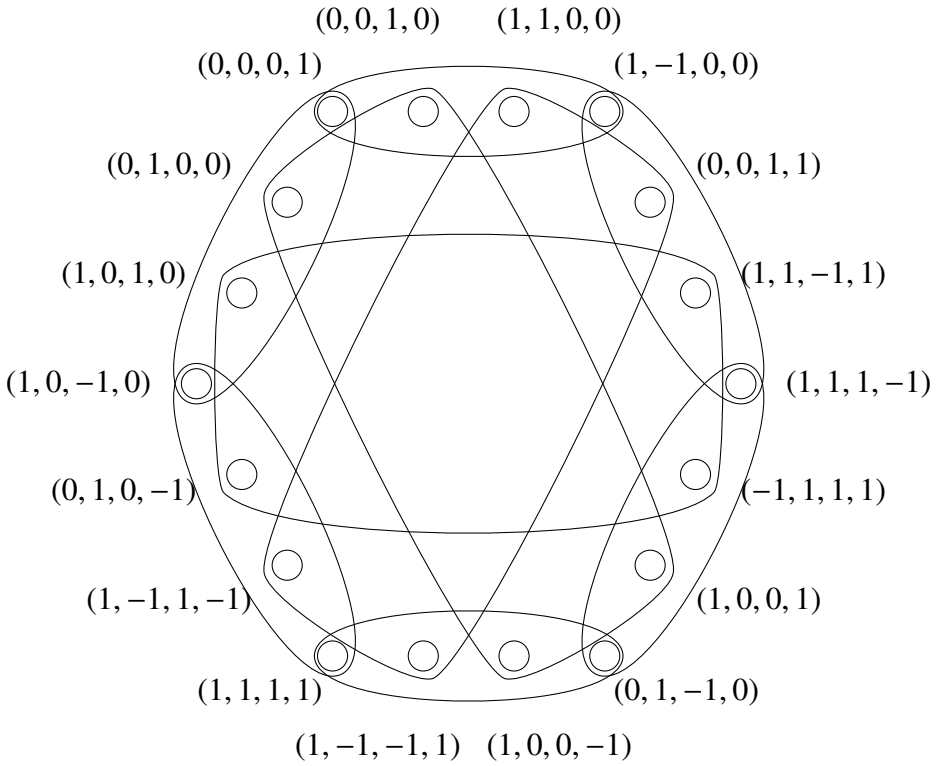
In the case of spatially separated events, the mathematical assumtion of factorizability can be justified by relativity theory, which prohibits objects to affect anything outside of their future light cone. Therefore, if relativity theory is correct, Bell's experiment does not admit any non-local hidden variable theory, whether deterministic or stochastic.

It was experimentally verified that the outcome statistics of experiments violate the CHSH equality, as predicted by quantum mechanics [HBD+15], [GVW+15]. Therefore, it is not only the theory of quantum mechanics that cannot be replicated by a local hidden variable theory; this is the case for *any* theory that explains such experiments.

Still, there are various implicit assumptions that could be dropped in order to maintain locality. One is the assumption that Alice and Bob have a free will. If the universe would be super-deterministic, as suggested by 't Hooft [tH] and the choices that Alice and Bob make are predetermined, then a local hidden variable model that takes the predetermined choices into account would be possible. The other assumption is causality. If, for instance, an event in the future could determine events in the past, then a local hidden variable theory would also be possible. This concept, called retro-causality, was advocated by [Pri12]. This would simply take some values into account which lie in an intersection of the future light cones of Alice and Bob after Alice's measurement. That way, Bob's measurement setting can influence the state of Alice's particle. In such scenarios, the choice of Alice and Bob is no longer independent from the measurement outcomes they obtain, which means that any statistical behaviour could be justified.

Contextuality of Quantum Mechanics

Bell [Bel01] and Kochen and Specker [KS67] showed that no deterministic hidden variable theory that is independent from the choice of the measurement setting can replicate the statistics of measurement outcomes in quantum mechanics. This holds in a larger class of scenarios, where the measurement setting does not necessarily arise from spatially separated joint measurements. In that sense, it is more general than non-locality; however, in such settings, one cannot justify the assumption of factorizability from relativity theory. This phenomenon of quantum mechanics is called contextuality. We will give a simplified version of the Kochen-Specker proof by Cabello, Estebaranz and Garcia-Alcaine [CEGA96], based on the hypergraph below.



Recall that an outcome to a measurement corresponds to a basis vector in the quantum formalism. Such a basis vector can be part of various different bases to the same state space. The 18 nodes in the graph depict basis elements of a 4-dimensional Hilbert space. The 9 hyperedges, marked by the loops, represent the bases that correspond to measurements - we will call these the **measurement contexts**. A hidden variable model that is independent of the measurement contexts would assign exactly one node to each hyperedge as the measurement outcome to that context. One can encode this as a value assignment of 0 or 1 to each of the nodes, such that exactly one node in each hyperedge receives a 1. This node is the outcome of the measurement. It is not possible to make such an assignment, as there is an odd number of hyperedges and each node is contained in exactly two of them. Therefore, there exists no set of predetermined measurement outcomes for this set of measurements. One can derive that any deterministic hidden variable theory for this set of measurements must depend on the choice of the measurement.

Can Factorizability be Justified in Contextuality Scenarios?

Whether one accepts factorizability as a valid assumption or not, the example demonstrates curious characteristics of the microscopic world: either it is inherently indeterministic, or it is contextual.

To resolve this issue, Spekkens proposed a general notion of contextuality which does not presuppose outcome-determinism [Spe05]. Within this framework, factorizability is derived from the notion of contextuality, only for those measurements for which the outcomes can be predicted with certainty, if the quantum system is in a particular state. However, as we will discuss in Chapter 2, one needs to introduce additional assumptions to derive the Bell-Kochen-Specker theorem from this general notion.

Frameworks for Contextuality

Since the discovery of contextuality, various abstract formalisms of different scope and nature have been proposed [AB11b, Spe05, CSW14, AFLS15, DK16, SU15] to generalise and expand the range of contextual scenarios. Such frameworks aim to capture the principle of contextuality abstractly, independent from the quantum formalism. The mathematical formulations facilitate the utilisation of various theorems and tools in graph-theory [CSW14, AFLS15] and sheaf-cohomology [AB11b, Rou16]. They enable applications beyond the world of physics, such as experimental psychology and linguistics [DK16, AS14]. While some of the approaches are known to be equivalent [dS15, AFLS15], this is not the case in general.

The Computational Power of Contextuality

The lack of predictability of quantum systems, or their dependence on other systems may seem to be a disadvantage; however, it turns out to be a source for computational power in various scenarios. It was shown in [Rau13, HCLB11] that contextuality is necessary for non-linear computations in mod-2 measurement-based quantum computation. Contextuality is essential for magic state distillation [HWVE14], which is an experimental method that enables fault-tolerant quantum computation. Furthermore, contextuality provides a speed-up over classical algorithms for specific problems, such as constraint satisfaction, graph isomorphisms, and certain questions in game-theory and communication complexity, as shown in [ABdSZ] [ABM17], [BCVD01]. In other schemes of quantum computing, such as the circuit model, the reason why quantum resources provide an advantage is still an open problem. Therefore, we have no conclusive evidence that contextuality is the cause of a quantum advantage in computation.

While the answer to this question is beyond the scope of this thesis, we take a step towards a universal understanding of contextuality, by unifying two main frameworks. We hope that one day this will lead to a deeper understanding of contextuality within the circuit model. In the meantime, we apply this unified framework to demonstrate the role

of contextuality in communication complexity. Thereby, we add to the accumulating evidence that contextuality in quantum computing increases computational power.

1.3.2 Modeling Quantum Protocols

One of the challenges of the development of quantum computing lies in the tools we have available to describe protocols. In the Hilbert space formalism, a quantum protocol, which is a sequence of quantum operations, corresponds to a multiplication of matrices. The size of such matrices increases exponentially with regards to their input, which makes them hard to grasp for the human brain.

To design and reason more easily about quantum protocols, more intuitive ways to visualise or process them have been developed, such as the circuit model. Other tools for specific facets of quantum computation include the Bloch Sphere [Blo46], for single qubit operations; tensor networks, to compute the ground state of one-dimensional quantum spin models for many particle systems [Orú14]; the ZX-calculus for surface codes lattice surgery in quantum error correction [dBH17] and the measurement calculus for measurement-based quantum computing [DKP07].

One can generalise the circuit model using monoidal categories [AC04], which provide an abstract language for the description of processes. The objects of a monoidal category represent the different states that something can be in, and the morphisms represent transformations from one state to another. The tensor product of two transformations represents the parallel execution of the transformations. The coherence equations ensure that the different ways in which processes can be composed correspond to the same compound process. Additional structure on a monoidal category such as a braiding or dagger functor is used to describe the characteristics of a specific process theory.

Symmetric monoidal dagger categories capture the essential characteristics of Hilbert spaces, such as the tensor product, transposition, conjugation, the inner product and the trace. Therefore, one can describe many essential elements of quantum theory independently from the Hilbert Space formalism. Examples are product states, maximally mixed states, measurements, the Born rule and perfect correlation. This allows one to prove various properties and theorems, such as quantum teleportation, quantum key distribution, dense coding, non-locality, no-cloning and no-broadcasting [CK17]. Most proofs are considerably easier, sometimes even trivial, in the diagrammatic language compared to their counterparts in the Hilbert space formalism.

Like the circuit model, monoidal categories do not capture Schrödinger's equation, which describes exactly how quantum states evolve over time. Schödinger's equation is essential for experiments in the lab, or the construction of quantum computers, as

it tells us how to create and transform specific quantum states. From a programmer's point of view, it is only important to know which operations are possible on a given computer, not how these operations are implemented. Therefore, monoidal categories have the right level of simplicity for an operational language of quantum protocols.

Monoidal categories give rise to an intuitive diagrammatic language, which is similar to the circuit model. This language is sound and complete [Sel09, Theorem 3.12], which means that any statement that can be proven diagrammatically is true in the categorical model and vice versa. This guarantees that one can design and reason about quantum protocols, by drawing and manipulating their corresponding diagrams. The diagrammatic language can be processed by computer programs, such as Quantomatic [KZ15] and Globular [BKV16], which increases the ease of dealing with large inputs or extensive sequences of operations. Various advancements in quantum information have been derived through the framework of monoidal categories [dBH17, CW18, DP10, VV18].

Additionally, monoidal closed categories are used as the semantics for quantum programming languages [Sel04, GLR$^+$13, LMZ18]. They generalise Cartesian closed categories, which serve as the semantics for classical functional programming languages. A Cartesian closed category is merely a monoidal closed category where the tensor is the categorical product.

To summarize, symmetric monoidal dagger categories allow us to describe quantum processes in an intuitive way. They capture exactly the facets that are needed from a programmer's point of view, without the complexity that arises from large matrix multiplications. Furthermore, they are essential in the development of higher level programming languages.

One thing that cannot be expressed explicitly in monoidal categories is the probabilistic branching of protocols due to measurements. Each measurement has a number of possible outcomes, each of which leads to a different evolution, called a branch of the protocol, and possibly a different outcome. One would like to keep track of all the different branches; a natural way to do this, is by using bicategories, as described in [Vic12]. Bicategories are a generalisation of monoidal categories, which have an extra dimension to store classical information, such as classical control or input bits, and measurement outcomes. This makes them particularly useful for modelling the interaction between classical and quantum information. This interaction is essential for various fundamental operations in quantum computing. It is needed for the creation of inputs and the recording of outputs of algorithms, as well as for controlled operations - operations that are conditional on previous measurement outcomes or classical input bits.

In the last two chapters of this thesis, we provide the mathematical foundation for such bicategorical models, based on modules that act on algebras. We prove that they have all the desired properties for a model of quantum computation. The algebras are a generalisation of C*-algebras on a Hilbert space, which capture classical and quantum data types as different instances of the same structure. Modules allow one to consider probability distributions over different outcome states. This provides a simple way of expressing the entire set of probabilistic branches of a quantum protocol, without the need to specify the actual outcome. In the next section we give a brief introduction to C*-algebras.

C*-algebras as a Formalism for Quantum Mechanics

There is an elegant mathematical way to unify the classical and the quantum world using C*-algebras as a generalization of the mixed-state formalism. Notions of states, measurements and evolutions have a simple description in this formalism. We can distinguish classical systems from quantum systems as those algebras that are commutative.

We will briefly set out how classical and quantum systems give rise to the C*-algebras listed below. More details can be found in [Heu17].

- Any state space in the density matrix formalism gives rise to an operator algebra.
- Any classical system can be represented by a commutative C*-algebra.

Definition 1.3.2. A normed vector space, is a vector space A, with a morphism $|-| : A \to \mathbb{R}$. For any two vectors a, b, and for any scalar λ, the following equalities hold:

$$|\lambda \cdot x| = |\lambda| \cdot |x| \tag{1.3.3}$$

$$|a + b| \leq |a| + |b| \tag{1.3.4}$$

We call the morphism $|-|$ a norm.

Note that a norm induces a metric, given by $d(a, b) = |a - b|$

Definition 1.3.5. A Banach space is a normed vector space which is complete. That is, every Cauchy sequence - a sequence whose elements become arbitrarily close to each other as the sequence progresses - converges.

We define C*-algebras as algebras on a Banach space that respect all structure of the space, and in addition, the C*-condition:

Definition 1.3.6. A C*-algebra is an algebra on a Banach space which satisfies the triangle inequality $||a \cdot b|| \leq ||a|| \cdot ||b||$, and is equipped with an antilinear morphism $* : A \to A$, such that:

$$(a + b)^* = a^* + b^* \tag{1.3.7}$$

$$||a^* a|| = ||a||^2 \tag{1.3.8}$$

One can verify that C*-algebras are closed under appropriately chosen tensor products and direct sums.

There are two important examples of C*-algebras: commutative C*-algebras, and the space $B(H)$ of bounded operators on a Hilbert space. We will discuss these below.

Classical Structures as Commutative C*-algebras

Classical structures can be characterized as commutative C*-algebras. As we discuss below, finite commutative C*-algebras are isomorphic to $\oplus_{i=1}^{n} \mathbb{C}$ for some n, which means they represent classical data types.

Let X be a compact Hausdorff space - a topological space in which distinct points have disjoint neighbourhoods. The space of continuous operators $C(X) = \{f : X \to \mathbb{C}\}$, is a C*-algebra with the following multiplication and unit:

$$f \cdot g : X \longrightarrow \mathbb{C} \tag{1.3.9}$$

$$x \longrightarrow f(x) \cdot g(x) \tag{1.3.10}$$

$$1 : X \longrightarrow \mathbb{C} \tag{1.3.11}$$

$$x \longrightarrow 1 \tag{1.3.12}$$

$C(X)$ is a vector space for function addition and scalar multiplication. The conditions that operators should be continuous and X should be compact guarantee completeness of this vector space. The norm is inherited from $\mathbb{C}$. The *-morphism is defined as

$$*(f) : X \longrightarrow \mathbb{C} \tag{1.3.13}$$

$$x \longrightarrow \overline{f(x)} \tag{1.3.14}$$

As multiplication in $\mathbb{C}$ is commutative, this is a commutative C*-algebra. By the Gelfand duality, every commutative C*-algebra is *-isomorphic to $C(X)$ for some Hausdorff space X, see Theorem 9.18 of [Tak02]. Therefore, this is a complete classification of commutative C*-algebras. When X is a finite Hausdorff space of n elements, $C(X)$ is the complex linear space on n generators. This is isomorphic to $\mathbb{C}^n$

Quantum Structures as Operator Algebras

The second important example of a C*-algebra is the space of continuous linear operators on a Hilbert space. Let H be a Hilbert space. The space $B(H)$ of bounded linear operators forms a C*-algebra with function composition and the identity function as multiplication and unit. A linear operator $f : H \to H'$ is **bounded** if exists some $M \geq 0$ such that for all $vi \in H$

$$\left\|f(v)\right\| \leq M\|v\|$$

Bounded linear operators form a vector space under addition and scalar multiplication. The norm $\|f\|$ of a function f in this space is defined as $\sup\{\|f(x)\| : \|x\| = 1\}$. The condition that operators should be bounded guarantees completeness of this vector space. The antilinear morphism $* : B(H) \to B(H)$ of the C*-condition is induced by the adjoint in H:

$$*(f) : H \to H \tag{1.3.15}$$

$$*(f)(x) := (f(x))^* \tag{1.3.16}$$

The remaining conditions are straightforward. Direct sums of operator algebras are C*-algebras themselves, which may arise from degenerate measurements. In that case it expresses the fact that we have partial information about the state.

Transformations in the algebraic formalism for quantum mechanics are given by completely positive maps on C*-algebras. For finite-dimensional C*-algebras, these are morphisms of the form below.

$$\sum_i c_i \left|\phi_i\right\rangle \left\langle\phi_i\right| \mapsto \sum_j d_j \left|\psi_i\right\rangle \left\langle\psi_i\right| \tag{1.3.17}$$

These maps are probabilistic mixtures of evolutions of closed quantum states. Such a map can always be represented as

$$f(\rho) = \sum_i E_i \rho E_i^\dagger$$

A completely positive map is **trace preserving** if $\sum_i E_i^\dagger E_i = I$. For each C*-algebra A, a **quantum state** can be recovered as a trace preserving completely positive map $\mathbb{C} \to A$. The image of this map is a positive element of the operator space, which is a density matrix.

A **measurement** corresponds to a completely positive map from a non-commutative C^*-algebra to a commutative C^*-algebra.

Chapter 2

Towards a Universal Description of Contextuality

Non-locality and contextuality are curious phenomena of physics. While nature seems to contradict itself, the fact that not everything can be observed at the same time keeps the universe coherent.

Following Bell and Kochen-Specker, numerous examples and proofs of contextuality in quantum mechanics were discovered, such as Hardy's paradox [Har92, Har93] and Mermin's All-versus-nothing argument [Mer90]. Each of these examples is specific to the Hilbert space formalism for quantum mechanics. In the last decade, various formalisms of different scope and nature have been proposed, which generalise these examples of contextuality in a more abstract framework: [AB11b, AFLS15, CSW14, DK16, Spe05, SU15]. These approaches share the goal of expressing the notion of non-contextuality in a manner that is independent of the quantum formalism. They are applicable to any high-level description of an experimental setting. The relation between some of the formalisms has been studied in [dS15, SU15].

In this chapter, which is based on work published in [Wes17], we unify the sheaf-theoretic formalism by Abramsky and Brandenburger [AB11b] with the equivalence-based notion of contextuality developed by Spekkens in [Spe05]. The mathematical framework of sheaf-theory provides algorithmic methods based on sheaf-cohomology to detect contextuality [AMB11], as well as means of quantifying contextuality [ABM17] and a structural method for deriving non-contextuality inequalities [AH12]. The equivalence-based approach provides simple critera to define contextuality for preparations, transformations and for (unsharp) measurements. The formalism does not presuppose outcome assignments in a hidden-variable model to be deterministic; it derives it from different assumptions about convexity in probabilistic samples. Additionally, it gives rise to different non-contextuality inequalities [Kun17], [MPK$^+$16]. In Section 2.1 we

recall the equivalence-based approach to contextuality. We discuss how known examples of contextuality and non-locality arise in this formalism by imposing additional assumptions which force the outcome assignments in an ontological model to be deterministic. We analyse the notion of contextuality beyond theories where outcome-determinism of ontological representations is justified. As an illustration, we discuss Mermin's All Versus Nothing argument and Bell's scenario in the equivalence-based model. In Section 2.2, we recall the sheaf-theoretic approach. We extend the framework to incorporate preparations. In Section 2.3, we introduce a method for constructing a canonical non-contextual ontological representation for any non-contextual empirical theory. We prove that such a canonical non-contextual ontological representation exists whenever the theory admits a factorizable non-contextual ontological representation. In Section 2.4 we introduce the categories $\mathcal{E}mp$ of empirical theories, $\mathcal{O}T$ of operational theories, and $\mathcal{O}R$ of ontological representations. We show how the correspondence between empirical and operational theories gives rise to a categorical isomorphism, which maps the subcategory of non-contextual empirical theories to the subcategory of operational theories that can be realised by a factorizable non-contextual ontological representation. In Section 2.5, we discuss contextuality for unsharp measurements and give an example for which the two notions of contexuality are different.

2.1 The Equivalence-Based Approach

Contextuality in the equivalence-based approach is defined as the non-existence of certain hidden variable models, called 'ontological representations', of operational theories. An operational theory is a high-level description of an experimental setting. An ontological representation represents physical systems as they really are, while the operational theory merely describes the operations we can perform on the system. We may be able to obtain information about the system through the outcomes of such operations, but this information may not be accurate or complete. To be non-contextual, an ontological representation must be determined by the statistical data of the experiment only. It cannot depend on any additional data, regarded as the 'context'. This gives a natural explanation for operational equivalence of measurements and preparations: we cannot distinguish them because they correspond to the same ontological values. The formalism distinguishes three different types of contextuality: contextuality for preparations, transformations and for (unsharp) measurements. Unlike traditional notions of contextuality, the formalism does not presuppose outcome assignments in a hidden-variable model to be deterministic.

Operational Theories

Consider two sets, P and M, of preparation procedures and measurement procedures, respectively. For each measurement $m \in M$ there is a finite set O^m of possible measurement outcomes. For each pair $(p, m) \in P \times M$, there exists a probability distribution $d_{p,m} : O^m \to [0, 1]$ over the set of possible outcomes O^m. The value $d_{p,m}(k)$ should be understood as the probability of obtaining the outcome k when a preparation p is performed, followed by a measurement m. We write D for the indexed set of probability distributions $\{d_{p,m}\}_{p\in P, m\in M}$. An **operational theory** is defined by a tuple (P, M, D, O), where $O = \cup_m O^m$. In [Spe05], operational theories also contain a set of transformation procedures, but we will not consider these here. We can still account for any transformation followed by a measurement by considering it as a new measurement. However, we cannot account for contextuality that arises from statistical equivalences, which are the result of the composition of transformations.

Preparations and measurements are **statistically equivalent** when they are not distinguishable based on the measurement statistics in the operational theory. Let $p, p' \in P$ be preparations, let $m, m' \in M$ be measurements and let $k \in O^m, k' \in O^{m'}$ be measurement outcomes, this is expressed below.

$$
\begin{array}{llll}
\forall p, p' & p \sim p' \Leftrightarrow & d_{p,m} = d_{p',m} & \forall m \in M \\
\forall m, m' & m \sim m' \Leftrightarrow & d_{p,m} = d_{p,m'} & \forall p \in P \\
\forall (m, k), (m', k') & (m, k) \sim (m', k') \Leftrightarrow & d_{p,m}(k) = d_{p,m'}(k') & \forall p \in P
\end{array}
$$

Example 2.1.1 (Quantum Mechanics). The standard example of an operational theory is the Hilbert space formalism for quantum mechanics. Equivalence classes of preparation procedures correspond to density matrices. Equivalence classes of measurement procedures correspond to POVM's. Different decompositions of density matrices or POVM's correspond to different preparation or measurement procedures, respectively. Joint measurements correspond to the tensor product of POVM's The outcome set of each measurement procedure corresponds to the index set of the POVM elements. The indexed set of distribution functions D is derived from the Born rule.

An **ontological representation** of the operational theory $A = (P, M, D, O)$ consists of a set of ontological values Ω, together with sets of discrete distribution functions $\mu = \{\mu_p : \Omega \to [0, 1]\}_{p\in P}$ and $\xi = \{\xi_m(\lambda) : O^m \to [0, 1]\}_{\lambda\in\Omega, m\in M}$. The distribution functions are such that they realise the measurement statistics of A, which is expressed by the formula below.

$$\sum_{\lambda\in\Omega} \xi_m(\lambda)(k)\mu_p(\lambda) = d_{p,m}(k) \qquad \forall p \in P, m \in M \tag{2.1.2}$$

In this paper, we will assume that all distribution functions μ are of finite support and that all ontological values can be obtained by performing some preparation procedure. This means that for all $p \in P$, the set $\{\lambda \in \Omega | \mu_p(\lambda) > 0\}$ is finite and for all $\lambda \in \Omega$ there exists a preparation $p \in P$, such that $\mu_p(\lambda) > 0$.

Definition 2.1.3. An **ontological representation** is called **preparation non-contextual** if $\mu_p = \mu_{p'}$, whenever $p \sim p'$; it is called **measurement non-contextual** if $\xi_m(k) = \xi_{m'}(k')$, whenever $(m, k) \sim (m', k')$; it is called **non-contextual** if it is preparation non-contextual as well as measurement non-contextual. An **operational theory** is called **non-contextual** whenever there exists a non-contextual ontological representation that realises the theory. When there exists no such ontological representation, the operational theory is called contextual.

Contextuality is characterised as the impossibility of *any* non-contextual hidden variable model. Therefore, one would want to consider non-discrete distributions of unbounded support as well. We conjecture that all results can be generalised to hold for general probability measures. We leave this for future work.

Nevertheless, the notion of non-contextuality without any further restrictions is too permissive. We can find a non-contextual ontological representation for any operational theory with discrete sets P, M. This covers all classic examples of contextuality mentioned so far. The ontological representation is defined as follows:

$$\Omega := \{[p]\}_{p\in P} \quad \mu_q([p]) := \delta_{p,q} \quad \xi_m([p])(k) := d_{p,m}(k) \tag{2.1.4}$$

Here, $[p]$ is the statistical equivalence class of $p \in P$. One could ask whether it is possible to find a non-contextual ontological representation that satisfies specific properties. These can either be derived from the formalism or justified by physical principles. In the rest of this section, we discuss which additional properties we need to derive known examples of contextuality from the equivalence-based definition.

Deriving Contextuality Arguments From Convex Structure

The following assumption is required for the contextuality proof of preparations and unsharp measurements of 2-dimensional quantum systems given in [Spe05].

Assumption 1 (Preservation of Convexity)**.** *Let $p, p_1, p_2 \in P$ be preparation procedures, such that $p = cp_1 + (1-c)p_2$ is a convex combination of p_1 and p_2; let $m, m_1, m_2 \in M$ be measurement procedures, such that $m = cm_1 + (1-c)m_2$ is a convex combination of m_1 and m_2. We have the following equalities of distribution functions:*

$$\mu_{cp_1+(1-c)p_2} = c\mu_{p_1} + (1-c)\mu_{p_2} \tag{2.1.5}$$

$$\xi_{cm_1+(1-c)m_2} = c\xi_{m_1} + (1-c)\xi_{m_2} \tag{2.1.6}$$

Example 2.1.7. In any physical experiment, the convex combination of two operations can be seen as a probabilistic sample of these operations. In the Hilbert space formalism for quantum mechanics, it is the convex combination of a set of density matrices or observables, respectively.

The contextuality examples in [Spe05] arise from the fact that POVM's and mixed density matrices can be written as different convex combinations of projectors and pure density matrices, respectively. It is not possible that the convex decompositions are preserved at the ontological level for all combinations at once. We will discuss the two examples in detail in section 2.2.

Deriving Traditional Notions of Contextuality and Non-locality

An ontological representation is **outcome-deterministic** if $\xi_m(\lambda)(k) \in \{0, 1\}$ for all $m \in M, k \in O$ and $\lambda \in \Omega$. In [Spe05] it was shown that every non-contextual ontological representation for PVM's in the Hilbert space formalism for quantum mechanics must be outcome-deterministic. We generalise this argument below for operational theories. To characterize a class of operational theories in which outcome-determinism can be justified, we generalise the notion of sharp measurements and the maximally mixed state in quantum mechanics to the operational notions below.

Definition 2.1.8. A measurement procedure m with outcome set O^m is **perfectly predictable** if for all $k \in O^m$ there exists a preparation p_k, such that $d_{p_k,m}(k') = \delta_{k,k'}$.

Definition 2.1.9. A preparation p^{mix} is **maximally mixed** if the following two conditions hold.

(i) For every preparation procedure p', p^{mix} is statistically equivalent to some preparation procedure which is a convex combination of preparations containing p'.

(ii) For every perfectly predictable measurement procedure m, p^{mix} is statistically equivalent to some measurement procedure which is a convex combination of p_k for $k \in O^m$.

Example 2.1.10 (Quantum Mechanics). In quantum theory, PVM's are perfectly predictable. In the Hilbert space model for quantum theory of a fixed dimension d, any preparation of the maximally mixed state $I/2^d$ is a maximally mixed preparation.

Lemma 2.1.11. *Let m be a perfectly predictable measurement procedure in an operational theory that satisfies Assumption 1 and contains a maximally mixed preparation. If the distribution function ξ_m is part of a preparation non-contextual ontological representation, it is outcome-deterministic.*

Proof. Let $\Omega_p := \{\lambda \in \Omega | \mu_p(\lambda) > 0\}$ be the support of μ_p. Perfect predictability implies that for each measurement m and outcome k of m, there exists a preparation p_k, such that $d_{p_k,m}(k') = \sum \xi_m(\lambda)(k')\mu_{p_k}(\lambda) = \delta_{k,k'}$ for all $k' \in O^m$. If $k = k'$, this means that $\xi_m(\lambda)(k) = 1$ for all $\lambda \in \Omega_{p_k}$, since μ_{p_k} is a probability distribution and $\xi_m(\lambda)(k) \leq 1$. For $k \neq k'$, this implies that $\xi_m(\lambda)(k) = 0$ for $\lambda \in \Omega_{p_{k'}}$. As a result, $\xi_m(\lambda)(k) \in \{0, 1\}$ for $\lambda \in \cup_k \Omega_{p_k}$.

It is left to prove that $\Omega = \cup_k \Omega_{p_k}$. By preparation non-contextuality, there is one probability distribution $\mu_{p^{mix}}$ for all preparations that are statistically equivalent to the maximally mixed preparation p^{mix}. We use this to show that $\Omega = \Omega_{p^{mix}}$. It is clear that $\Omega_{p^{mix}} \subset \Omega$, so we need to show that for all $\lambda \in \Omega$, it is true that $\lambda \in \Omega_{p^{mix}}$. By our earlier assumption, for every element $\lambda \in \Omega$ there exists a preparation p, such that $\lambda \subset \Omega_p$. By the first condition of the maximally mixed preparation and Assumption 1, we know that $\lambda \subset \Omega_{p^{mix}}$. It follows that $\Omega = \Omega_{p^{mix}}$. By the second condition and Assumption 1, we know that $\mu_{p^{mix}} = \mu_{\sum c_k p_k}$. It follows from the definition of the support, that $\Omega_{p^{mix}} = \Omega_{\sum c_k p_k} = \cup \Omega_{c_k p_k} = \cup \Omega_{p_k}$. As a result, $\Omega = \cup \Omega_{p_k}$, hence ξ_m is outcome-deterministic. □

Another crucial structure in various contextuality examples is the notion of joint measurements. We recall the following recursive definition given in [LSW11].

Definition 2.1.12. A set of N measurements $\{m_1, m_2, ..., m_N\}$ is **jointly measurable** if there exists a measurement m with the following features:
(i) The outcome set of m is the Cartesian product of the outcome sets of $m_1, ..., m_N$
(ii) Let S be a subset of the index set $\{1, ..., N\}$. The outcome distributions for every joint measurement of any subset $\{m_s | s \in S\} \subset \{m_1, ..., m_N\}$ is recovered as the marginal of the outcome distribution of m for all preparations $p \in P$. Denoting a joint measurement of the subset S by m_S with a corresponding outcome $k_S \in O^{m_S}$, the condition can be expressed as

$$\forall S, \forall p : d_{p,m_S}(k) = \sum_{k \in O^m : \pi_S(k) = k_S} d_{p,m}(k). \tag{2.1.13}$$

Here, π_S is the projection function on the subset $O^{m_S} \subset O^m$.

Note that the notion of joint measurement defines a preorder on the set M. We restrict our attention to operational theories where each joint measurement m corresponds to a chosen set of measurements $\{m_1, m_2, ..., m_N\}$, that satisfies the requirements of Definition 2.1.12. We regard m as the unique joint measurement of $m_1, m_2, ..., m_N$.

An ontological representation is called **parameter independent** if for each measurement the effect on the ontological states is independent of any other measurement performed simultaneously. We can restrict the distribution function of m to a subset m'. The corresponding distribution, which we denote by $\xi_{m|_{m'}}$, is defined as $\xi_{m|_{m'}}(k')(\lambda) := \sum_{k:\pi_{m'}(k)=k'} \xi_m(k)(\lambda)$, where $\pi_{m'} : O^m \to O^{m'}$ projects the outcomes of m to the set of outcomes of m'. Parameter independence means that for two joint measurements m, n, the equality $\xi_m|_{m\cap n} = \xi_n|_{m\cap n}$ holds.

Lemma 2.1.14. *Any measurement non-contextual representation of an operational theory (P, M, D, O) is parameter independent. That is, for all joint measurements $\{m, n\}$, we have the following equalities:*

$$\xi^k_m|_{m\cap n}(\lambda) = \xi^k_{m\cap n}(\lambda) = \xi^k_n|_{m\cap n}(\lambda) \tag{2.1.15}$$

Proof. Let $m = \{m_1, ..., m_N\}$ be a jointly measurable set of measurement procedures of M, let p be a preparation procedure, let K_s be the set $\{k \in O^m | \pi_s(k) = k_s\}$, for some $s \in \{1, ..., N\}, k_s \in O^{m_s}$.

By joint measurability and basic probability theory, we have the following sequence of equalities on the operational level:

$$\begin{aligned} d_{m_s,p}(k_s) &= \sum_{k\in K_s} d_{m,p}(k) \\ &= d_{m,p}(K_s) \end{aligned}$$

It then follows from measurement non-contextuality that

$$\begin{aligned} \xi_{m_s}(k_s) &= \xi_m(K_s) \\ &= \sum_{k|\pi_s(k)=k_s} \xi_m(k) \\ &=: \xi_{m|m_s}(k_s) \end{aligned}$$

□

A stronger restriction on ontological representations is factorizability. We call an ontological model **factorizable** when for joint measurements $m = (m_1, ..., m_n)$, we can write $\xi_m(\lambda)(o) = \prod_{i=1,...,n} \xi_{m_i}(\lambda)(\pi_i(o))$. It was shown in Theorem 6 of [LSW11] that any ontological model which is outcome-deterministic and measurement non-contextual, is factorizable. In fact, we will show in Section 2.3 that an operational theory admits a factorizable non-contextual ontological representation if and only if it admits a deterministic non-contextual ontological representation. This is a generalisation of Fine's theorem [Fin82] for the equivalence-based notion of contextuality.

Bell's Scenario

We derive Bell's non-locality proof as a special case of equivalence-based contextuality. Consider the following experiment, where two parties can each choose from two different measurements with outcome set $\{1, -1\}$: a and a' for the first party; b and b' for the second party. The outcome statistics of each possible combination of measurements after a preparation p is organised in the table below. Each entry $a_{i,j}$ of the table represents the probability of obtaining outcome i for measurement j.

	(1,1)	(-1,1)	(1,-1)	(-1,-1)
(a, b)	1/2	0	0	1/2
(a', b)	3/8	1/8	1/8	3/8
(a, b')	3/8	1/8	1/8	3/8
(a', b')	1/8	3/8	3/8	1/8

(2.1.16)

This setup can be realised in the operational theory given by the Hilbert space formalism of quantum mechanics. Consider the quantum states below.

$$\phi_{a_+}, \phi_{b_+} = (|0\rangle + |1\rangle)/\sqrt{2}) \qquad \phi_{a_-}, \phi_{b_-} = (|0\rangle - |1\rangle)/\sqrt{2})$$
$$\phi_{a'_+}, \phi_{b'_+} = (|0\rangle + e^{\pi/3i}|1\rangle)/\sqrt{2}) \qquad \phi_{a'_-}, \phi_{b'_-} = (|0\rangle + e^{(\pi/3+\pi)i}|1\rangle)/\sqrt{2})$$
$$\phi_{GHZ} = (|00\rangle + |11\rangle)/\sqrt{2}$$

Let P_{x_+} and P_{x_-} be observables that project onto the state ϕ_{x_+} and ϕ_{x_-}, respectively and consider the PVM $x := (P_{x_+}, P_{x_-})$ for $x \in \{a, b, a', b'\}$.

We are interested in measurement procedures (a, b), (a', b), (a, b'), and (a', b') corresponding to the PVM's $a \otimes b, a' \otimes b, a \otimes b'$ and $a' \otimes b'$, respectively, as well as the restriction to each of the components for each of the measurements, which are obtained by taking the partial trace.

We have seen before that the Hilbert space formalism of fixed dimension has a well-defined notion of convex combinations and contains a maximally mixed preparation. Furthermore, all measurements are perfectly predictable as they are PVM's. The tuples are joint measurements of their restrictions, which fall into four equivalence classes a, a', b, b'. Since any non-contextual ontological representation is in particular preparation non-contextual, it follows that any such a representation must be outcome-deterministic under Assumption 1, hence factorizable. As a result, every ontological state can be associated with a function $\{a, a', b, b'\} \to \{0, 1\}$ from the set of equivalence classes of elementary measurements to the outcome set. This morphism maps each measurement to the outcome that occurs with probability 1 when the system is in ontological state λ. In other words, we can identify each ontological value λ with the outcome $(\alpha, \beta, \alpha', \beta') \in \{0, 1\}^4$. We obtain the presupposed probability that $a = \alpha, b = \beta, a' = \alpha', b' = \beta'$, by summing over all ontological values that correspond to this outcome, according to equation 2.1.2. We denote this probability by $p_{\alpha\beta\alpha'\beta'}$. These probabilities should add up to the values given in the table. The entries $a_{1,1}, a_{2,2}, a_{3,3}$, and $a_{1,4}$, give us the 4 equations below.

$$a_{1,1} : p_{0000} + p_{0010} + p_{0001} + p_{0011} = 1/2 \qquad a_{2,2} : p_{0010} + p_{1010} + p_{0011} + p_{1011} = 1/8$$
$$a_{3,3} : p_{0001} + p_{0101} + p_{0011} + p_{0111} = 1/8 \qquad a_{1,4} : p_{0000} + p_{0100} + p_{1000} + p_{1100} = 1/8$$

The left-hand-side of the sum of $a_{2,2}, a_{3,3}$ and $a_{1,4}$ should be greater than $1/2$, since it contains all summands of $a_{1.1}$. However, the right-hand side of these equations sums to $3/8$. As a result, the equations cannot be satisfied. As a consequence of this contradiction, a non-contextual ontological representation cannot exist.

Mermin's All Versus Nothing Argument

For the next example, we again consider the operational theory defined by the Hilbert space formalism of quantum mechanics. Suppose that we are given a GHZ state $\phi_{GHZ} = (|000\rangle + |111\rangle)/\sqrt{2}$ and we may perform Pauli X or Y measurements on each of its components. One can verify that for a choice of joint measurements, the following equalities hold with certainty. The right-hand-side of the equalities are given by the product of the outcomes of the three individual measurements:

$$X_1Y_2Y_3 = -1 \qquad Y_1Y_2X_3 = -1 \qquad Y_1X_2Y_3 = -1 \qquad X_1X_2X_3 = 1$$

As in the previous example, the measurements are perfectly predictable, and the operational theory contains a maximally mixed state. Furthermore, the triples are joint measurements of their restrictions to the three different components, given by the partial trace. These restrictions fall into the equivalence classes $X_1, Y_1, X_2, Y_2, X_3, Y_3$. We will show that no ontic state λ in a non-contextual representation allows for probability distributions $\xi_-(\lambda)$ that are consistent with this scenario. Suppose there exists a non-contextual ontological representation for this operational theory. In particular, this representation is preparation non-contextual. Perfect predictability and the maximally mixed preparation imply outcome determinism and factorizability. Hence, $\xi_{X_1Y_2Y_3} = \xi_{X_1}\xi_{Y_2}\xi_{Y_3}$, and similarly for the other joint measurements. Given any ontological state λ of such representation, we can identify each distribution function $\xi_{X_i}(\lambda), \xi_{Y_i}(\lambda)$ with the outcome that occurs with certainty. We will denote this constant function by ξ'_{X_i} and ξ'_{Y_i}, respectively. As a result, ξ'_{X_i} and ξ'_{Y_i} assign -1 or 1 to λ, in a way that the equalities below are satisfied.

$$\begin{aligned} \xi'_{X_1}(\lambda)\xi'_{Y_2}(\lambda)\xi'_{Y_3}(\lambda) &= -1 & \xi'_{Y_1}(\lambda)\xi'_{Y_2}(\lambda)\xi'_{X_3}(\lambda) &= -1 \\ \xi'_{Y_1}(\lambda)\xi'_{X_2}(\lambda)\xi'_{Y_3}(\lambda) &= -1 & \xi'_{X_1}(\lambda)\xi'_{X_2}(\lambda)\xi'_{X_3}(\lambda) &= 1 \end{aligned}$$

It is easy to see that this is impossible: The product of the expressions on the left-hand-side of the equations must equal 1, since every component occurs twice, while the product of the right-hand-sides equals -1.

2.2 The Sheaf Approach

In the sheaf approach to contextuality, one defines contextuality as the non-existence of a joint probability distribution over the outcomes of a set of measurements. It is formulated within the mathematical framework of sheaf theory as the non-existence of a global section for a presheaf of distributions over measurement outcomes. This approach provides algorithmic methods based on sheaf-cohomology to detect contextuality [AMB11], as well as means of quantifying contextuality [ABM17] and a structural method for deriving non-contextuality inequalities [AH12].

In this section, we recall the sheaf-theoretic approach to contextuality and non-locality, which was introduced by Abramsky and Brandenburger in [AB11b] and [AB11a].

A sheaf is a mathematical tool for describing how local data can be combined to obtain global information about a system. In the sheaf approach, this is applied to sets of outcome probabilities in an experiment. A **measurement scenario** consists of a discrete set L of measurement labels, together with a **measurement cover** $\mathcal{M} = \{C_i\}_{i\in I}$ and an

outcome set O. The measurement cover $\mathcal{M}$ is an antichain of subsets $C_i \subset L$, such that $\cup_{i\in I} C_i = L$. This means that for $C, C' \in \mathcal{M}$, we have the implication $C \subset C' \implies C = C'$. The measurement cover $\mathcal{M}$ represents the maximal sets of measurements that can be performed jointly. It gives rise to a simplicial set $\downarrow \mathcal{M}$, consisting of all subsets of the elements of the measurement cover. The outcome set O is the union of the sets of possible outcomes for each of the measurements in L. For each set of measurements $U \subset L$, a **section over** U is a function $U \to O$. We write O^U for the set of sections over U. The assignment $U \mapsto O^U$ defines a sheaf $\mathcal{E} : \mathcal{P}(L) \to Set$, which is a contravariant functor over the powerset $\mathcal{P}(L)$. We call this the **sheaf of events**, as it assigns every context to a set of outcomes. Furthermore, it maps every subset to a restriction function of the outcomes to that subset, as defined below.

$$\rho^U_{U'} := \mathcal{E}(U \subset U') : O^{U'} \mapsto O^U :: s \to s|_U$$

We call elements of $\mathcal{E}(L)$ **global sections** of measurement outcomes. Each global section consists of an assignment of an outcome to each of the measurements.

For any commutative semiring R and set L, an R-distribution d on L is a map $d : L \to R$ of finite support, such that

$$\sum_{x\in L} d(x) = 1$$

We write $\mathcal{D}_R(X)$ for the set of R-distributions on a set X. For a function of sets $f : X \to Y$, we define

$$\mathcal{D}_R(f) : \mathcal{D}_R(X) \to \mathcal{D}_R(Y) :: d \mapsto [y \mapsto \sum_{f(x)=y} d(x)]$$

It is easy to see that $\mathcal{D}_R$ is functorial. Hence, we can compose $\mathcal{E}$ with $\mathcal{D}_R$ to obtain a presheaf $\mathcal{D}_R\mathcal{E} : \mathcal{P}(L) \to Set$, which maps each set of measurements to the set of R-distributions over their sections. When R is the ring of non-negative reals $\mathbb{R}_+$, $\mathcal{D}_R\mathcal{E}(m)$ corresponds to probability distributions over the outcomes of m; if R is the ring of Booleans $\mathbb{B}$, it represents the possibility of obtaining each of the outcomes of m.

An **empirical model** for a measurement scenario $(L, \mathcal{M}, O)$ is a collection of distribution functions $\{\sigma_C \in \mathcal{D}_R\mathcal{E}(C)\}_{C\in\mathcal{M}}$. An empirical model is called **no-signalling** when for all $C, C' \in \mathcal{M}$

$$\sigma_C|_{C\cap C'} = \sigma_{C'}|_{C\cap C'}$$

When an empirical model σ is no-signalling, the restriction $\sigma_{C|_m}$ for $m \in L$ corresponds to the same probability distribution for each $C \in \mathcal{M}$. We will denote this distribution by σ_m. A quantum state can be expressed as a no-signalling empirical

model, but is not uniquely determined by one. A **state** is a label for an empirical model. There may be various states that correspond to the same empirical model. States that correspond to the same empirical model are **statistically equivalent states**.

An **empirical theory** comprises a measurement scenario $(L, \mathcal{M}, O)$, together with a set of states S and a function assigning an empirical model over $(L, \mathcal{M}, O)$ to each state in S. For simplicity, in this chapter we will elide the function and informally conflate states with the empirical models that they label. We will refer to empirical theories as tuples $(L, \mathcal{M}, O)$. A **global section** for the presheaf $\mathcal{D}_R\mathcal{E}$ is given by an indexed set $d = \{d^\sigma\}_{\sigma \in S}$, such that for each $\sigma \in S$, $d^\sigma \in \mathcal{D}_R\mathcal{E}(L)$ and we have the following equality

$$d^\sigma_m := d^\sigma_L|_m = \sigma_m \qquad\qquad \forall \sigma \in S$$

We define **contextuality of an empirical theory** as the non-existence of a global section for the presheaf $\mathcal{D}_R\mathcal{E}$.

Example 2.2.1 (Quantum Mechanics). The Hilbert space model for quantum mechanics gives rise to an empirical theory. The measurement labels correspond to POVMs; the measurement cover consists of maximal sets of joint measurement as in Definition 2.1.12; and states are given by density matrices, which determine the corresponding families of probability distributions according to the Born rule.

Example 2.2.2 (Quantum Mechanics 2). An alternative way to express the Hilbert space formalism as an empirical theory, is to take the projectors as measurement labels and sets of orthogonal projectors as the measurement cover. These sets form the ordinary measurements in the Hilbert space formalism. The outcome set of a measurement label is $\{0, 1\}$, where '1' represent the event that the image of the projector is the outcome of the measurement and '0' represents the event that it is not. The distributions σ_m are only non-zero on a section s that assigns a 1 to exactly one of the measurement labels in a measurement cover. Otherwise there would not be a unique outcome to the measurement m on the state σ.

We will usually interpret quantum mechanics as the empirical theory of example 2.2.1. However, we will see that the perspective of example 2.2.2 can be useful in specific situations.

2.3 Unifying Approaches

In this section, we will explore the relation between empirical theories, operational theories, and ontological representations. We establish a link between general equivalence-based contextuality and sheaf-theoretic contextuality. Specifically, we connect theo-

ries that admit no ontological representation that is simultaneously preparation non-contextual and measurement non-contextual according to equivalence-based formalism, and theories that admit no global section $d \in \mathcal{D}_{\mathbb{R}}(\mathcal{E}(L))$ in the sheaf-theoretic formalism, respectively.

Recall that we only consider operational theories where each joint measurement m corresponds to a chosen set of measurements $\{m_1, m_2, ..., m_N\}$, that satisfies the requirements of Definition 2.1.12. Any no-signalling empirical theory $A = (L_A, \mathcal{M}_A, S_A, O_A)$ corresponds to an operational theory $\mathscr{O}p(A) = (P_{\mathscr{O}p(A)}, M_{\mathscr{O}p(A)}, D_{\mathscr{O}p(A)}, O_A)$ defined below.

$$
\begin{aligned}
P_{\mathscr{O}p(A)} &:= S_A \\
M_{\mathscr{O}p(A)} &:=\downarrow \mathcal{M}_A \\
d_{m,\sigma}(k) &:= \sigma_m(s) \qquad\qquad \text{for } s(m) = k
\end{aligned}
$$

Conversely, every set of preparation procedures P together with the set of distributions D gives rise to a set of states S; every set of measurement procedures M gives rise to the measurement cover $\mathcal{M}$, which consists of all maximal joint measurements. It gives rise to the set of measurement labels L, which is the set of all minimal joint measurements.

Remark 2.3.1. Signalling empirical theories cannot be described as operational theories. The reason is that operational theories are defined by their outcome statistics. While the 'same' measurement can have different outcome statistics in the empirical theory, depending on the context, in an operational theory, it can have only one outcome distribution for each preparation. One could get around it by treating restrictions of a context to a measurement as elementary measurements.

We will show that every sheaf-theoretic non-contextual empirical theory A gives rise to a non-contextual ontological representation for $\mathscr{O}p(A)$. We will call this a canonical ontological representation for the operational theory. Finally, we prove the theorem below, which connects sheaf-theoretic contextuality to equivalence-based contextuality. This theorem generalises the result in [AB11b], as well as Fine's Theorem [Fin82], to the more general setup of sheaf-theoretic contextuality in empirical theories and equivalence-based contextuality in operational theories.

Theorem 2.3.2. *The following statements are equivalent for any no-signalling empirical theory A and its corresponding operational theory* $\mathscr{O}p(A)$

(i) The empirical theory A admits a global section

(ii) The operational theory $\mathscr{O}p(A)$ *admits a canonical non-contextual ontological representation*

(iii) The operational theory $\mathcal{O}p(A)$ admits a factorizable non-contextual ontological representation

A Canonical Ontological Representation

As a warm-up, we recall the canonical ontological representation for empirical models with a global section d, which was introduced in [AB11b].

$$\Omega := \mathcal{E}(L) \qquad \mu_\sigma(s) := d(s) \qquad \xi_m(s)(k) := \delta_{s|_m(m),k}$$

This ontological representation is generally not non-contextual, for the reason set out below. Consider two statistically equivalent measurements $m \sim n$. While for each state σ the outcome distributions σ_m, σ_n over the local sections are the same, a global section s, may assign different outcomes to m and n. Suppose that s is a section of measurement outcomes such that $s|_m \neq s|_n$ for $m \sim n$, then $\xi_m(s)(k) \neq \xi_n(s)(k)$. Hence, $\xi_m \neq \xi_n$, which means that the ontological representation is contextual.

To get around this, we will prove that whenever a global section exists, we can find another global section that depends on equivalence classes of measurements only. It is not hard to see that the same holds for states.

Statistical Equivalence in Empirical Theories

We call two states $\sigma, \sigma' \in S$ and two measurement labels $m, m' \in L$ **statistically equivalent** when $\sigma_m = \sigma'_m$ for all $m \in L$ and $\sigma_m = \sigma_{m'}$ for all $\sigma \in S_A$, respectively. In that case we write $\sigma \sim \sigma'$ and $m \sim m'$.

Let $A = (L_A, \mathcal{M}_A, S_A, O_A)$ be an empirical theory. We construct a new empirical theory $\tilde{A} := (L_A/\sim, \mathcal{M}_A/\sim, \tilde{S}_A), O_A$ by taking the quotients of the set of measurement labels L_A and the measurement cover $\mathcal{M}_A$ by the equivalence relation. For each measurement label $[m]$ of $L_A/\sim$ and each section $s \in \mathcal{E}(m)$, we define a (not necessarily unique) section $\tilde{s}$, such that $\tilde{s}([m]) := s(m)$. Likewise, we define a section $\tilde{s}$ for each section s over an element of $\downarrow \mathcal{M}$. We take $\tilde{S}_A$ to be the set $\{\tilde{s} | s \in \mathcal{E}(m), m \in \downarrow \mathcal{M}\}$. The set $\tilde{S}_A$ is well-defined, because $[C] = [D]$ if and only if $\sigma_C = \sigma_D$ for each $\sigma \in S_A$.

Lemma 2.3.3. *Any empirical theory A admits a global section if and only if it admits a global section that only depends on equivalence classes of measurements of A.*

We will prove this Lemma formally in Section 2.4. Intuitively, it can be understood as follows: Any global section d of S_A can be restricted to a global section over a subset of L_A of representatives of $L_A/\sim$. This restriction defines a global section for

$\tilde{S}_A$. Conversely, any global section $\tilde{d}$ of $\tilde{A}$ defines a global section d for A, defined as $d(s) := \tilde{d}(\tilde{s})$ when s assigns the same value to all elements of an equivalence class, and $d(s) := 0$ otherwise.

We have shown how to deal with equivalence on the level of measurements. However, individual outcomes of measurements can be statistically equivalent, even when the measurements as a whole are not. This means that for some $s \in O^m$ and $s' \in O^{m'}$, $\sigma_m(s) = \sigma_{m'}(s')$ for all $\sigma \in S_A$. To eliminate this last form of statistical redundancy, we rewrite any such system type A as a system type A' with outcome set $\{0, 1\}$, as laid out in example 2.2.2. The measurement labels of A' are given by the individual measurement outcomes for each experiment. We denote each measurement label by a tuple (m, k) of a measurement and an outcome, so $L_{A'} := \{(m, k)\}_{m \in L_A, k \in O}$. The measurement cover is given by the sets of measurement outcomes of measurements in the original cover: $\mathcal{M}_{A'} := \{\{(m, k) | k \in O, m \in C\}_{C \in \mathcal{M}_A}\}$. Joint measurements are defined analogously. The outcomes 0 and 1 indicate whether the outcome corresponding to the observable is observed, hence $S_{A'} := \{\sigma' | \sigma'_{(m,k)}(1) = \sigma_m(k)\}$. Recall that the support $\mathcal{E}(m)$ of each measurement m consists of those sections where exactly one observable in each measurement is assigned a 1, and all others are assigned a 0.

Note that the model A has a global section if and only if A' has a global section under the given restrictions. As a consequence of Lemma 2.3.3, A has a global section if and only if $\tilde{A}'$ has a global section. Hence, A contains a global section induced by a global section d for $\tilde{A}'$, which is only defined on equivalence classes.

Non-contextual Canonical Ontological Representations

We can now define a canonical ontological representation that preserves non-contextuality. Let A be an empirical theory with a global section d_σ for each state $\sigma \in S_A$, which only depends on the equivalence classes of the preparations. We make use of the minimal empirical theory $\tilde{A}'$ and its induced global sections $\tilde{d}_{\tilde{\sigma}}$ to define the canonical ontological representation $\mathscr{R}(A) = (\Omega_A^{NC}, \{\mu_\sigma^{NC}\}_{\sigma \in S_A}, \{\xi_m^{NC}\}_{m \in \downarrow \mathcal{M}})$:

$$\Omega_{\mathscr{R}(A)} := \mathcal{E}(L/\sim), \qquad \mu_\sigma^{NC}(s) := \tilde{d}_{\tilde{\sigma}}(\tilde{s}), \qquad \xi_m^{NC}(s)(k) := \begin{cases} \delta_{\tilde{s}([m]),[k]} & \text{if s is a section over m} \\ 0 & \text{otherwise} \end{cases}$$

This representation generates the required outcome statistics, as shown below.

$$\begin{aligned}\sum_{s\in\Omega_A^{NC}} \mu_\sigma^{NC}(s)\xi_m^{NC}(s)(k) &= \sum_{\tilde{s}\in\mathcal{E}(L/\sim)} \tilde{d}_{\tilde{\sigma}}(\tilde{s})\delta_{\tilde{s}|_{[m]}([m]),[k]} \\ &= \sum_{s\in\mathcal{E}(L)} d_\sigma(s)\delta_{s|_m(m),k} \\ &= d^A_{\sigma,m}(k)\end{aligned}$$

The first equality holds by unfolding definitions of the canonical representation. The second equality holds because $d_\sigma(s)$ is only nonzero on those sections s that assign the same outcome to all equivalent measurements; therefore, we can extend the sum over $\mathcal{E}(L/\sim)$ to the sum over $\mathcal{E}(L)$. The last equality holds as both expressions are equal to $\sigma_m(s)(k)$.

This canonical ontological representation is by definition preparation non-contextual. On measurements, it is defined such that $m \sim m'$ implies $\xi_m^{NC} = \xi_{m'}^{NC}$; hence it is measurement non-contextual.

It is left to determine under which conditions an operational theory can be realised by a non-contextual empirical theory. To this end, we generalise Theorem 8.1 of [AB11b].

Lemma 2.3.4. *For every factorizable, non-contextual ontological representation B, there exists an empirical theory A with a global section, such that $\mathscr{R}(A)$ and B realise the same operational theory.*

Proof. Let B be a factorizable, measurement non-contextual ontological representation. The operational theory realised by B induces an empirical theory A where the set of measurement labels L_A of A is given by the minimal elements of the preorder of joint measurements. By Lemma 2.1.14, B is parameter independent. Every preparation $p \in P_B$ realises a state σ_p with a global section d_p for the sheaf of distributions induced by A. These are defined below for $r \in \mathcal{E}(m)$ and $s \in \mathcal{E}(L)$:

$$\sigma_p(r) := \sum_{\lambda\in\Omega_B} \xi_m(\lambda)(r(m))\mu_P(\lambda) \qquad d_p(s) := \sum_{\lambda\in\Omega_B} \prod_{m\in L_A} \xi_m(\lambda)(s|_m(m))\mu_P(\lambda) \tag{2.3.5}$$

We need to verify that $\mathscr{R}(A)$ and B realise the same measurement statistics. This follows from the equalities below, where we denote the canonical ontological representation by Ω'_A, μ', and ξ'.

$$\begin{aligned}
\sum_{\tilde{s}\in\Omega'_A} \xi'_m(\tilde{s})(k)\mu'_p &= \sum_{\tilde{s}\in\mathcal{E}(L_A/\sim)} \delta_{\tilde{s}|_{[m]}([m]),[k]}\left[\tilde{d}_{\tilde{\sigma}_P}(\tilde{s})\right] \\
&= \sum_{s\in\mathcal{E}(L_A)} \delta_{s|_m(m),k}\left[\sum_{\lambda\in\Omega_B}\prod_{n\in L_A}\mu_p(\lambda)\xi_n(\lambda)(s|_n(n))\right] \\
&= \sum_{\lambda\in\Omega_B} \xi_m(\lambda)(k)\left[\sum_{s\in\mathcal{E}(L_A\setminus m)}\prod_{n\in L_A\setminus m}\xi_n(\lambda)(s|_n(n))\right]\mu_p(\lambda) \\
&= \sum_{\lambda\in\Omega_B} \xi_m(\lambda)(k)\mu_p(\lambda)
\end{aligned}$$

The first two equalities result from expanding definitions. For the third, we apply the discrete version of Fubini's theorem, split the sum and product, and rewrite the expression. The last equality holds because probability distributions sum to one over all the inputs. □

Proof of Theorem 2.3.2. For any empirical theory A, the canonical non-contextual ontological representation for $\mathscr{O}p(A)$ is given by $\mathscr{R}(A)$, which means that 1) $\Rightarrow$ 2). The canonical ontological representation $\mathscr{R}(A)$ is factorizable; therefore, 2) $\Rightarrow$ 3). Finally, 3) $\Rightarrow$ 1) holds by Lemma 2.3.4. □

Corollary 2.3.6. *For the class of perfectly predictable operational theories with a maximally mixed preparation, an operational theory is non-contextual if and only if its canonical ontological representation is non-contextual.*

Proof. By Lemma 2.1.11, all preparation non-contextual ontological representations of operational theories in this class are outcome-deterministic. By Theorem 6 of [LSW11] that implies that all non-contextual ontological representations are factorizable. The result follows directly from Theorem 2.3.2. □

2.4 A Categorical Isomorphism

In this section, we show that the two formalisms can be used to represent the no-signalling world in equivalent ways. To give a formal proof, we use the mathematical framework of category theory. We show that the correspondence between no-signalling empirical theories, operational theories and ontological representations discussed in the previous section gives rise to functors between suitable categories. In particular, there is an isomorphism between the categories $\mathcal{E}mp_{ns}$ of no-signalling empirical theories and OT operational theories. This isomorphism maps non-contextual empirical theories to operational theories that admit a factorizable non-contextual ontological representation.

The Category of Empirical Theories

We will define the category $\mathcal{E}mp$ of empirical theories and transformations of empirical theories. The category $\mathcal{E}mp$ is an extension of the category of empirical models introduced in [AB11a].

Definition 2.4.1. A transformation of empirical theories $f : A \to B$ is given by a triple $f = (f^S, f^{\mathcal{M}}, f^O)$ of maps $f^S : S_A \to S_B$ between the set of states, $f^O : O_A \to O_B$ between the set of outcomes, respectively and a simplicial map $f^{\mathcal{M}} :\downarrow \mathcal{M}_A \to\downarrow \mathcal{M}_B$ between the simplicial sets generated by the measurement covers. This guarantees that the image of each joint measurement is a joint measurement itself. Since $f^{\mathcal{M}}$ is a simplicial map, it gives rise to a function $f^{\mathcal{M}}|_C : C \to f^{\mathcal{M}}(C)$ for each context $C \in \mathcal{M}$. The triple f should satisfy the equality below for all $C \in\downarrow \mathcal{M}$ and for each section $s \in \mathcal{E}(C)$.

$$\sigma_C(s) = f^S(\sigma)_{f^{\mathcal{M}}(C)}(s') \qquad \text{for } s' \in \mathcal{E}(f^{\mathcal{M}}(C)) \text{ such that } f^O \circ s = s' \circ f^{\mathcal{M}}|_C \quad (2.4.2)$$

Note that $f^O \circ s$ and $s' \circ f^{\mathcal{M}}|_C$ are both sections over C that take values in O_B. We write f for either of the three components when it is clear from the context which one we mean.

Lemma 2.4.3. *Let $f : A \to B$ be a transformation of empirical theories and let σ be a state of A. If σ does not admit a global section, then $f(\sigma)$ does not admit a global section.*

Proof. Suppose that $f(\sigma) \in B$ has a global section $\delta' \in D_R\mathcal{E}(L_B)$, then $\delta := \delta'|_{f(L_A)}$ is a section in $D_R\mathcal{E}(f(L_A))$ such that $\delta|_{C'} = f(\sigma)_{C'}$ for all $C' \in L_A$. This induces a global section for σ, given by $\gamma(s) = \delta|_{f(L_A)}(s')$ in $D_R(\mathcal{E}(L_A))$, where $s' \in \mathcal{E}(L_B)$ satisfies $s' \circ f^{\mathcal{M}}|_{L_B} = f^O \circ s$.

□

Note that it follows from Equation 2.4.2 and the notion of statistical equivalence **??**, that f preserves statistical equivalences.

$$m \sim m' \;\Rightarrow\; f(m) \sim f(m') \qquad \sigma \sim \sigma' \;\Rightarrow\; f(\sigma) \sim f(\sigma') \quad (2.4.4)$$

We can now prove the statement in Lemma 2.3.3, that any global section gives rise to a global section defined on equivalence classes.

Proof of Lemma 2.3.3. Consider the quotient map $A \xrightarrow{q} \tilde{A}$ and any inclusion map $\tilde{A} \xrightarrow{i} A$, which is defined such that $\tilde{\sigma}$ is mapped to σ. It is easy to see that q and i are morphisms in $\mathcal{E}mp_{ns}$. consequently, the proof follows from Lemma 2.4.3. □

Remark 2.4.5. Another way to define transformations between empirical theories is given in [AH13]. Here, empirical models are defined in terms of Chu spaces and the function on states goes in the opposite direction. By that definition, contextuality of states would only be preserved by transformations that are surjective on states.

In the rest of this paper we will restrict our attention to the subcategory $\mathcal{E}mp_{ns}$ of no-signalling empirical theories. We write $\mathcal{E}mp_{ns}^{NC}$ for the subcategory of non-contextual empirical theories.

The Category of Operational Theories

Operational theories form a category $\mathcal{O}t$. Morphisms are triples $f = (f^M, f^P, f^O) : A \to B$ of maps, such that $f^M : M_A \to M_B$, $f^P : P_A \to P_B$ and $f^O : O_A \to O_B$ preserve outcome statistics:

$$d_{f^P(p),f^M(m)}(f^O(k)) = d_{p,m}(k) \tag{2.4.6}$$

As a consequence, morphisms in $\mathcal{O}t$ preserve statistical equivalence:

$$m \sim m' \Rightarrow f(m) \sim f(m') \qquad p \sim p' \Rightarrow f(p) \sim f(p') \tag{2.4.7}$$

One can see this by combining the notion of statistical equivalence **??** with equation 2.4.7. This category is similar to the category of operational theories defined in [AH13].

The Category of Ontological Representations

Objects in the category $\mathcal{O}R$ of ontological representations correspond to a pair of an ontological representation and its induced operational theory. Morphisms consist of triples (f, f^μ, f^ξ), where $f : A \to B$ is a morphism of operational theories, and $f^\xi : \xi \mapsto \xi'$ and $f^\mu : \mu \mapsto \mu'$ are functions of sets. We require that the image of (f, f^μ, f^ξ) realises the operational theory in the image of f. This means that the images of the elements of μ and ξ coincide with the elements corresponding to the images of f^P and f^M. We express this as $f^\mu(\mu_p) = f^\mu(\mu)_{f^P(p)}$ and $f^\xi(\xi_m) = f^\xi(\xi)_{f^M(m)}$. In addition, one can deduce from equations 2.1.2 and 2.4.6 that the equality below holds.

$$\sum_{\lambda \in \Omega_B} f^\xi(\xi_m)(\lambda)(f^O(k)) f^\mu(\mu_p)(\lambda) = \sum_{\lambda \in \Omega_A} \xi_m(\lambda)(k)\mu_p(\lambda) \tag{2.4.8}$$

Remark 2.4.9. Note that the morphisms do not contain a component that maps between the sets of ontological values. This is because our goal is not to understand individual ontological representations, but to explore the existence of certain classes of ontological representations for operational theories.

There is a forgetful functor $G : \mathcal{OR} \to \mathcal{OT}$ that maps each ontological representation to its corresponding operational theory. More precisely, it maps (Ω, ξ, μ) to $(\{\mu_p\}_{p\in P}, \{\xi_m\}_{m\in M}, D, O)$, where $d_{p,m} := \sum_{\lambda\in\Omega} \mu_p(\lambda)\xi_m(\lambda)$. The elements μ_P and ξ_M no longer represent distribution functions, but merely label the preparations and measurements.

Lemma 2.4.10. *Contextuality of operational theories is preserved by morphisms in $\mathcal{OT}$*

Proof. Let $f : A \to B$ be a morphism of operational theories. Let $(\Omega_B, \{\mu_p\}_{p\in P_B}, \{\xi_m\}_{m\in M_B})$ be a non-contextual ontological representation of B. This induces an ontological representation $(\Omega_B, \{\mu'_p\}_{p\in P_A}, \{\xi'_m\}_{m\in M_A})$, which is defined as $\mu'_p := \mu_{fp}$, $\xi'_m := \xi_{fm}$. Non-contextuality of this ontological representation is guaranteed by the equivalence preservation condition on f. It follows by contradiction that when A is contextual, B must be contextual. □

The Isomorphism

The map $A \mapsto \mathscr{O}p(A)$ that assigns an operational theory to each no-signalling empirical theory described in Section 2.3 gives rise to the functor below.

$$\begin{aligned} \mathcal{E}mp_{ns} &\xrightarrow{\qquad\qquad\mathscr{O}p\qquad\qquad} \mathcal{OT} \\ A &\longmapsto \mathscr{O}p(A) \\ (f^S, f^{\mathcal{M}}, f^{O_A}) &\longmapsto (f^M, f^P, f^{O_{\mathscr{O}p(A)}}) \end{aligned}$$

Here, f^M is defined as the assignment of $f^{\mathcal{M}}$ on the 0-simplices of $\downarrow \mathcal{M}$, $f^P := f^S$ and $f^{O_{\mathscr{O}p(A)}} := f^{O_A}$, since $O_A = O_{\mathscr{O}p(A)}$. To verify that this is well-defined on morphisms, one needs to check that equation 2.4.6 holds. This follows directly from equation 2.4.2. Functoriality is straightforward.

Proposition 2.4.11. *The functor $\mathcal{E}mp_{ns} \xrightarrow{\mathscr{O}p} \mathcal{OT}$ is an isomorphism*

Proof. As discussed in section 2.3, the assignment is bijective on objects. To see that it is injective on morphisms, note that the simplicial map $f^{\mathcal{M}}$ is completely determined by its assignments on 0-simplices. Therefore, if $\mathscr{O}p(f^{\mathcal{M}}) = \mathscr{O}p(g^{\mathcal{M}})$, then $f^{\mathcal{M}} = g^{\mathcal{M}}$. Surjectivity follows from the fact that equation 2.4.2 implies equation 2.4.6. □

We will show that the isomorphism $\mathcal{E}mp_{ns} \xrightarrow{\mathscr{O}p} \mathcal{OT}$ maps non-contextual empirical theories to operational theories that admit a factorizable non-contextual ontological representation. In order to do so, we first examine how the canonical ontological representation described in Section 2.3 gives rise to an equivalence functor $\mathcal{E}mp_{ns}^{NC} \xrightarrow{\mathscr{R}} \mathcal{OR}$. This equivalence maps each non-contextual empirical model to its canonical non-contextual ontological representation, which is factorizable. We show that the composition $\mathcal{E}mp_{ns}^{NC} \xrightarrow{\mathscr{R}} \mathcal{OR} \to \mathcal{OT}$ of the equivalence with the forgetful functor equals $\mathcal{E}mp_{ns} \xrightarrow{\mathscr{O}p} \mathcal{OT}$ on the class of non-contextual empirical models.

Proposition 2.4.12. *For any choice of a global section δ, the assignment $A \mapsto \mathscr{R}(A)$ defines an equivalence between the subcategory of non-contextual empirical theories and the subcategory of non-contextual, factorizable ontological representations. The image $\mathscr{R}f = (\mathscr{O}p(f), (\mathscr{R}f)^{\mu}, (\mathscr{R}f)^{\xi})$ of each morphism $f = (f^S, f^{\mathcal{M}}, f^O)$ has the following components*

$$(\mathscr{R}f)^{\mu}(\sigma_m) := f\sigma_{f(m)}, \qquad (\mathscr{R}f)^{\xi}(\xi_m)(s)(k) := \delta_{s(f(m)),k}$$

Proof. We need to verify that for each $f : A \to B$ in $\mathcal{E}mp_{ns}$, $\mathscr{R}f : \mathscr{R}(A) \to \mathscr{R}(B)$ is a well-defined morphism in the category of ontological representations. By the following equations, $\mathscr{R}f$ satisfies equation 2.4.8.

$$\sum_{\lambda \in \Omega_{\mathscr{R}(A)}} \xi_m(\lambda)(k)\mu_\sigma(\lambda) = \sum_{\lambda \in \mathcal{E}(m)} \delta_{\lambda(m),k}\sigma_m(\lambda) \tag{2.4.13}$$

$$= \sum_{\lambda' \in \mathcal{E}(f(m))} \delta_{\lambda'(f(m)),f^O(k)} f\sigma_{f(m)}(\lambda') \tag{2.4.14}$$

$$= \sum_{\lambda' \in \Omega_{\mathscr{R}(B)}} Ff(\xi_m)(\lambda')(f^O(k))\mathscr{R}f(\mu_\sigma)(\lambda') \tag{2.4.15}$$

The equalities are obtained by unfolding definitions, application of equation 2.4.2 and rewriting the summation.

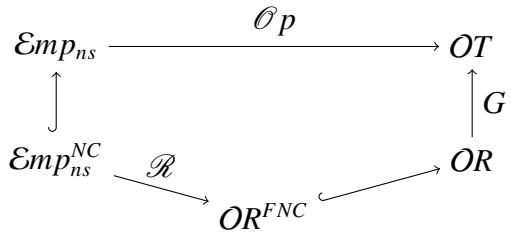
By Lemma 2.3.4, $\mathscr{R}$ is essentially surjective on the subcategory of factorizable non-contextual ontological representations. We will show that the functor $\mathscr{R}$ is injective on hom-sets. First of all, $\delta_{s(f(\{m\})),k} = \delta_{s(g(\{m\})),k)}$ for all $k \in O$ implies that $f^S = g^S$. Similarly, $\mathscr{R}(f)^{\mu} = \mathscr{R}(g)^{\mu}$ implies $f^{\mathcal{M}} = g^{\mathcal{M}}$. We will prove that F is surjective on hom-sets. Let $(g, g^{\mu}, g^{\xi}) : \mathscr{R}A \to \mathscr{R}B$ be a morphism in $\mathcal{OR}$. This corresponds to the morphism $g' : A \to B$ in $\mathcal{E}mp_{ns}$ with components $g'^{\mathcal{M}}(\{m\}) = g^M(m)$ and $g'^S(\sigma)_{g'^{\mathcal{M}}(\{m\})}(s) = g^P(\mu_\sigma)(s)$ for $s \in \mathcal{E}(m)$. Finally, to show that equation 2.4.7 holds, we take equation 2.4.8 and unfold the definitions of Ω_A, Ω_B, $g(\xi_M)$, and ξ_M. This gives us the equality below, which reduces to the second condition for transformations of empirical theories.

$$\sum_{s\in\mathcal{E}(m)} \delta_{s(m),k}\mu_\sigma(s) = \sum_{s\in\mathcal{E}(f(m))} \delta_{s(f(m)),k} g_\mu(\mu_\sigma)(s) \tag{2.4.16}$$

□

Theorem 2.4.17. *The isomorphism $\mathscr{O}p$ restricts to an isomorphism between the subcategory of non-contextual empirical theories and the subcategory of operational theories that do not admit a factorizable non-contextual ontological representation.*

Proof. Note that the following diagram commutes, where we write $\mathcal{E}mp_{ns}^{NC}$ and $\mathcal{O}R^{FNC}$ for the subcategories of non-contextual empirical theories and factorizable non-contextual ontological representations, respectively.



□

Corollary 2.4.18. *For models with perfectly predictable measurements and a maximally mixed preparation, $\mathscr{R}$ restricts to an isomorphism between non-contextual empirical theories and non-contextual operational theories.*

2.5 Non-Factorizable Representations and POVM's

In general, equivalence-based measurement contextuality implies sheaf-theoretic contextuality, but not necessarily the other way around. The two formalisms coincide in any scenario where factorizability can be justified, such as in the following three cases:

- For theories with perfectly predictable measurements and a maximally mixed preparation, non-contextuality of an ontological representation implies factorizability.
- Any non-local scenario rules out non-factorizable ontological representations, as these would violate local causality.

- In theories that do not contain joint measurements, the notion of factorizability is vacuous.

The following example, which is known as Specker's Triangle, shows that the two formalisms are not equal for all scenarios.

Example 2.5.1 (Specker's Triangle). There are three parties, A, B, C, that each conduct a measurement with two outcomes, $\{0, 1\}$. It is possible for two parties to apply the measurement at the same time, but it is not possible to apply all three measurements simultaneously. The measurement statistics is such that for any joint measurement, the obtained outcome is $(0, 1)$ half of the time, and $(1, 0)$, half of the time.

Lemma 2.5.2. *The scenario in Example 2.5.1 is contextual in the sheaf sense, but non-contextual in the equivalence-based sense*

Proof. The marginal probabilities for each of the individual measurements are $\frac{1}{2}$ for either of the outcomes. It follows that all measurements are statistically equivalent, and hence, should not be distinguishable on the ontological level. This means that we can define the set $\Omega := \{*\}$ to be a singleton set. We set $\mu_p(*) = 1$ for any preparation of this scenario, $\xi_m(*)(0) = \xi_m(*)(1) = \frac{1}{2}$ for each of the elementary measurements, and $\xi_m(*)(0, 1) = \xi_m(*)(1, 0) = \frac{1}{2}$, for each of the joint measurements. On the other hand, it is not possible to define a factorizable non-contextual ontological representation. It is easy to see this, since without loss of generality, any global section of measurement outcomes to the presheaf describing this scenario must assign the same outcome to measurement A and B. But that means that it does not marginalise to an admissible outcome for the joint measurement of A and B. □

This scenario cannot be realised by sharp measurements in quantum mechanics. However, one can find a POVM for each joint measurement that margnalises to the required outcomes: $(0 \cdot P_{0,0}, \frac{1}{2} \cdot P_{0,1}, \frac{1}{2} \cdot P_{1,0}, 0 \cdot P_{1,1})$, where $P_{i,j}$ is the projector onto outcome (i, j). Note however, that this POVM can be classically realised, by flipping a coin to decide between outcomes $(0, 1)$ or $(1, 0)$.

Whether such POVM's are within the scope of scenarios that are of interest is up for debate. As we have shown before, in the absence of perfect predictability or any convex structure, there is always a universal non-contextual ontological representation 2.1.4. Therefore, contextuality for scenarios like these is trivial. Perhaps a more restrictive notion of what a measurement can constitute would resolve the difference between the two notions of contextuality.

Chapter 3

Contextuality in Communication Complexity

In this section, we take a structural approach to clarify the role of contextuality in communication complexity of one-way protocols.

We use the sheaf-theoretic framework by Abramsky and Brandenburger to provide a general notion of classical and quantum communication protocols. This formulation allows one to determine the contextuality of a protocol. We draw from various results on sheaf-theoretic contextuality [AH12], [ABM17] [Wes17], [ABdSZ], to develop criteria that specify when a contextual protocol offers a communication complexity advantage.

This work reduces questions regarding the existence of quantum advantages in communication complexity to questions about the realisability of contextual scenarios in quantum mechanics. The question of realisability for a general empirical model in a Hilbert space of arbitrary finite dimension, or as a limit of realisations in finite dimensional Hilbert spaces, has been demonstrated to be undecidable [Slo17]. However, realisability is known for specific empirical models [ABC$^+$17], [ABCP17]. Solving this question for scenarios described in this paper would result in the discovery of new quantum protocols with optimal communication complexity.

Scientific Context

Communication complexity for 2-party distributed functions was introduced by Yao in [Yao79]. It is concerned with lower bounds on the required amount of communication between two parties that perform a distributed computation. In order to achieve this, the parties may perform local operations before communicating their respective output. We talk about classical communication complexity when the parties only have access to classical resources. This may include having an initial shared random bit string - a bit string that is stochastically generated by a probability distribution and a

classical computer. In the case of quantum communication complexity, the parties can also access quantum resources, such as (entangled) qubits. They may perform quantum operations and measurements on these qubits. In both scenarios, the parties communicate or broadcast classical bits. A different scenario, where the parties can communicate qubits, was proposed in [Yao93]. As one can perform the communication of a qubit by using a quantum teleportation protocol with an entangled state, this scenario is fundamentally the same. Some examples of quantum communication protocols have been proposed, which offer a communication complexity advantage over any classical protocol [BCW98] [CVDNT99] [BCVD01] [RK11], [BCG$^+$16]. A plausible explanation for this advantage lies in the strength of correlations between measurement outcomes of different qubits, which exceed those of shared random bit strings. Such correlations can increase the probability of some outcomes over others in a way that is not possible classically. Such correlations characterize non-locality scenarios, which suggest a connection between comunication complexity and non-locality. In fact, it was shown in [BCG$^+$16] that any two-party quantum protocol with a lower communication complexity than any classical protocol for the same functions gives rise to a non-locality scenario.

Communication Protocols

A **one-way communication complexity** protocol for n parties is set up as follows. Let $f : X_1 \times ... \times X_n \to Z$ be a function. The n different parties jointly want to compute the output $z = f(\mathbf{x})$ for an input $\mathbf{x} = (x_1, ..., x_n) \in X_1 \times ... \times X_n$, with minimal communication between the parties. The ith party only has access to the input $x_i \in X_i$. Each party can apply computations to their input and broadcast the output of these computations once. After broadcasting their output, all parties must be able to compute $f(\mathbf{x})$ with some minimal success probability P. This generalisation of one-way communication protocols between two parties by [Yao79], was used in [BvDHT99]. It should not be confused with Chandra and Ashok's "numbers on the forehead" model, where each party has knowledge of all inputs but their own [CFL83].

The **complexity of a communication protocol** corresponds to the minimum number of bits that each party needs to broadcast to complete the computation.

Definition 3.0.1. An **(n,i,o)- distributed function** is a function $f : X_1 \times ... \times X_n \to Z$, where $X_j = \{0,1\}^i$ for $j \in \{1, ..., n\}$ and $Z = \{0,1\}^o$, for some $n, i, o \in \mathbb{N}_+$. A k-bit **classical communication protocol (CCP)** for a (n,i,o)-function f is a tuple $(\mathbf{a}, g, d)$, where $\mathbf{a}$ is a set of functions $\{a_i : \Lambda_i \times X_i \to \{0,1\}^k\}_{i=1,...,n}$, g is a function $\{0,1\}^k \times ... \times$

$\{0,1\}^k \to Z$ and d is a probability distribution $d : \prod_{i=1}^n \Lambda_i \to [0,1]$. Each set Λ_i equals $\{0,1\}^l$, for some $l \in \mathbb{N}$.

The protocol is successful if $g(a_1(\lambda_1, x_1), ..., a_n(\lambda_n, x_n)) = f(x_1, ..., x_n)$ for some random bit string $\lambda = (\lambda_1, ..., \lambda_n) \in \Lambda = \prod_{i=1}^n \Lambda_i$, generated according to the distribution d. The success probability for each of the inputs can be computed by the formula below.

$$P_f^S(\mathbf{a}, g, d)(\mathbf{x}) = \sum_{\lambda \in \prod_{i=1}^n \Lambda_i : g(\lambda, \mathbf{x}) = f(\mathbf{x})} d(\lambda) \tag{3.0.2}$$

We say that the **success probability P_f^S of the protocol**$(\mathbf{a}, g, d)$ is defined as the average success probability below.

$$P_f^S(\mathbf{a}, g, d) := \frac{1}{|X|} \sum_{\mathbf{x} \in X} P_f^S(\mathbf{a}, g, d)(\mathbf{x})$$

Definition 3.0.3. Let ψ be an n-partite quantum state and let $\{\{P^i_{x_i}\}_{x_i \in X_i}\}_{i \in \{1,...,n\}}$ be a set of projective measurements, each with outcome set $O_i = \{0,1\}^k$. the set is indexed by the input x_i for each party i. A k-bit **quantum communication protocol (QCP)** is given by a tuple $(\psi, \{P^i_{x_i}\}_{i \in \{1,..,n\}, x_i \in X_i}, \mathrm{g})$.

For each input $\mathbf{x} = (x_1, ..., x_n)$, each party i applies $P^i_{x_i}$ to their part of the quantum state ψ and broadcasts the outcome o_i. The outcome of the protocol is then given by $g(o_1, ..., o_n)$ for some classical function $g : O_1 \times .... \times O_n \to Z$.

We can calculate the **success probability** from the probabilities of each of the measurement outcomes. Let $\mathrm{Prob}\left[(P^1_{x_1} \otimes P^2_{x_2} \otimes ... \otimes P^n_{x_n})(\psi) = \mathbf{o}\right]$ be the probability that the set of measurements $P^1_{x_1}, ..., P^n_{x_n}$ on the state ψ gives the outcome $\mathbf{o}$. The average success probability $P_f^S(\psi, \{P^i_{x_i}\}_{i \in \{1,..,n\}, x_i \in X_i}, g)$ of the protocol is given by the probability below.

$$P_f^S(\psi, \{P^i_{x_i}\}, g) := \frac{1}{|X|} \sum_{\mathbf{x} \in X^n} \sum_{\mathbf{o} \in O^n | f(\mathbf{x}) = g(\mathbf{o})} \mathrm{Prob}\left[(P^1_{x_1} \otimes P^2_{x_2} \otimes ... \otimes P^n_{x_n})(\psi) = \mathbf{o}\right] \tag{3.0.4}$$

Example 3.0.5. Fix $X = \{(\mathbf{x}, \mathbf{y}) \in \{0,1\}^2 \times \{0,1\}^2\}$, $f = x_1 \oplus y_1 \oplus (x_2 \wedge y_2)$ and $g(a_1, a_2) = a_1 \oplus a_2$. As shown in [BCVD01], there is a quantum protocol to compute this function with only one bit of communication per party and success probability $P^S = cos^2(\pi/8) = \frac{\sqrt{2+\sqrt{2}}}{2}$. The protocol is based on the non-locality scenario in [CHSH69], which allows one to compute the function $(x_2, y_2) \mapsto (o_1, o_2)$ in a distributed setting, such that $x_2 \wedge y_2 = o_1 \oplus o_2$ with success probability $\frac{\sqrt{2+\sqrt{2}}}{2}$. Subsequently, the parties broadcast $x_1 \oplus o_1$ and $y_1 \oplus o_2$. Finally, they compute $(x_1 \oplus o_1) \oplus (o_2 \oplus y_2)$.

The scenario that enables this distributed function is set up as follows: The two parties share the entangled state $\frac{1}{\sqrt{2}}(|00\rangle - |11\rangle)$. They are able to perform the following rotation to their qubit:

$$R(\theta) := \begin{pmatrix} cos\theta & -sin\theta \\ sin\theta & cos\theta \end{pmatrix}$$

The first party applies the $R(-\pi/16)$ if their second input is $x_2 = 0$ and $R(-3\pi/16)$ if their second input is $x_2 = 1$. The second party applies the $R(\pi/16)$ if their second input is $y_2 = 0$ and $R(3\pi/16)$ if their second input is $y_2 = 1$. Afterwards, they both measure in the computational basis. The state after the rotation is $\cos(\phi)^2(|00\rangle+|11\rangle)+\sin(\phi)^2(|01\rangle+|10\rangle)$ where $\phi = \pi/8$ for the input $(x_2, y_2) = (0,0), (x_2, y_2) = (1,0)$, $\phi = -\pi/8$ for the input $(x_2, y_2) = (0,1)$ and $\phi = 3\pi/8$ for the input $(x_2, y_2) = (1,1)$. The **probability table** below shows the probabilities that the two parties obtain each of the outcomes in the first row for each of the inputs in the first column. In this table, $p = \cos^2(\pi/8) = \frac{\sqrt{2+\sqrt{2}}}{2}$, which means that $1 - p = \frac{\sqrt{2-\sqrt{2}}}{2}$.

(x_2, y_2) \ (o_1, o_2)	(0,0)	(0,1)	(1,0)	(1,1)
$(0,0)$	$\frac{p}{2}$	$\frac{1-p}{2}$	$\frac{1-p}{2}$	$\frac{p}{2}$
$(0,1)$	$\frac{p}{2}$	$\frac{1-p}{2}$	$\frac{1-p}{2}$	$\frac{p}{2}$
$(1,0)$	$\frac{p}{2}$	$\frac{1-p}{2}$	$\frac{1-p}{2}$	$\frac{p}{2}$
$(01,1)$	$\frac{1-p}{2}$	$\frac{p}{2}$	$\frac{p}{2}$	$\frac{1-p}{2}$

One can check that for each pair of inputs (x_2, y_2) and each pair of outputs (o_1, o_2), the outcome probability is $\frac{\sqrt{2+\sqrt{2}}}{4}$ if $x_2 \wedge y_2 = o_1 \oplus o_2$ and it is $\frac{\sqrt{2-\sqrt{2}}}{4}$ if $x_2 \wedge y_2 \neq o_1 \oplus o_2$

Outline

In section 3.1 we describe a general notion of a communication protocol, using the sheaf-theoretic framework for contextuality by Abramsky and Brandenburger [AB11b]. We show that non-contextual protocols correspond to protocols that can be realised classically. In section 3.2 we use a connection between sheaf-theoretic contextuality and constraint satisfaction problems to describe a bound on the success probability of classical communication protocols. We give a description of contextual protocols with maximal success probability for each distributed function. In section 3.3 we give a complete characterization of the set of $(2, 2, 1)$-distributed functions where contextual protocols provide a communication complexity advantage. For (n, i, o)-functions, we can give a more abstract description of functions that admit a contextual communication

complexity advantage, in terms of hypergraph colouring problems. In Section 3.4, we quantify the relationship between the contextual fraction of a protocol - a measure for the amount of contextuality - and its success probability.

3.1 General Communication Protocols

We will describe communication protocols as scenarios in the sheaf-theoretic formalism of contextuality, introduced in Section 2.2. Observe that in a QCP, the individual input value of each party determines their choice of quantum measurement. The joint input values make up the different contexts of the individual measurements. We generalise this observation to describe a k-bit communication protocol (CP) of a function $f : X_1 \times ... \times X_n \to Z$ as a tuple (e, g), of a no-signalling empirical model e and a function $g : \prod_{i=1}^{n} \{0,1\}^k \to Z$. The measurement scenario for e is defined below.

$$
\begin{aligned}
L &= \sqcup_{i=1,...,n} X_i \\
\mathcal{M} &= \{\{x_1, ..., x_n\} | x_i \in X_i\} \\
O &= \{0, 1\}
\end{aligned}
$$

We write $X := X_1 \times ... \times X_n$. Note that we can identify every element $\mathbf{x} \in X$ with an element $\{x_1, ..., x_n\} \in \mathcal{M}$. For readability, we will denote the context $\{x_1, ..., x_n\}$ by $\mathbf{x}$. Every section s over a context $\mathbf{x} \in \mathcal{M}$ can be identified with a bit string $(s(x_1), ..., s(x_n))$, which we will denote by $s(\mathbf{x}) \in O^n$. The corresponding outcome distribution $e_{\mathbf{x}}(s)$ of the empirical model determines the probabilities of each bit string $s(\mathbf{x})$ to be broadcasted. The success probability $P_f^S(g, e)(\mathbf{x})$ of a communication protocol (g, e) for the input $\mathbf{x} \in X$ is the sum of the probabilities $e_{\mathbf{x}}(s)$ for those s such that $f(\mathbf{x}) = g(s(\mathbf{x}))$.

$$
P_f^S(g, e)(\mathbf{x}) = \sum_{\mathbf{x} \in X, s \in \mathcal{E}(\mathbf{x}) | f(\mathbf{x}) = g(s(\mathbf{x}))} e_{\mathbf{x}}(s)
$$

We can describe a QCP $(\psi, \{P^i_{x_i}\}_{i \in \{1,...,n\}, x_i \in X_i, g})$ as the empirical model defined below.

$$
e_{\mathbf{x}}(s) = \text{Prob}\left[(P^1_{x_1}, ..., P^n_{x_n})(\psi) = (s(x_1), ..., s(x_n)) \right] \tag{3.1.1}
$$

A CCP $(\mathbf{a}, g, d)$ can be described as an empirical model with outcome distributions given by the equation below, where Λ and $\mathbf{a}$ are as in Definition 3.0.1.

$$
e_{\mathbf{x}}(s) = \sum_{\lambda \in \Lambda : \mathbf{a}(\lambda, \mathbf{x}) = (s(x_1), ..., s(x_n))} d(\lambda) \tag{3.1.2}
$$

Example 3.1.3. The QCP in Example 3.0.5 corresponds to the measurement scenario with a set of measurement labels $L = \{0,1\}^2 \sqcup \{0,1\}^2$, a measurement cover $\mathcal{M} = \{\{x_1, x_2\}\}_{(x_1,x_2)\in X}$, and outcome set $O = \{0,1\}$. Note that we have switched from the notation $(\mathbf{x}, \mathbf{y}) \in X$ to the standard notation $(x_1, x_2) \in X$ for the input bit strings. The empirical model is expressed in the probability table below, where $p = \frac{\sqrt{2+\sqrt{2}}}{2}$. The entries $a_{(x_1,x_2),o}$, where $\{x_1, x_2\}$ is the context in the first column and o is the outcome in the first row, correspond to the probabilities $e_{\{x_1,x_2\}}(s)$ for the section s such that $s(\{x_1, x_2\}) = o$.

	(0,0)	(0,1)	(1,0)	(1,1)
(00, 00)	p/2	(1-p)/2	(1-p)/2	p/2
(00, 01)	p/2	(1-p)/2	(1-p)/2	p/2
(00, 10)	(1-p)/2	p/2	p/2	(1-p)/2
(00, 11)	(1-p)/2	p/2	p/2	(1-p)/2
(01, 00)	p/2	(1-p)/2	(1-p)/2	p/2
(01, 01)	(1-p)/2	p/2	p/2	(1-p)/2
(01, 10)	(1-p)/2	p/2	p/2	(1-p)/2
(01, 11)	p/2	(1-p)/2	(1-p)/2	p/2
(10, 00)	(1-p)/2	p/2	p/2	(1-p)/2
(10, 01)	(1-p)/2	p/2	p/2	(1-p)/2
(10, 10)	p/2	(1-p)/2	(1-p)/2	p/2
(10, 11)	p/2	(1-p)/2	(1-p)/2	p/2
(11, 00)	(1-p)/2	p/2	p/2	(1-p)/2
(11, 01)	p/2	(1-p)/2	(1-p)/2	p/2
(11, 10)	p/2	(1-p)/2	(1-p)/2	p/2
(11, 11)	(1-p)/2	p/2	p/2	(1-p)/2

In general, one can calculate the success probability of the communication protocol directly from its probability table. In order to do so, one sums over all entries $p_{\mathbf{x},o}$ of the probability table such that $f(\mathbf{x}) = g(o)$ and divides by the number of inputs. For the example above, this gives us $P^S = \frac{\sqrt{2+\sqrt{2}}}{2}$.

Proposition 3.1.4. *Let (e, g) be a k-bit CP for a (n,i,o)-function f. The empirical model e admits a global section, if and only if there exists a k-bit CCP $(\mathbf{a}, g, d)$ for f such that $P^S_f(g, e)(\mathbf{x}) = P^S_f(\mathbf{a}, g, d)(\mathbf{x})$ for all $\mathbf{x} \in X$.*

Proof. Recall that a CCP for a (n,i,o)-function $f : X \to Z$ corresponds to a set of functions $\{a_i : \Lambda \times X_i \to \{0,1\}^k\}_{i=1}^n$, a function $g : \{0,1\}^{k\times n} \to Z$ and a probability distribution $d : \Lambda \to [0,1]$; a CP corresponds to an empirical model e for the measurement scenario $L = \sqcup_{i=1}^n X_i$, $\mathcal{M} = \{\{x_1, ..., x_n\} | (x_1, ..., x_n) \in X\}$ and $O = \{0,1\}^k$ and a function $g : \prod_{i=1}^n \{0,1\}^k \to Z$; furthermore, any CCP (**a**, g, d) gives rise to a CP where $e_{\mathbf{x}}(s) = \sum_{\lambda\in\Lambda^n : a(\lambda,\mathbf{x})=(s(x_1),...,s(x_n))} d(\lambda)$.

We will first show that a CP with a global section gives rise to a CCP. Let e be an empirical model of a CP with a global section δ. Given some binary enumeration of the sections $s \in \mathcal{E}(X_i)$, we can define functions $a_i : \mathcal{E}(X_i) \times X_i \to \{0,1\}^k$ as $a_i(s, x_i) := s(x_i)$. To define the distribution $d : \prod_i \mathcal{E}(X_i) \to [0,1]$, note that every $s \in \mathcal{E}(\sqcup_{i=1}^n X_i)$ gives rise to a function $\mathbf{s} \in \prod_{i=1}^n \mathcal{E}(X_i)$, that maps each $\mathbf{x} \in X$ to $\mathbf{s}(\mathbf{x}) := (s(x_1), ..., s(x_n))$. We define the distribution d as $d(\mathbf{s}) := \delta(s)$ for each such $\mathbf{s}$ that can be obtained from some $s \in \mathcal{E}(\sqcup_{i=1}^n X_i)$ and $d(\mathbf{s}) := 0$ for all other functions $\mathbf{s} \in \prod_{i=1}^n \mathcal{E}(X_i)$. The success probability of $(\mathbf{a}, g, d)$ equals the success probability of (e, g) by the equations below, where we simply apply equations 3.0.2,3.1.2 and rewrite the summations. We write $s_o \in \mathcal{E}(\mathbf{x})$ for the specific section $s_o \in \mathcal{E}(\sqcup_{i=1}^n X_i)$, such that $(s_{\mathbf{o}}(x_1), ..., s_{\mathbf{o}}(x_n)) = \mathbf{o}$, for $\mathbf{o} \in \{0,1\}^{k \times n}$.

$$
\begin{aligned}
P^S(\mathbf{a}, g, d)(\mathbf{x}) &:= \sum_{\substack{\mathbf{s} \in \prod_{i=1}^n \mathcal{E}(X_i): \\ g(a_1(s_1,x_1),...,a_n(s_n,x_n)) = f(\mathbf{x})}} d(\mathbf{s}) \\
&= \sum_{\mathbf{o}: g(\mathbf{o}) = f(\mathbf{x})} \sum_{\substack{s \in \mathcal{E}(\sqcup_{i=1}^n X_i) \\ (s(x_1),...,s(x_n)) = \mathbf{o}}} \delta(s) \\
&= \sum_{\mathbf{o}: g(\mathbf{o}) = f(\mathbf{x})} \delta|_{\mathbf{x}}(s_o) \\
&= \sum_{\mathbf{o}: g(\mathbf{o}) = f(\mathbf{x})} e_{\mathbf{x}}(s_o) \\
&= \sum_{\substack{s \in \mathcal{E}(\mathbf{x}): \\ g(s(\mathbf{x})) = f(\mathbf{x})}} e_{\mathbf{x}}(s) \\
&:= P^S(e, g)(\mathbf{x})
\end{aligned}
$$

Conversely, we show that any CCP gives rise to a non-contextual, factorizable ontological representation in the equivalence-based sense of contextuality, defined in [Spe05] and[Wes17].

We consider the operational theory where $P = X$ and $M = \mathcal{P}(\{a_i\}_{i=1...n})$. The ontological representation, has a set of ontological states $\Omega = \{(\lambda, \mathbf{x})\}_{\mathbf{x} \in X, \lambda \in \Lambda}$. The distribution functions for the inputs are $\mu_{\mathbf{x}}(\lambda, \mathbf{y}) = \delta_{\mathbf{x},\mathbf{y}} d(\lambda)$. The distribution functions for the outputs are $\xi_{\mathbf{a}}(\lambda, \mathbf{x})(\mathbf{o}) = \delta_{\mathbf{a}(\lambda,\mathbf{x}),\mathbf{o}}$ and $\xi_{a_i}(\lambda, \mathbf{x})(o) = \delta_{a_i(\lambda,\mathbf{x}),o}$. This ontological representation is clearly non-contextual and factorizable by [Wes17, Definition 1]; therefore, it gives rise to a non-contextual empirical model with the same outcome statistics by Lemma 6 of [Wes17]. □

3.2 Bounding the Success Probability of Classical Protocols

In this section, we give a CP with optimal success probability for each distributed function f. Furthermore, we bound on the success probability of a non-contextual CP, based on the structure of the probability table of this optimal protocol.

Each probability table of an empirical model e gives rise to a **possibility table** for e. This is a table where the entries are either 0 or 1, indicating the possibility of obtaining the outcomes in the first row for the inputs in the first column. The entry $a_{\mathbf{x},o} = 1$, when $e_C(s) > 0$ for $s(\mathbf{x}) = o$, this means that the outcome o can be obtained for the input $\mathbf{x}$. Otherwise, $a_{\mathbf{x},o} = o$, which means we cannot obtain this outcome. The possibility table for an empirical model e corresponds to a different type of empirical model e', where the probability distributions $e_{\mathbf{x}}$ are replaced by distribution functions over the ring $\mathbb{B}$ of Booleans. This is called a **possibilistic empirical model**. If the empirical model e' is contextual, this implies that e is also contextual, but not necessarily vice versa.

We give a necessary and sufficient condition for a CP (g,e) to have maximal success probability $P_f^S(g, e) = 1$.

Lemma 3.2.1. *Let (g, e) be a communication protocol for a function f. The following two statements are equivalent:*

- $P_f^S(g, e) = 1$
- $e_{\mathbf{x}}(s) \geq 0 \Rightarrow f(\mathbf{x}) = g(s(\mathbf{x}))$

Proof. By the expression for the success probability $P_f^S(g, e)$ 3.1, $P_f^S(g, e) = 1$ if and only if for all $\mathbf{x} \in X$

$$\sum_{s \in \mathcal{E}(\mathbf{x}) | f(\mathbf{x}) = g(s(\mathbf{x}))} e_{\mathbf{x}}(s) = 1$$

This implies that $e_{\mathbf{x}}(s) = 0$ for all $s \in \mathcal{E}(\mathbf{x})$ such that $f(x) \neq g(s(\mathbf{x}))$. Hence, by contradiction, we know that $P_f^S(g, e) = 1$ if and only if $e'_{\mathbf{x}}(\mathbf{x})(\mathbf{o}) = 1 \Rightarrow f(\mathbf{x}) = g(\mathbf{o})$. □

Definition 3.2.2. Let $f : X_1 \times ... \times X_n \to Y$ be a distributed function. We define the possibilistic empirical model $e^{f,g}$ as

$$e_{\mathbf{x}}^{f,g}(s) = \begin{cases} 1, & \text{iff } f(\mathbf{x}) = g(s(\mathbf{x})) \\ 0, & \text{otherwise} \end{cases} \tag{3.2.3}$$

Note that for any probabilistic no-signalling empirical model e that gives rise to $e^{f,g}$, (e, g) is a CP for f with success probability 1. If $e^{f,g}$ is no-signalling, one can always find such an empirical model, by taking the uniform distribution over all sections $s \in \mathcal{E}(\mathbf{x})$ such that $e^{f,g}_{\mathbf{x}}(s) = 1$ for each $\mathbf{x} \in X$. However, $e^{f,g}$ is not necessarily no-signalling. When it is not, there exists no quantum realisation.

We can define any possibility table as a constraint satisfaction problem where we regard the measurement labels $m \in L$ as variables that take values $o \in O$ [ABdSZ]. For any section s, we can define the following constraint on the possible assignments of L.

$$\phi_s = \bigwedge_{o \in O} \bigwedge_{m \in C|s|_m(m)=o} (m == o)$$

If we take the section $s : (a, e) \mapsto (0, 0)$ in the upper left corner of the possibility table of Example 3.2.5below, we get $\phi_s = (a == 0) \wedge (e == 0)$. This constraint is satisfied by any assignment $r : L \to O$ such that $r(a) = 0$ and $r(e) = 0$.

The set of all possible sections over a context C, specified by the row of the table with label C, corresponds to the formula $\phi_C := \bigvee_{s \in \mathcal{E}(C)|\sigma_C(s)=1} \phi_s$. For the context (a, e) this corresponds to $(a == 0 \wedge e == 0) \vee (a == 1 \wedge e == 1)$.

The possibility table as a whole corresponds to the set of formulas for each of the contexts.

$$\Phi_e = \{\phi_C\}_{C \in \mathcal{M}} \tag{3.2.4}$$

For dichotomic measurements, we can write this as Boolean formulas, interpreting 0 as False and 1 as True.

$$\phi_s = \bigwedge_{m \in C|s|_m(m)=0} m \wedge \bigwedge_{m \in C|s|_m(m)=0} \neg m$$

For example, the first row of the table in the example below corresponds to $(a \wedge e) \vee (\neg a \wedge \neg e)$, which can be written more concisely as $a \leftrightarrow e$.

Example 3.2.5. The possibility table of the empirical model $e^{f,\oplus}$ for the function f in Example 3.0.5 is given below. We have relabelled the inputs $00, 01, 10, 11$ to a, b, c, d, respectively, for party 1 and to e, f, g, h, respectively, for party 2. One can check that $p_{\mathbf{x},o} = 1$ iff $f(\mathbf{x}) = g(o)$. Note that this empirical model is no-signalling. The table on the right of the possibility table contains the list of logical formulas defining the

restrictions corresponding to each of the rows.

$e^{f,\oplus}$	**(0,0)**	**(0,1)**	**(1,0)**	**(1,1)**	$\phi_{\mathbf{x}}$
(a,e)	1	0	0	1	$a \leftrightarrow e$
(a,f)	1	0	0	1	$a \leftrightarrow f$
(a,g)	0	1	1	0	$a \oplus g$
(a,h)	0	1	1	0	$a \oplus h$
(b,e)	1	0	0	1	$b \leftrightarrow e$
(b,f)	0	1	1	0	$b \oplus f$
(b,g)	0	1	1	0	$b \oplus g$
(b,h)	1	0	0	1	$b \leftrightarrow h$
(c,e)	0	1	1	0	$c \oplus e$
(c,f)	0	1	1	0	$c \oplus f$
(c,g)	1	0	0	1	$c \leftrightarrow g$
(c,h)	1	0	0	1	$c \leftrightarrow h$
(d,e)	0	1	1	0	$d \oplus e$
(d,f)	1	0	0	1	$d \leftrightarrow f$
(d,g)	1	0	0	1	$d \leftrightarrow g$
(d,h)	0	1	1	0	$d \oplus h$

(3.2.6)

We define the K**-consistency** $K(\Phi_e)$ as the cardinality of the largest subset $S \subset \Phi_e$ that is satisfiable. Every formula Φ_e gives rise to an inequality, as shown in [AH12, Proposition V.1]. This inequality is of the form below, where
$supp(C) := \{s \in \mathcal{E}(C) | \sigma_C(s) > 0\}$.

$$\sum_{C \in \mathcal{L}} \sum_{s \in supp(C)} e_C(s) \leq K(\Phi_e)$$

We bound the success probability of any CCP $(\mathbf{a}, g, d)$ for a function f by a measure of the 'hardness' of f compared to g. This is a function of the size of the input of f and the K-consistency of $\Phi_{e_{f,g}}$. Here, $e^{f,g}$ is the possibilistic empirical model that satisfies $e^{f,g}_{\mathbf{x}}(s) = 1 \Leftrightarrow f(\mathbf{x}) = g(s(\mathbf{x}))$. We denote the K-consistency by $K(f,g) := K(\Phi_{e^{f,g}})$. It follows that any k-bit CP (e, g) for f such that $P^S_f(e, g)$ is larger than this bound is contextual.

Lemma 3.2.7. *Let (e, g) be a non-contextual k-bit CP for the function f. The success probability of (e, g) is bounded by the inequality below.*

$$P^S_f(e, g) \leq \frac{K(g, f)}{|X|}$$

Proof. By Lemma 3.1.4, there exists a CP (e, g) with a global section such that $p^S_f(e, g) = P^S_f(\mathbf{a}, g, d)$. This follows from the (in)equalities below, where first is merely unfolding

the definition of the success probability and the inequality holds by Proposition V.1 of [AH12].

$$\begin{aligned}\sum_{\mathbf{x}\in X} P_f^S(e,g)(\mathbf{x}) &= \frac{1}{|X|} \sum_{\mathbf{x}\in X, s\in\mathcal{E}(\mathbf{x})|f(\mathbf{x})=g(s(\mathbf{x}))} e_{\mathbf{x}}(s) \\ &\leq \frac{1}{|X|} \sum_{\mathbf{x}\in X, s\in supp(e_{f,g})} e_{\mathbf{x}}^{f,g}(s) \\ &\leq \frac{1}{|X|} K(f,g)\end{aligned}$$

□

Solutions to constraint satisfaction problems are computable, but NP-hard. Therefore, Lemma 3.2.7 provides algorithmic methods for finding optimal classical protocols - if they exist. This may be useful for protocols with a small input. Most known quantum communication protocols have only single-digit numbers of input bits. Therefore, this new approach promises to be useful to extend our current knowledge of QCPs.

Example 3.2.8. We use Lemma 3.2.7 to demonstrate that the example in section 3.0.5 would have a lower success probability, were it not contextual. We regroup the logical formulas 3.2.6 in the sets of 4 below.

$$\begin{array}{llll} a\leftrightarrow e & b\leftrightarrow h & a\oplus g & c\oplus e \\ b\leftrightarrow e & c\leftrightarrow h & a\oplus h & c\oplus f \\ a\leftrightarrow f & c\leftrightarrow g & d\leftrightarrow g & d\leftrightarrow f \\ b\oplus f & b\oplus g & d\oplus h & d\oplus e \end{array} \tag{3.2.9}$$

Any valuation of the variables can only satisfy at most 3 out of the 4 formulas in each of the rows. Hence, the K-consistency is at most 12.

As a result of Lemma 3.2.7, the maximal success probability of any non-contextual CP $(e,\oplus)$ is $\frac{3}{4}$.

3.3 Functions With a Contextual Advantage

We will give a set of necessary conditions for (2,2,1)-functions f to ensure that contextual 1-bit CPs have an advantage over non-contextual 1-bit CPs. We generalise this statement to (n,i,o)-functions k-bit communication protocols. Lemma 3.2.7 tells us when a contextual CP (e,g) has an advantage over all non-contextual CP's (e',g). To verify that there is no non-contextual CP (e',g') with the same success probability, it seems that we need to check the consistency of $\Phi_{e^{f,g}}$ for all $g:\prod_{j=1}^{n}\{0,1\}^k\times\{0,1\}^k\to\{0,1\}^o$. However, it turns out that we can restrict this set drastically, as only the global structure of the functions g is of interest for our purpose.

Definition 3.3.1. We define the order $\prec$ on the set $\{g : O_1 \times ... \times O_n \to Z\}$ as $g' \prec g$ if $g' = g \circ (h_1, ..., h_n)$ for some tuple of functions $h_i : \{0,1\}^k \to \{0,1\}^k$. We denote $M_{\prec}(n,k,o)$ as the set of maximal elements of $\{g : \prod_{i=1}^{n}\{0,1\}^k \to \{0,1\}^o\}$ for the ordering $\prec$.

Lemma 3.3.2. *Let f be a (n,i,o)-distributed function. The inequality below holds for any k-bit CCP $(\mathbf{a}, g, d)$.*

$$P_f^S(\mathbf{a}, g, d) \leq \max_{g' \in M_{\prec}(n,k,o)\}} \frac{K(g', f)}{2^{in}}$$

Proof. Let $g, g' : O_1 \times ... \times O_n \to Z$ be functions such that $g' \prec g$ and let $(\mathbf{a}, g, d)$ be a CCP. The composition $(\mathbf{h} \circ \mathbf{a}, g, d)$ is another CCP. Since $g \circ \mathbf{h} = g'$. It follows that $P_f^S(\mathbf{a}, g', d) = P_f^S(\mathbf{h} \circ \mathbf{a}, g, d) \leq \frac{K(g,f)}{|X|}$.

Now we derive the inequalities below from Lemma 3.2.7.

$$\begin{aligned} P_f^S(\mathbf{a}, g, d) &\leq \max_{\substack{\mathbf{a}:\{0,1\}^i \times ... \times \{0,1\}^i \to \{0,1\}^o, \times \{0,1\} \\ g':\{0,1\}^k \times ... \times \{0,1\}^k \to \{0,1\}}} P_f^S(\mathbf{a}, g', d) \\ &\leq \max_{g' \{0,1\}^k \times ... \times \{0,1\}^k \to \{0,1\}} \frac{K(g', f)}{2^{in}} \\ &= \max_{g' \in M_{\prec}(n,k,o)} \frac{K(g', f)}{2^{in}} \end{aligned}$$

□

Any QCP that violates this bound offers a communication complexity advantage over all classical protocols, since any classical protocol will need more communication bits to achieve the same success probability.

Lemma 3.3.3. *Let f be a (2,i,1)- distributed function. The inequality below holds for any 1-bit CCP $(\mathbf{a}, g, d)$.*

$$P_f^S(\mathbf{a}, g, d) \leq \max_{g' :\in \{\oplus, \wedge, \vee\}} \frac{K(g', f)}{2^{i2}}$$

Proof. A simple case analysis based on the table below shows that for every $g : \{0,1\} \times \{0,1\} \to \{0,1\}$, one of the following three statements holds:

$$g \prec \oplus$$
$$g \prec \wedge$$
$$g \prec \vee$$

The columns of the table show the outcomes of each of the 16 functions in the set $\{g : \{0,1\} \times \{0,1\} \to \{0,1\}\}$ for each of the 4 inputs in the first row.

	F	$a \wedge b$	$a \wedge \neg b$	$a \wedge T$	$\neg a \wedge b$	$T \wedge b$	$a \oplus b$	$a \vee b$	$\neg a \wedge \neg b$	$a \leftrightarrow b$	$T \wedge \neg b$	$a \vee \neg b$	$\neg a \wedge T$	$\neg a \vee b$	$\neg a \vee \neg b$	T
00	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1
01	0	0	0	0	1	1	1	1	0	0	0	0	1	1	1	1
10	0	0	1	1	0	0	1	1	0	0	1	1	0	0	1	1
11	0	1	0	1	0	1	0	1	0	1	0	1	0	1	0	1

The rest follows immediately from Lemma 3.3.2. □

The result above characterizes the set of $(2, i, 1)$-distributed functions that admit a communication complexity advantage for contextual CPs, as a set of constraint satisfaction problems. We will reformulate this in terms of properties on a set of bipartite graphs. The graphs provide a visual illustration and allow us to deduce the sets of formulas $\Phi_{e^{f,g}}$ directly from the functions f and g without working out the possibility tables for $e^{f,g}$. From the graphs, we derive an explicit characterization of functions f that allow a communication complexity advantage for contextual CP's.

Note that for each g, the set $\Phi_{e^{f,g}}$ specified in equation 3.2.4 can be written as the union $\{\Phi_g^0(C)\}_{C\in\mathcal{M}|f(C)=0} \cup \{\Phi_g^1(C)\}_{C\in\mathcal{M}|f(C)=1}$, where for $i \in \{0,1\}$, $\Phi_g^i(C)$ is defined below.

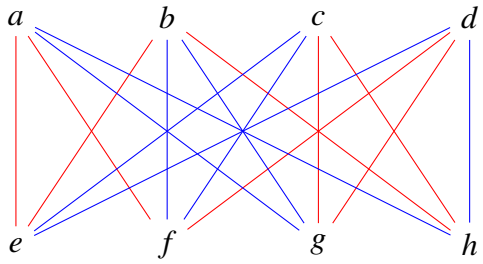
$$\Phi_g^i(C) = \bigvee_{\substack{s\in\mathcal{E}(C)\\ g(s(C))=i}} \phi_s \tag{3.3.4}$$

We will prove this in full generality in Lemma 3.3.7. Applying this expression to $g = \oplus, \wedge$ and $\vee$ gives us the following formulas:

$$\Phi_\oplus^0(a_i, b_j) = a_i \Leftrightarrow b_j \qquad \Phi_\oplus^1(a_i, b_j) = a_i \oplus b_j$$
$$\Phi_\wedge^0(a_i, b_j) = \neg a_i \vee \neg b_j \qquad \Phi_\wedge^1(a_i, b_j) = a_i \wedge b_j$$
$$\Phi_\vee^0(a_i, b_j) = \neg a_i \wedge \neg b_j \qquad \Phi_\vee^1(a_i, b_j) = a_i \vee b_j$$

For a fixed $f : X_1 \times X_2 \to \{0,1\}$ and g, the consistency of a set $\Phi_{e^{f,g}}$ corresponds to a colouring problem on a tuple of bipartite graphs (G_f^0, G_f^1) on the set $L = X_1 \cup X_2$ of vertices, where $(a_i, b_j) \in e(G_f^0)$ iff $f(a_i, b_j) = 0$ and $(a_i, b_j) \in e(G_f^1)$ iff $f(a_i, b_j) = 1$. The colouring problem is defined as follows: one needs to assign a 0 or a 1 to each vertex, such that for each edge $(a_i, b_j) \in e(G_f^0)$, the formula $\Phi_g^0(a_i, b_j)$ holds and for each edge $(a_i, b_j) \in e(G_f^1)$, the formula $\Phi_g^1(a_i, b_j)$ holds.

Example 3.3.5. The pair of bipartite graphs for the function $f : \{0,1\}^2 \times \{0,1\}^2 \to \{0,1\}$ where $f(a_1, a_2, b_1, b_2) = a_1 \oplus b_1 \oplus (a_2 \wedge b_2)$ in Section 3.0.5, is given below, as well as the derived sets of logical formulas for each of the functions $g = \oplus, \wedge, \vee$.



$\Phi_{f,\oplus}$		$\Phi_{f,\wedge}$		$\Phi_{f,\vee}$	
$a \leftrightarrow e$	$a \oplus g$	$\neg a \vee \neg e$	$a \wedge g$	$\neg a \wedge \neg e$	$a \vee g$
$a \leftrightarrow f$	$a \oplus h$	$\neg a \vee \neg f$	$a \wedge h$	$\neg a \wedge \neg f$	$a \vee h$
$b \leftrightarrow e$	$b \oplus f$	$\neg b \vee \neg e$	$b \wedge f$	$\neg b \wedge \neg e$	$b \vee f$
$b \leftrightarrow h$	$b \oplus g$	$\neg b \vee \neg h$	$b \wedge g$	$\neg b \wedge \neg h$	$b \vee g$
$c \leftrightarrow g$	$c \oplus e$	$\neg c \vee \neg g$	$c \wedge e$	$\neg c \wedge \neg g$	$c \vee e$
$c \leftrightarrow h$	$c \oplus f$	$\neg c \vee \neg h$	$c \wedge f$	$\neg c \wedge \neg h$	$c \vee f$
$d \leftrightarrow f$	$d \oplus e$	$\neg d \vee \neg f$	$d \wedge e$	$\neg d \wedge \neg f$	$d \vee e$
$d \leftrightarrow g$	$d \oplus h$	$\neg d \vee \neg g$	$d \wedge h$	$\neg d \wedge \neg g$	$d \vee h$

To show that the sets are inconsistent, we make the following observations:

- We can find closed loops of edges in G_f^0 and G_f^1, corresponding to the 4 groups of formulas 3.2.9. Each of these closed loops contains an odd number of edges in G_f^1. As a result, any attempt to colour such a subset leads to a contradiction. Therefore, $\Phi_{f,\oplus}$ is not satisfiable.

- The set $\Phi_{f,\wedge}$ is not satisfiable, as each blue edge forces both vertices in that edge to be 1, while each red edge forces at least one of the two vertices to be 0. Any blue edge is connected to a red edge through both of its vertices; hence, neither of the two vertices can be 1, which is a contradiction.

- For the set $\Phi_{f,\vee}$, we can give a similar argument. Now each red edge forces at least one of the two vertices to be 0, while each blue edge forces both vertices in that edge to be 1. Each blue edge is connected to red edges through each of the two vertices; hence, both vertices in the blue edge must be 0, which is a contradiction.

We generalize the observations above to give a set of necessary conditions for $(2, i, 1)$-distributed functions f, for which there is no contextual advantage in communication complexity. An inversion of the conditions provides neccessary conditions for functions that allow an advantage for contextual CPs.

Lemma 3.3.6. *The following three statements are equivalent for a* $(2, i, 1)$*−distributed function f:*

1) *There exists a non-contextual CP for* f *with maximal success probability.*

2) *The function f satisfies at least one of the following three requirements:*

   i *The function* f *is mod-2 linear: There exist* $c_1, c_2 \in \{0,1\}^i$ *such that* $f(a_i, b_j) = c_1 a_i + c_2 b_j (mod\ 2) \forall (a_i, b_j) \in X$.

   ii *The kernel Ker(f) is a product* $Ker(f) = X_1' \times X_2'$ *for some* $X_1' \subset X_1$, $X_2' \subset X_2$

   iii *The kernel Ker(f) is the complement of a product* $Ker(f) = X \backslash (X_1' \times X_2')$ *for some* $X_1' \subset X_1$, $X_2' \subset X_2$

3) *The pair of bipartite graphs* (G_f^0, G_f^1) *satisfies one of the following requirements:*

   i *Any closed loop of edges in* $e(G_f^0) \cup e(G_f^1)$ *has an even number of edges from each of the two graphs*

   ii *If* $(a_i, b_j) \in e(G_f^0)$ *then either*

   - $(a_i', b_j) \in e(G_f^0) \forall a_i' \in X_1$, *or*
   - $(a_i, b_j') \in e(G_f^0) \forall b_j' \in X_2$

   iii *If* $(a_i, b_j) \in e(G_f^1)$ *then either*

   - $(a_i', b_j) \in e(G_f^1) \forall a_i' \in X_1$, *or*
   - $(a_i, b_j') \in e(G_f^1) \forall b_j' \in X_2$

Proof of Lemma 3.3.6. First, we will prove that 1) $\Leftrightarrow$ 3). By Lemma 3.3.3, 1) holds iff $\Phi_{f,g}$ is consistent for $g = \oplus$, $g = \wedge$ or $g = \vee$. We show that each of the three cases is equivalent to one of the three conditions of 3).

i $\Phi_{f,\oplus}$ is satisfiable iff any closed loop of edges in $e(G_f^0) \cup e(G_f^1)$ has an even number of edges from each of the two graphs.
To see that this is true, note that every closed loop in a bipartite graph has an even number of edges, so it is sufficient to show that there is an even number of blue edges in each closed loop iff $\Phi_{f,\oplus}$ is satisfiable. A blue edge (a_i, b_j) implies that a_i and b_j must have different colour assignments. Since there are only two possible values, a closed loop with an odd number of blue edges leads to a contradiction. The result follows.

ii $\Phi_{f,\wedge}$ is consistent iff $(a_i, b_j) \in e(G_f^0)$ implies

- $(a'_i, b_j) \in e(G^0_f) \forall a'_i \in X_1$, or
- $(a_i, b'_j) \in e(G^0_f) \forall b'_j \in X_2$

To see this, note that $(a_i, b_j) \in e(G^0_f)$ implies $\neg a_i \vee \neg b_j$. If without loss of generality, for some b'_j, $(a_i, b'_j) \in e(G^1_f)$, then a_i must be 1. Hence, b_j must be 0, which implies that $(a'_i, b_j) \in e(G^0_f)$ for all $a'_i \in X_1$. Conversely, we assign 0 to a vertex if all edges containing the vertex are in G^0_f. We assign a 1 to all other vertices. This colouring satisfies $\Phi_{f,\wedge}$

iii $\Phi_{f,\vee}$ is consistent iff $(a_i, b_j) \in e(G^1_f)$ implies

- $(a'_i, b_j) \in e(G^1_f) \forall a'_i \in X_1$, or
- $(a_i, b'_j) \in e(G^1_f) \forall b'_j \in X_2$

To see this, note that $(a_i, b_j) \in e(G^1_f)$ implies $a_i \vee b_j$. If without loss of generality, if for some b'_j, $(a_i, b'_j) \in e(G^0_f)$, then a_i must be 0. Hence, b_j must be 1, which implies that $(a'_i, b_j) \in e(G^1_f)$ for all $a'_i \in X_1$. Conversely, we assign 1 to the vertices such that all edges containing the vertex are in G^1_f; we assign a 0 to all other vertices. This colouring satisfies $\Phi_{f,\vee}$.

Now we will prove that 3) $\Leftrightarrow$ 2) by showing that the three conditions for each of the statements are equivalent, respectively.

2)i $\Leftrightarrow$ 3)i For any closed loop, $L = \{(a_1, b_1), (a_2, b_1), (a_2, b_2), ..., (a_n, b_n), (a_1, b_n)\}$, the following equality holds for any $c_1, c_2 \in \{0, 1\}^i$, because each summand appears twice.

$$\sum_{(a_i,b_j)\in L} c_1 a_i + c_2 b_j (\text{mod } 2) = 0$$

It follows that $f(a_i, b_j) = 1$ for an even number of edges in this loop iff f is mod-2-linear. Since the total number of edges in a closed loop of a bipartite graph is even, this is the case iff there is an even number of edges in G^0_f and G^1_f.

2)ii $\Leftrightarrow$ 3)ii Unfolding definitions shows that 3)*ii* holds iff the kernel $Ker(f)$ is of the form $\bigcup_{i\in I}(a_i \times X_2) \cup \bigcup_{j\in J}(X_1 \times a_j)$. This is the case, iff $Ker(f) = X'_1 \times X'_2$ for some $X'_1 \subset X_1$ and $X'_2 \subset X_2$.

2)iii $\Leftrightarrow$ 3)iii Let f' be defined as $f' := f \oplus 1$, then 3)ii holds for f' iff 3)iii holds for f. By the argument above, this is the case iff $Ker(f') = X'_1 \times X'_2$ for some $X'_1 \subset X_1$ and $X'_2 \subset X_2$. The result follows from the observation that $Ker(f) = X \backslash Ker(f')$.

□

For general (n, i, o)-distributed functions, we provide an abstract description of the necessary set of functions that admit a contextual advantage for n-bit communication protocols. This description is in terms of colourings of sets of directed hypergraphs.

Every (n, i, o)-distributed function $f : X_1 \times ... \times X_n \to Z$ gives rise to a set of disjoint directed n-partite hypergraphs $\{G_f^z\}_{z \in Z}$. The set of nodes for the hypergraph corresponds to the set of measurement labels $L := \cup_{i=1}^n X_i$. The set of directed hyperedges for each graph G_f^z corresponds to $\{(x_1, ..., x_n) \in X | f(x_1, ..., x_n) = z\}$. The union of these hypergraphs forms a complete n-partite hypergraph on L. For each edge $\mathbf{x} \in G_f^z$, we have a formula $\Phi_g^z(\mathbf{x})$. The **K-consistency** $K(G_f, \Phi_g)$ is the number of edges of the largest subgraph G of the complete n-partite hypergraph on L, such that there exists a colouring $c : L \to \{1, .., 2^k\}$ for which $\Phi_g^z(\mathbf{x})$ holds for every hyperedge $\mathbf{x}$ of G in G_f^z and for every $z \in Z$.

Lemma 3.3.7. *Let $f : X \to Z$ be a (n, i, o)-distributed function. The following equality holds for any $g : Y \to Z$.*

$$K(\Phi_{e^{f,g}}) = K(G_f, \Phi_g)$$

Proof. We can write the colouring problem of $\{G_f^z\}_{z \in Z}$ for the formulas $\{\Phi_g^z\}$ as the constraint satisfaction problem $\cup_{z \in Z} \{\Phi_g^z(\mathbf{x})\}_{\mathbf{x} \in e(G_f^z)}$. This is equivalent to $\Phi_{e^{f,g}}$, as shown by the equations below. An analogous argument shows that a subgraph of $\cup_{z \in Z} \{G_f^z\}$ defines a subset of $\Phi_{e^{f,g}}$ and vice versa.

$$\begin{aligned}
\Phi_{e^{f,g}} &= \{\Phi_{\mathbf{x}}\}_{\mathbf{x} \in M} \\
&= \cup_{z \in Z} \{\Phi_{\mathbf{x}}\}_{\mathbf{x} \in \mathcal{M} | f(\mathbf{x}) = z} \\
&= \cup_{z \in Z} \{ \bigvee_{\substack{s \in \mathcal{E}(\mathbf{x})| \\ e_{\mathbf{x}}^{f,g}(s) \geq 0}} \phi_s \}_{\mathbf{x} \in \mathcal{M} | f(\mathbf{x}) = z} \\
&= \cup_{z \in Z} \{ \bigvee_{\substack{s \in \mathcal{E}(\mathbf{x})| \\ g(s(\mathbf{x})) = z}} \phi_s \}_{\mathbf{x} \in \mathcal{M} | f(\mathbf{x}) = z} \\
&= \cup_{z \in Z} \{\Phi_g^z(\mathbf{x})\}_{\mathbf{x} \in \mathcal{M} | f(\mathbf{x}) = z}
\end{aligned}$$

□

It follows that a function f admits a contextual advantage if the following two conditions are met. In that case, any CP (e, g') for any e that gives rise to the possibilistic empirical model $e^{f,g}$ attains the maximum contextual advantage.

(i) $\max_{g \in M_<(n,k,o))} \frac{K(G_f, \Phi_g)}{2^{in}} \leq 1$

(ii) The maximum $\max_{g \in M_{\prec}(n,k,o)} \frac{K(G_f, \Phi_g)}{2^{in}}$ is attained by a function g' such that $e^{f,g'}$ is no-signalling

3.4 Complexity Bounds From the Contextual Fraction

In this section we explore how the amount of contextuality in a communication protocol influences its success probability.

In [ABM17], the contextual fraction of an empirical model was introduced as a measure for the amount of contextuality. The authors show that an increase in the amount of contextuality corresponds to an increase in the success probability for probabilistic quantum protocols in measurement-based quantum computing, as well as for certain non-local games. Here, we will make a similar argument to show that an increase in contextuality of an empirical model corresponds to an increase in the upper bound of the success probability a corresponding quantum communication protocol. We will derive such a bound for the success probability of any k-bit CP (e, g) for a function f, based on the contextual fraction of e and the K-consistency $K(f, g)$

We call an empirical model **strongly contextual** if there exists no global section of measurement outcomes $s \in \mathcal{E}(L)$ in the support of e, which is defined as $supp(e) := \{s \in \mathcal{E}(\sigma_C(s|_C) > 0 \quad \forall C \in \mathcal{M}\}$. Any strongly contextual model is contextual, but not vice versa. Furthermore, strongly contextual models correspond to maximal violations of Bell-inequalities: by Proposition III.2 of [AH12], if $K(f, g) < 1$, then the inequality derived from and empirical model e is only maximally violated by a strongly contextual model. Hence, if $P_f^S(e, g) = 1$ and $\Phi_{e^{f,g}}$ is not consistent, then (e, g) must be strongly contextual.

The notion of the contextual fraction of an empirical model e is based on a convex decomposition $e = \lambda e^{NC} + (1 - \lambda)e^{SC}$, where e^{NC} is a non-contextual empirical model and e^{SC} is a strongly contextual empirical model. It was proven in [AB11b] that such a decomposition always exists, but may not be unique. The **non-contextual fraction** of the empirical model e is the maximum possible value λ for which such a decomposition exists. We denote the non-contextual fraction of e by $NCF(e)$. The **contextual fraction**, which we denote by $CF(e)$ is equal to $1 - NCF(e)$. Hence, we can decompose any empirical model e as $e = NFC(e)e^{NC} + CF(e)e^{SC}$ for some non-contextual empirical model e^{NC} and some strongly contextual empirical model e^{SC}.

Theorem 1. *Let (e, g) be a k-bit CP for a function f, such that $e^{f,g}$ is no-signalling. We have the following bound on the success probability of (e, g)*

$$P_f^S(e, g) \leq 1 - \frac{NCF(e)(|X| - K(f, g))}{|X|}$$

Proof. We know that $P^S(e^{NC}, g) \leq \frac{K(f,g)}{|X|}$, while $P^S(e^{SC}, g) \leq 1$. Following [ABM17][Theorem 4], we can bound the probability of failure $1 - P^S$ for an arbitrary protocol based on the amount of contextuality, as derived below. The inequality shows that one can improve the bound on the failure of a protocol by increasing the amount of contextuality

$$\begin{aligned}
1 - P^S(e, g) &= 1 - \Big(NCF(e)P^S(e^{NC}, g) + CF(e)P^S(e^{SC}, g)\Big) \\
&\geq 1 - \Big(NCF(e)\frac{K(f,g)}{|X|} + CF(e)\Big) \\
&= 1 - \Big(NCF(e)\frac{K(f,g)}{|X|} + (1 - NCF(e))\Big) \\
&= NCF(e) - NCF(e)\frac{K(f,g)}{|X|} \\
&= \frac{NCF(e)(|X| - K(f,g))}{|X|}
\end{aligned}$$

□

When the non-contextual fraction is 0, the upper bound for the protocol is 1. If the non-contextual fraction is bigger than 0, and $K(f,g) < |X|$, the upper bound is strictly smaller than 1. It follows that if we want to improve the success probability of a protocol, we need to decrease the non-contextual fraction, which means increasing the contextual fraction. We conclude that contextuality is the resource that enables quantum protocols to achieve an advantage in communication complexity.

Chapter 4

Constructing Symmetric Monoidal Bicategories Functorially

We turn our attention away from contextuality to study the nature of general quantum protocols. Our aim is to develop the mathematical foundation proposed by the author in [Wes13] for the higher categorical semantics for quantum protocols introduced in [Vic12].

Specifically, we will establish the existence of a symmetric monoidal structure for bicategories underlying the semantics, and functors between them. This allows for the description of compound and parallel protocols and guarantees that compound protocols are preserved by transformations between different models. The definition of a symmetric monoidal bicategory [GPS95, Gur06, KV94b, KV94a, BN96, DS97, Cra98, McC00, Gur] is time-consuming to verify in any example, let alone a monoidal pseudo functor, monoidal transformation or a monoidal modification. Double categories, on the other hand, are hardly more difficult to construct than symmetric monoidal categories. Therefore, we make use of the method developed in [Shu10] to construct symmetric monoidal bicategories from symmetric monoidal double categories and extend it to pseudo functors, pseudo natural transformations and modifications. The main result of [Shu10] is the following theorem:

Theorem (Theorem 1.2 of [Shu10])**.** *If $\mathbb{D}$ is a fibrant monoidal double category, then its underlying bicategory $\mathcal{L}(\mathbb{D})$ is a monoidal bicategory. If $\mathbb{D}$ is braided or symmetric, so is $\mathcal{L}(\mathbb{D})$.*

In this chapter, which is based on joint work with Michael Shulman, we improve and extend this theorem to the one below. We make use of locally cubical bicategories, which are bicategories enriched in the bicategory $\mathcal{D}bl$ of double categories. This is the simplest higher categorical structure containing monoidal bicategories, monoidal pseudo functors, monoidal pseudo transformations and monoidal modifications.

Our result provides a method for constructing pseudofunctors, pseudo transformations and modifications between bicategories from their double categorical counter parts. The construction preserves all different kinds of composition possible in a locally cubical bicategory, as well as any braided, sylleptic and symmetric monoidal structure.

Theorem 4.0.1. *If $\mathbb{D}$ is a monoidal double category, of which the monoidal constraints have loosely strong companions and conjoints, then its underlying bicategory $\mathcal{L}(\mathbb{D})$ is a monoidal bicategory. If $\mathbb{D}$ is braided or symmetric, so is $\mathcal{L}(\mathbb{D})$. Furthermore, the assignment $\mathcal{L}$ extends to a functor of locally cubical bicategories, which preserves all monoidal structures as well as compositions.*

There are three versions of this result, depending on whether the functors and transformations are chosen to be lax, colax, or strong with respect to the monoidal structure. In fact, we derive the more abstract result that *any* product preserving functor of locally cubical bicategories preserves all braided, sylleptic and symmetric monoidal structure.

In §4.1 we review the definition given in [Shu10] of fibrant symmetric monoidal double categories and their loose bicategories. In addition, we define symmetric monoidal pseudo double functors and transformations. In §4.2 we show that $\mathcal{L}$ forms a product-preserving functor of locally cubical bicategories. In §4.3 we define monoidal structures abstractly on the elements of a locally cubical bicategory and show that monoidal objects and higher cells form a new locally cubical bicategory. The abstract notions generalise simultaneously the locally cubical bicategory of monoidal bicategories, as well as that of monoidal double categories. We prove that any product-preserving functor of locally cubical bicategories preserves all monoidal structures. We apply this result to the functor $\mathcal{L}$ to derive a functorial method for constructing braided and symmetric monoidal bicategories, pseudo functors, pseudo transformations and modifications.

4.1 Fibrant Symmetric Monoidal Double Categories

In this section, we recall notions of fibrant monoidal double categories and their corresponding bicategories from [Shu10]. We define braided, symmetric and monoidal double functors as well as braided, symmetric and monoidal transformations between them.

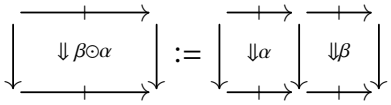
Definition 4.1.1. A **double category** $\mathbb{D}$ consists of the following elements:

- A pair of categories $\mathbb{D}_0, \mathbb{D}_1$,
- A *unit* functor $U\colon \mathbb{D}_0 \to \mathbb{D}_1$
- A *source* and *target* functor $S, T\colon \mathbb{D}_1 \rightrightarrows \mathbb{D}_0$
- A *composition* functor $\odot\colon \mathbb{D}_1 \times_{\mathbb{D}_0} \mathbb{D}_1 \to \mathbb{D}_1$ from the pullback over $\mathbb{D}_1 \xrightarrow{T} \mathbb{D}_0 \xleftarrow{S} \mathbb{D}_1$, that satisfies $S(U_A) = A$, $S(M \odot N) = SN$, $T(U_A) = A$, $T(M \odot N) = TM$, naturally.
- Natural isomorphisms called the *associator* $\alpha : (M \odot N) \odot P \xrightarrow{\cong} M \odot (N \odot P)$, the left *unitor* $\lambda : U_B \odot M \xrightarrow{\cong} M$, and the right *unitor* $\rho : M \odot U_A \xrightarrow{\cong} M$, such that $S(\alpha)$, $T(\alpha)$, $S(\lambda)$, $T(\lambda)$, $S(\rho)$, and $T(\rho)$ are identities, which satisfy the coherence axioms 1.2.1 1.2.2.

Let's unfold this definition. The double category contains **objects** or **0-cells**, which are the objects of $\mathbb{D}_0$; **tight 1-morphisms** $f\colon A \to B$, which are the morphisms of $\mathbb{D}_0$; **loose 1-cells** $M\colon A \nrightarrow B$, corresponding to the objects M of $\mathbb{D}_1$ with $S(M) = A$ and $T(M) = B$; **2-morphisms**, which correspond to a morphism $\alpha\colon M \to N$ of $\mathbb{D}_1$ with $S(\alpha) = f$ and $T(\alpha) = g$.

$$\begin{array}{ccc} A & \overset{M}{\nrightarrow} & B \\ {\scriptstyle f}\downarrow & \Downarrow\alpha & \downarrow{\scriptstyle g} \\ C & \underset{N}{\nrightarrow} & D \end{array} \tag{4.1.2}$$

We distinguish two different ways in which elements of a double category can be composed: **tight composition**, '$\circ$' of tight 1-morphisms $A \xrightarrow{f} B \xrightarrow{g} C$ and of 2-morphisms $M \xrightarrow{\alpha} N \xrightarrow{\beta} P$, given by composition in the respective categories. We write tight composition as $g \circ f$ and $\beta \circ \alpha$, or sometimes just gf and $\beta\alpha$; **loose composition**, '$\odot$' of 1-cells and 2-morphisms, which we write as $A \overset{N\odot M}{\nrightarrow} C := A \overset{M}{\nrightarrow} B \overset{N}{\nrightarrow} C$ and



Tight composition is strictly associative and unital, while loose composition is only weakly associative and unital. Tight and loose composition of 2-morphisms obey an interchange law, by the functoriality of $\odot$:

$$(M_1 \odot M_2) \circ (N_1 \odot N_2) = (M_1 \circ N_1) \odot (M_2 \circ N_2).$$

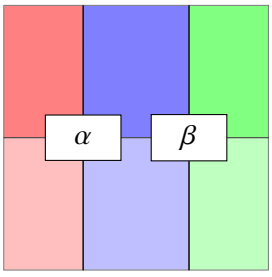
Every object A and every loose 1-cell has a tight *identity* 1_A and 1_M, respectively. This is the respective identity morphism in $\mathbb{D}_0$ and $\mathbb{D}_1$. Every object A and every tight 1-morphism f has a loose *unit* U_A, U_f. These are the images $U(A)$, $U(f)$, respectively. By funtoriality of U, we have the equality $1_{U_A} = U_{1_A}$.

Example 4.1.3. There is a double category $\mathbb{M}\mathsf{od}$ where the objects are rings, the tight 1-morphisms are ring homomorphisms, the loose 1-cells are bimodules, and the 2-morphisms are equivariant bimodule maps. Its loose bicategory $\mathcal{M}od = \mathcal{L}(\mathbb{M}\mathsf{od})$ is the bicategory of rings, bimodules and bimodule homomorphisms.

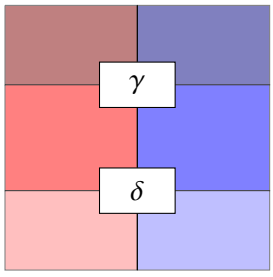
Example 4.1.4. There is a double category $\mathbb{P}\mathsf{rof}$ where the objects are categories, the tight 1-morphisms are functors, the loose 1-cells are *profunctors* (a profunctor $A \nrightarrow B$ is a functor $B^{op} \times A \to \mathbf{Set}$), and the 2-morphisms are natural transformations.

Sometimes it is useful to draw the Poincaré dual of the diagram [Mye16]. In these diagrams, the regions are objects, the vertical lines are 1-cells, the horizontal lines are 1-morphisms and the boxes are 2-morphisms. Below we depict loose and tight composition of 2-cells.

Loose composition



Tight composition



Every double category $\mathbb{D}$ has a **loose bicategory** $\mathcal{L}(\mathbb{D})$ consisting of the objects, loose 1-cells, and globular 2-morphisms, which are 2-morphisms (4.1.2) where f and g are identities. In the literature, this is often called the "horizontal" or "vertical" bicategory of a double category, depending on the direction in which the loose 2-cells are drawn. We have chosen to use the terms 'loose' and 'tight', to avoid any confusion that may arise from different diagrammatic conventions.

The diagrams corresponding to the loose bicategories have all the elements of the diagrams for double categories, without the horizontal lines. They correspond to the ones given in Equation 1.2.3 which generate the calculus for monoidal bicategories described in [BMS13].

Definition 4.1.5. Let $\mathbb{D}$ and $\mathbb{E}$ be double categories. A **pseudo double functor** $F\colon \mathbb{D} \to \mathbb{E}$ consists of the following elements:

- Two functors $F_0\colon \mathbb{D}_0 \to \mathbb{E}_0$ and $F_1\colon \mathbb{D}_1 \to \mathbb{E}_1$, which satisfy $S \circ F_1 = F_0 \circ S$ and $T \circ F_1 = F_0 \circ T$.
- Two globular natural isomorphisms $F_\odot\colon F_1 M \odot F_1 N \to F_1(M \odot N)$ and $F_U\colon U_{F_0 A} \to F_1(U_A)$, which satisfy coherence axioms 4.1.20, 4.1.21.

Composition of pseudo double functors is strictly associative and unital; hence, double categories form a category, which we denote by **Dbl**.

Definition 4.1.6. A **tight transformation** between two functors $\alpha : F \to G : \mathbb{D} \to \mathbb{E}$ consists of two natural transformations $\alpha_0\colon F_0 \to G_0$ and $\alpha_1\colon F_1 \to G_1$, such that $S(\alpha_M) = \alpha_{SM}$ and $T(\alpha_M) = \alpha_{TM}$, which satisfy the following equality for all 1-cells $M\colon A \nrightarrow B$, $N\colon B \nrightarrow C$ and for each object A.

$$
\begin{array}{ccc}
FA & \overset{FM}{\longmapsto} & FB \\
\| & \Downarrow F_\odot & \| \\
FA & \xrightarrow{F(N\odot M)} & FC \\
{\scriptstyle \alpha_A}\downarrow & \Downarrow \alpha_{N\odot M} & \downarrow{\scriptstyle \alpha_C} \\
GA & \underset{G(N\odot M)}{\longrightarrow} & GC
\end{array}
\overset{FN}{\longmapsto} FC
\quad = \quad
\begin{array}{ccc}
FA & \overset{FM}{\longmapsto} & FB \\
{\scriptstyle \alpha_A}\downarrow & \Downarrow \alpha_M & \downarrow{\scriptstyle \alpha_B} \\
GA & \underset{GM}{\longmapsto} & GB \\
\| & \Downarrow G_\odot & \| \\
GA & \underset{G(N\odot M)}{\longrightarrow} & GC
\end{array}
\overset{FN}{\longmapsto}
\begin{array}{c} FC \\ \Downarrow \alpha_N \\ \downarrow{\scriptstyle \alpha_C} \\ GC \end{array}
\qquad
\begin{array}{ccc}
FA & \xrightarrow{U_{FA}} & FA \\
\| & \Downarrow F_U & \| \\
FA & \xrightarrow{F(U_A)} & FA \\
{\scriptstyle \alpha_A}\downarrow & \Downarrow \alpha_{U_A} & \downarrow{\scriptstyle \alpha_A} \\
GA & \underset{G(U_A)}{\longrightarrow} & GA
\end{array}
\quad = \quad
\begin{array}{ccc}
FA & \xrightarrow{U_{FA}} & FA \\
{\scriptstyle \alpha_A}\downarrow & \Downarrow U_{\alpha_A} & \downarrow{\scriptstyle \alpha_A} \\
GA & \xrightarrow{U_{GA}} & GA \\
\| & \Downarrow G_U & \| \\
GA & \underset{G(U_A)}{\longrightarrow} & GA.
\end{array}
$$

We often drop the subscript and write α for either component of a tight transformation α_0, α_1. We write $\mathcal{D}bl$ for the 2-category of double categories, functors, and transformations.

Now, we recall the definition of a monoidal double category given in [Shu10].

Definition 4.1.7. A **monoidal double category** is a double category $\mathbf{D}$, equipped with the following data:

- A functor $\otimes\colon \mathbb{D} \times \mathbb{D} \to \mathbb{D}$, called the tensor product.
- A functor $I\colon * \to \mathbb{D}$, called the unit.
- Invertible tight transformations

  $\mathfrak{a} : \otimes \circ (\mathrm{Id} \times \otimes) \to \otimes \circ (\otimes \times \mathrm{Id})$, $\mathfrak{r} : \otimes \circ (\mathrm{Id} \times I) \to \mathrm{Id}$, $\mathfrak{l} : \otimes \circ (I \times \mathrm{Id}) \to \mathrm{Id}$, satisfying axioms 1.2.1 and 1.2.2.

A **braided monoidal double category** is a monoidal double category with a braiding isomorphism $\mathfrak{s} : \otimes \to \otimes \circ \tau$, where $\tau\colon \mathbb{D} \times \mathbb{D} \cong \mathbb{D} \times \mathbb{D}$ is the functor that maps $A \times B \mapsto B \times A$ and $f \times g \mapsto g \times f$. The braiding σ must satisfy the usual coherence axioms 1.2.14, 1.2.15.

A **symmetric monoidal double category** is a braided monoidal double category where the braiding is self-inverse.

Unfolding the definition tells us that a monoidal double category consists of two monoidal categories $\mathbb{D}_0$ and $\mathbb{D}_1$, such that U_I is the monoidal unit of $\mathbb{D}_1$[1], the functors S and T preserve the associativity and unit constraints and are strict monoidal, i.e. $S(M \otimes N) = SM \otimes SN$ and $T(M \otimes N) = TM \otimes TN$, and we have globular isomorphisms derived from $\otimes_\odot$ and $\otimes_U$

$$\mathfrak{x}\colon (M_1 \otimes N_1) \odot (M_2 \otimes N_2) \xrightarrow{\cong} (M_1 \odot M_2) \otimes (N_1 \odot N_2)$$

and

$$\mathfrak{u}\colon U_{A\otimes B} \xrightarrow{\cong} (U_A \otimes U_B)$$

such that the diagrams below commute.

$$\begin{array}{ccc}
((M_1 \otimes N_1) \odot (M_2 \otimes N_2)) \odot (M_3 \otimes N_3) & \xrightarrow{\mathfrak{x} \odot \mathrm{id}} & ((M_1 \odot M_2) \otimes (N_1 \odot N_2)) \odot (M_3 \otimes N_3) \\
\downarrow{\scriptstyle \mathfrak{a}} & & \downarrow{\scriptstyle \mathfrak{x}} \\
(M_1 \otimes N_1) \odot ((M_2 \otimes N_2) \odot (M_3 \otimes N_3)) & & ((M_1 \odot M_2) \odot M_3) \otimes ((N_1 \odot N_2) \odot N_3) \\
\downarrow{\scriptstyle \mathrm{id} \odot \mathfrak{x}} & & \downarrow{\scriptstyle \mathfrak{a} \odot \mathfrak{a}} \\
(M_1 \otimes N_1) \odot ((M_2 \odot M_3) \otimes (N_2 \odot N_3)) & \xrightarrow{\mathfrak{x}} & (M_1 \odot (M_2 \odot M_3)) \otimes (N_1 \odot (N_2 \odot N_3))
\end{array} \tag{4.1.8}$$

$$\begin{array}{ccc}
(M \otimes N) \odot U_{C\otimes D} & \xrightarrow{\mathrm{id} \odot \mathfrak{u}} & (M \otimes N) \odot (U_C \otimes U_D) \\
\downarrow{\scriptstyle \mathfrak{r}} & & \downarrow{\scriptstyle \mathfrak{x}} \\
M \otimes N & \xleftarrow{\mathfrak{r} \otimes \mathfrak{r}} & (M \odot U_C) \otimes (N \odot U_D)
\end{array} \tag{4.1.9}$$

$$\begin{array}{ccc}
U_{A\otimes B} \odot (M \otimes N) & \xrightarrow{\mathfrak{u} \odot \mathrm{id}} & (U_A \otimes U_B) \odot (M \otimes N) \\
\downarrow{\scriptstyle \mathfrak{l}} & & \downarrow{\scriptstyle \mathfrak{x}} \\
M \otimes N & \xleftarrow{\mathfrak{l} \otimes \mathfrak{l}} & (U_A \odot M) \otimes (U_B \odot N)
\end{array} \tag{4.1.10}$$

[1]It is sufficient that U_I is *isomorphic to* the monoidal unit of $\mathbb{D}_1$. However, we can choose the unit isomorphism $I_U : U_{I_{\mathbb{D}_0}} \to I_{\mathbb{D}_1}$ of the functor $I : * \to \mathbb{D}$ to be an identity, which makes U_I the monoidal unit.

$$\begin{array}{ccc}
((M_1 \otimes N_1) \otimes P_1) \odot ((M_2 \otimes N_2) \otimes P_2) & \xrightarrow{\mathfrak{a} \odot \mathfrak{a}} & (M_1 \otimes (N_1 \otimes P_1)) \odot (M_2 \otimes (N_2 \otimes P_2)) \\
\downarrow{\scriptstyle \mathfrak{x}} & & \downarrow{\scriptstyle \mathfrak{x}} \\
((M_1 \otimes N_1) \odot (M_2 \otimes N_2)) \otimes (P_1 \odot P_2) & & (M_1 \odot M_2) \otimes ((N_1 \otimes P_1) \odot (N_2 \otimes P_2)) \\
\downarrow{\scriptstyle \mathfrak{x} \otimes \mathrm{id}} & & \downarrow{\scriptstyle \mathrm{id} \otimes \mathfrak{x}} \\
((M_1 \odot M_2) \otimes (N_1 \odot N_2)) \otimes (P_1 \odot P_2) & \xrightarrow{\mathfrak{a}} & (M_1 \odot M_2) \otimes ((N_1 \odot N_2) \otimes (P_1 \odot P_2))
\end{array} \tag{4.1.11}$$

$$\begin{array}{ccc}
U_{(A \otimes B) \otimes C} & \xrightarrow{U_{\alpha_{A,B,C}}} & U_{A \otimes (B \otimes C)} \\
\downarrow{\scriptstyle \mathfrak{u}} & & \downarrow{\scriptstyle \mathfrak{u}} \\
U_{A \otimes B} \otimes U_C & & U_A \otimes U_{B \otimes C} \\
\downarrow{\scriptstyle \mathfrak{u} \otimes \mathrm{id}} & & \downarrow{\scriptstyle \mathrm{id} \otimes \mathfrak{u}} \\
(U_A \otimes U_B) \otimes U_C & \xrightarrow{\alpha_{U_A,U_B,U_C}} & U_A \otimes (U_B \otimes U_C)
\end{array} \tag{4.1.12}$$

$$\begin{array}{ccc}
(M \otimes U_I) \odot (N \otimes U_I) & \xrightarrow{\mathfrak{x}} & (M \odot N) \otimes (U_I \odot U_I) \\
\downarrow{\scriptstyle \rho_M \odot \rho_M} & & \downarrow{\scriptstyle \mathrm{id} \otimes \rho_{U_I}} \\
M \odot N & \xleftarrow{\rho_{M \odot N}} & (M \odot N) \otimes U_I
\end{array} \tag{4.1.13}$$

$$\begin{array}{ccc}
U_{A \otimes I} & \xrightarrow{\mathfrak{u}} & U_A \otimes U_I \\
& {\scriptstyle U_{\rho_A}} \searrow & \downarrow{\scriptstyle \rho_{U_A}} \\
& & U_A
\end{array} \tag{4.1.14}$$

$$\begin{array}{ccc}
(U_I \otimes M) \odot (U_I \otimes N) & \xrightarrow{\mathfrak{x}} & (U_I \odot U_I) \otimes (M \odot N) \\
\downarrow{\scriptstyle \lambda_M \odot \lambda_N} & & \downarrow{\scriptstyle \lambda_{U_I} \otimes \mathrm{id}} \\
M \odot N & \xleftarrow{\lambda_{M \odot N}} & U_I \otimes (M \odot N)
\end{array} \tag{4.1.15}$$

$$\begin{array}{ccc}
U_{I \otimes A} & \xrightarrow{\mathfrak{u}} & U_I \otimes U_A \\
& {\scriptstyle U_{\lambda_A}} \searrow & \downarrow{\scriptstyle \lambda_{U_A}} \\
& & U_A
\end{array} \tag{4.1.16}$$

Equations 4.1.8, 4.1.9 and 4.1.10 express that $\otimes$ is a pseudo double functor; equations 4.1.11 and 4.1.12 express that α is a tight transformation of double categories;

equations 4.1.13, 4.1.14, 4.1.15 and 4.1.16 express that the unit isomorphisms for $\otimes$ are transformations of double categories.

Similarly, a braided monoidal double category is a monoidal double category that consists of two braided monoidal categories $\mathbb{D}_0$ and $\mathbb{D}_1$, such that the functors S and T are strict braided monoidal and the diagrams below commute. These equations express that the braiding is a tight transformation of double categories.

$$\begin{array}{ccc} (M_1 \odot M_2) \otimes (N_1 \odot N_2) & \xrightarrow{\mathfrak{s}} & (N_1 \odot N_2) \otimes (M_1 \odot M_2) \\ \mathfrak{x} \uparrow & & \mathfrak{x} \uparrow \\ (M_1 \otimes N_1) \odot (M_2 \otimes N_2) & \xrightarrow{\mathfrak{s} \odot \mathfrak{s}} & (N_1 \otimes M_1) \odot (N_2 \otimes M_2) \end{array} \tag{4.1.17}$$

$$\begin{array}{ccc} U_A \otimes U_B & \xrightarrow{\mathfrak{u}} & U_{A \otimes B} \\ \mathfrak{s} \uparrow & & U_{\mathfrak{s}} \uparrow \\ U_B \otimes U_A & \xrightarrow{\mathfrak{u}} & U_{B \otimes A} \end{array} \tag{4.1.18}$$

Finally, a symmetric monoidal double category is a braided monoidal double category, such that $\mathbb{D}_0$ and $\mathbb{D}_1$ are symmetric monoidal.

We now move on to define functors and transformations of monoidal double categories.

Definition 4.1.19. Let $\mathbb{D}$, $\mathbb{E}$ be (braided/symmetric) monoidal double categories. A **(braided or symmetric) lax monoidal double functor** $F : \mathbb{D} \to \mathbb{E}$ is a pseudo double functor F, together with transformations $\phi : \otimes \circ (F, F) \to F \circ \otimes$ and $\phi_u : I_{\mathbb{E}} \to F \circ I_{\mathbb{D}}$ satisfying the usual axioms for (braided/symmetric) monoidal functors with respect to $\otimes$.

Unfolding the definitions tells us that F_0 and F_1 are (braided/symmetric) monoidal such that $F_0 \circ S_{\mathbb{D}} = S_{\mathbb{E}} \circ F_1$ and $F_0 \circ T_{\mathbb{D}} = T_{\mathbb{E}} \circ F_1$ are strict equalities of monoidal functors and the diagrams below commute.

$$\begin{array}{ccc} (FN \otimes FL) \odot (FM \otimes FK) & \xrightarrow{\phi \odot \phi} & F(N \otimes L) \odot F(M \otimes K) \\ \xi \downarrow & & F_{\odot} \downarrow \\ (FN \odot FM) \otimes (FL \odot FK) & & F((N \otimes L) \odot (M \otimes K)) \\ F_{\odot} \otimes F_{\odot} \downarrow & & F(\xi) \downarrow \\ F(N \odot M) \otimes F(L \odot K) & \xrightarrow{\phi} & F((N \odot M) \otimes (L \odot K)) \end{array} \tag{4.1.20}$$

$$\begin{array}{ccc} U_{FA\otimes FB} & \xrightarrow{U_\phi} & U_{F(A\otimes B)} \\ {\scriptstyle u}\downarrow & & \downarrow{\scriptstyle F_U} \\ U_{FA}\otimes U_{FB} & & F(U_{A\otimes B}) \\ {\scriptstyle F_u\otimes F_u}\downarrow & & \downarrow{\scriptstyle F\circ u} \\ F(U_A)\otimes F(U_B) & \xrightarrow{\phi} & F(U_A\otimes U_B) \end{array} \tag{4.1.21}$$

These diagrams express that ϕ is a transformation of double categories. When the natural transformations are in the opposite direction, the functor is **colax monoidal**, and when they are isomorphisms, the functor is **strong monoidal**.

Definition 4.1.22. Let $\mathbb{D}, \mathbb{E}$ be monoidal double categories and let $(F,\phi),(G,\psi) : \mathbb{D} \to \mathbb{E}$ be monoidal double functors. A **monoidal transformation** $\alpha : F \to G$ is a tight transformation such that α_0 and α_1 are monoidal natural transformations. Explicitly, this means (in the lax case) that the following equalities hold:

$$\begin{array}{ccc} FA\otimes FB & \overset{FM\otimes FN}{\longrightarrow} & FC\otimes FD \\ {\scriptstyle \phi_{A,B}}\downarrow & \Downarrow \phi_{M,N} & \downarrow{\scriptstyle \phi_{C,D}} \\ F(A\otimes B) & \overset{F(M\otimes N)}{\longrightarrow} & F(C\otimes D) \\ {\scriptstyle \alpha_{A\otimes B}}\downarrow & \Downarrow \alpha_{M\otimes N} & \downarrow{\scriptstyle \alpha_{C\otimes D}} \\ G(A\otimes B) & \underset{G(M\otimes N)}{\longrightarrow} & G(C\otimes D) \end{array} \quad = \quad \begin{array}{ccc} FA\otimes FB & \overset{FM\otimes FN}{\longrightarrow} & FC\otimes FD \\ {\scriptstyle \alpha_A\otimes\alpha_B}\downarrow & \Downarrow \alpha_M\otimes\alpha_N & \downarrow{\scriptstyle \alpha_C\otimes\alpha_D} \\ GA\otimes GB & \overset{GM\otimes GN}{\longrightarrow} & GC\otimes GD \\ {\scriptstyle \psi_{A,B}}\downarrow & \Downarrow \psi_{M,N} & \downarrow{\scriptstyle \psi_{C,D}} \\ G(A\otimes B) & \underset{G(M\otimes N)}{\longrightarrow} & G(C\otimes D) \end{array} \tag{4.1.23}$$

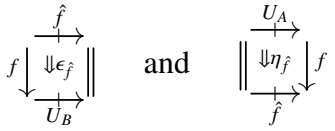
$$\begin{array}{ccc} I_{\mathbb{E}} & \xrightarrow{U_{I_{\mathbb{E}}}} & I_{\mathbb{E}} \\ {\scriptstyle \phi_{u_0}}\downarrow & \Downarrow \phi_{u_1} & \downarrow{\scriptstyle \phi_{u_1}} \\ F(I_{\mathbb{D}}) & \overset{F(U_{I_{\mathbb{D}}})}{\longrightarrow} & F(I_{\mathbb{D}}) \\ {\scriptstyle \alpha_{I_{\mathbb{D}}}}\downarrow & \Downarrow \alpha_{U_{I_{\mathbb{D}}}} & \downarrow{\scriptstyle \alpha_{I_{\mathbb{D}}}} \\ G(I_{\mathbb{D}}) & \underset{G(U_{I_{\mathbb{D}}})}{\longrightarrow} & G(I_{\mathbb{D}}) \end{array} \quad = \quad \begin{array}{ccc} I_{\mathbb{E}} & \xrightarrow{U_{I_{\mathbb{E}}}} & I_{\mathbb{E}} \\ {\scriptstyle \psi_u}\downarrow & \Downarrow \psi_{u_1} & \downarrow{\scriptstyle \psi_u} \\ G(I_{\mathbb{D}}) & \underset{G(U_{I_{\mathbb{D}}})}{\longrightarrow} & G(I_{\mathbb{D}}) \end{array} \tag{4.1.24}$$

A **braided or symmetric monoidal tight transformation** is a monoidal transformation between braided/symmetric monoidal functors.

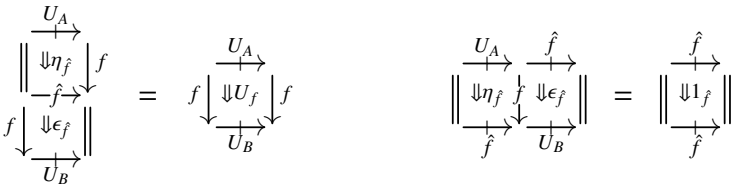
It is straightforward to verify that we have various 2-categories of monoidal double categories, depending on whether we take the objects to be braided, symmetric, or neither, and whether the morphisms are lax, colax, or strong.

The loose bicategory of a (symmetric) monoidal double category will in general not be symmetric monoidal, as the monoidal constraints are tight isomorphisms, which are discarded. In order to preserve (symmetric) monoidal structure, we need an appropriate way to turn such constraints into loose 2-cells. The following definition was given in [Shu10] for this purpose. The form of this definition is due to [GP04, DPP10], but the ideas date back to [BS76]; see also [BM99, Fio07]. In the terminology of these references, a *connection* on a double category is equivalent to a strictly functorial choice of a companion for each tight arrow.

Definition 4.1.25. A **companion** of a tight 1-morphism $f\colon A \to B$ in a double category $\mathbb{D}$ consists of a triple $(\hat{f},\ \epsilon_{\hat{f}},\ \eta_{\hat{f}})$, where $\hat{f}\colon A \nrightarrow B$ is a loose 1-cell and $\epsilon_{\hat{f}},\ \eta_{\hat{f}}$ are 2-morphisms of the form depicted below.



This data needs to satisfy the equalities below.



(4.1.26)

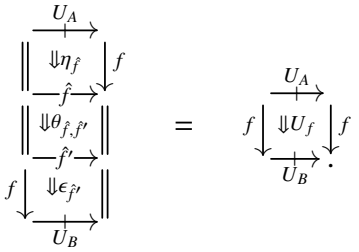
A **conjoint** $(\check{f}, \epsilon_{\check{f}}, \eta_{\check{f}})$ of f, is a companion of f in the double category $\mathbb{D}^{l\text{-op}}$. This is the category $\mathbb{C}$, with all loose 1-cells in the opposite direction; hence, $\check{f}$ is of the form $B \nrightarrow A$.

Note that the second equation in (4.1.26) requires an additional unit; we have left it out as we assume the double categories to be strict.

Definition 4.1.27. A double category is **fibrant** if every tight 1-morphism has a companion and a conjoint.

In [Shu10], it was shown that companions and conjoints give rise to a lifting from tight double transformations to loose 1-cells, which is unique up to isomorphism, canonical and coherent. We recall four lemmas, which we will use to prove that if **D** has sufficient companions and conjoints, the assignment $\mathcal{L} : \mathbb{D} \mapsto \mathcal{L}(\mathbb{D})$ lifts the monoidal structure functorially. These lemmas all have dual versions for conjoints.

Lemma 4.1.28. *Let $\hat{f}\colon A \nrightarrow B$ and $\hat{f}'\colon A \nrightarrow B$ be companions of f (that is, each comes* equipped with *2-morphisms as in Definition 4.1.25). Then there is a unique globular isomorphism $\theta_{\hat{f},\hat{f}'}\colon \hat{f} \xrightarrow{\cong} \hat{f}'$ such that*



(4.1.29)

We will often use this type of unique isomorphism, which we call a θ**-isomorphism**.

Lemma 4.1.30. *Suppose that $f\colon A \to B$ has a companion $\hat{f}$ and $g\colon B \to C$ has a companion $\hat{g}$. Then $\hat{g} \odot \hat{f}$ is a companion of gf.*

Lemma 4.1.31. *Let $F\colon \mathbb{D} \to \mathbb{E}$ be a functor between double categories and let $f\colon A \to B$ have a companion $\hat{f}$ in $\mathbb{D}$. Then $F(\hat{f})$ is a companion of $F(f)$ in $\mathbb{E}$.*

Lemma 4.1.32. *If $f\colon A \to B$ is a tight isomorphism with a companion $\hat{f}$, then $\hat{f}$ is a conjoint of its inverse f^{-1}.*

4.2 From Double Categories to Bicategories

In [Shu10], it was shown that the assignment $\mathcal{L} : \mathbb{D} \mapsto \mathcal{L}(\mathbb{D})$ on fibrant double categories gives rise to a trifunctor between the tricategory of double categories and the tricategory of bicategories. In this section, we show that it is in fact a *functor of locally cubical bicategories*. A locally cubical bicategory is a bicategory enriched in the 2-category $\mathcal{D}bl$ of double categories, double functors and tight transformations. In contrast, a tricategory is a bicategory enriched in the bicategory $\mathcal{B}icat$, which is a more complex structure, due to the additional coherence equations of the hom-bicategories.

In order to maintain consistency with the notation for double categories, we write the horizontal composition functor for bicategories as $\odot$. We make use of Theorem 4.1 and Theorem 4.6 of [Shu10], which we recall below. Here, $Conj(\mathcal{L}(\mathbb{D}), \mathcal{L}(\mathbb{E}))$ is the bicategory of pseudo functors from $\mathcal{L}(\mathbb{D})$ to $\mathcal{L}(\mathbb{E})$, conjunctional transformations and modifications. As discussed in Section 1.2.2, conjunctional transformations are merely lax natural transformations with a canonical choice of adjunction in the horizontal direction. When the tranformations are isomorphisms and the adjunctions are equivalences, this extra structure provides an explicit description of canonical horizontal inverses.

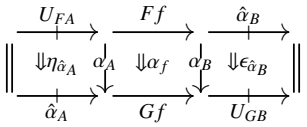
Theorem (Theorem 4.1 of [Shu10])**.** *If $\mathbb{D}$ is a double category, then $\mathcal{L}(\mathbb{D})$ is a bicategory, and any functor $F\colon \mathbb{D} \to \mathbb{E}$ induces a functor $\mathcal{L}(F)\colon \mathcal{L}(\mathbb{D}) \to \mathcal{L}(\mathbb{E})$. In this way $\mathcal{L}$ defines a functor of 1-categories* **Dbl** $\to$ **Bicat**.

Theorem (Theorem 4.6 of [Shu10])**.** *If $\mathbb{D}$ is a double category and $\mathbb{E}$ is a double category with chosen companions and conjoints for all transformations, we have a functor of bicategories*

$$\begin{aligned} \mathcal{D}bl(\mathbb{D}, \mathbb{E}) &\longrightarrow Conj(\mathcal{L}(\mathbb{D}), \mathcal{L}(\mathbb{E})) \\ F &\mapsto \mathcal{L}(F) \\ \alpha &\mapsto (\hat{\alpha} \prec \check{\alpha}). \end{aligned}$$

Moreover, if α is an isomorphism, then $\hat{\alpha} \prec \check{\alpha}$ is a pseudo natural adjoint equivalence.

In this result, the 1-category $\mathcal{D}bl(\mathbb{D}, \mathbb{E})$ is regarded as a bicategory with only identity 2-cells. The colax transformation $\hat{\alpha}$ is defined below, which has 1-cell components of the form $\hat{\alpha}_A := \widehat{\alpha_A}$.



(4.2.1)

The lax transformation $\check{\alpha}$ is defined using the data of the conjoint instead of the companion. All structure isomorphisms are constructed from the unique canonical isomorphisms between different companions of the same 1-morphism, Lemma 4.1.28.

While the theorem above relies on a choice of companions and conjoints, the resulting functor is unique up to equivalence, as shown in [Shu10, Theorem 4.8].

If the images $\hat{\alpha} \prec \check{\alpha}$ are pseudo natural adjoint equivalences, this pseudo functor can be upgraded to a functor of locally cubical bicategories. It is not sufficient for the images to be conjunctional transformations, as the interchange law does not hold strictly in this case. Therefore, we introduce the following definition.

Definition 4.2.2. We will say that a transformation α in $\mathcal{D}bl$ has **loosely strong companions and conjoints** if $\hat{\alpha}$ is a pseudo natural adjoint equivalence.

We write $\mathcal{D}bl_f$ for the sub-2-category of $\mathcal{D}bl$ containing the double categories, all functors between them, and only transformations with loosely strong companions. For the construction of (braided or symmetric) monoidal bicategories and pseudo functors, we only require the monoidal constraints to have loosely strong companions. As such constraints are isomorphisms by definition, this merely amounts to the existence of companions and conjoints for the monoidal constraints.

We are now ready to prove that $\mathcal{L}$ lifts to a functor of locally cubical bicategories. The definition of a locally cubical bicategory can be found in [GG09]. It can also be derived as a bicategory enriched in the monoidal 2-category $\mathcal{D}bl$. The 2-category $\mathcal{D}bl$ has finite products, which gives the monoidal structure.

Definition 4.2.3. Let $\mathcal{V}$ be a monoidal 2-category. A $\mathcal{V}$-enriched bicategory $\mathfrak{B}$ consists of the following elements:

- A collection of objects $\mathfrak{B} = \{A, B, C, ...\}$
- For each two objects A, B of $\mathfrak{B}$, an object $\mathfrak{B}(A, B)$ of $\mathcal{V}$.
- For each three objects A, B, C of $\mathfrak{B}$, a 1-cell $\circ : \mathfrak{B}(B, C) \otimes \mathfrak{B}(A, B) \to \mathfrak{B}(A, C)$ of $\mathcal{V}$.
- For each object A of $\mathfrak{B}$, a 1-cell $I_A : 1 \to \mathfrak{B}(A, A)$ of $\mathcal{V}$, where 1 is the initial object of $\mathcal{V}$.
- For each four objects A, B, C, D of $\mathfrak{B}$, a 2-cell of $\mathcal{V}$, depicted below.

$$\begin{array}{ccc} \mathbf{B}(C,D)\otimes\mathbf{B}(B,C)\otimes\mathbf{B}(A,B) & \xrightarrow{\mathrm{id}\otimes\circ} & \mathbf{B}(C,D)\otimes\mathbf{B}(A,C) \\ {\scriptstyle \circ\otimes\mathrm{id}}\downarrow & \Downarrow\alpha & \downarrow{\scriptstyle \circ} \\ \mathbf{B}(B,D)\otimes\mathbf{B}(A,B) & \xrightarrow[\circ]{} & \mathbf{B}(A,D) \end{array}$$

- For each two objects A, B of $\mathfrak{B}$, a natural isomorphisms

$$\begin{array}{ccc} 1\otimes\mathbf{B}(A,B) & & \\ {\scriptstyle I_B\otimes\mathrm{id}}\downarrow & \cong & \\ & \Downarrow\lambda & \searrow \\ \mathbf{B}(B,B)\otimes\mathbf{B}(A,B) & \xrightarrow[\circ]{} & \mathbf{B}(A,B) \end{array} \qquad \begin{array}{ccc} \mathbf{B}(A,B)\otimes 1 & & \\ {\scriptstyle \mathrm{id}\otimes I_A}\downarrow & \cong & \\ & \Downarrow\rho & \searrow \\ \mathbf{B}(A,B)\otimes\mathbf{B}(A,A) & \xrightarrow[\circ]{} & \mathbf{B}(A,B) \end{array}$$

This data needs to satisfy the usual axioms for bicategories from Section 1.2.2

When we apply the definition above to $\mathcal{D}bl$, we see that a locally cubical bicategory has objects, hom-double categories of 1-morphisms, tight 2-morphisms, loose 2-cells, and 3-cells, which fit in a square of tight and loose 2-cells. We have double functors $\circ$, I_A and tight isomorphisms α, ρ, λ.

Note that a locally cubical bicategory with one object is precisely a monoidal double category in the sense of 4.1, and thus the explicit description of the coherences in 4.1 can also be applied here. We will primarily be concerned with the following two examples.

Example 4.2.4. Any category can be regarded as a double category in the *loose* direction, with only identity tight morphisms and identity 2-cells. (Note that this is a *strict* double category, not a pseudo one.) This operation preserves products, and thereby any strict 2-category can be regarded as a locally cubical bicategory. Therefore, we can regard the 2-category $\mathcal{D}bl_{\mathbf{f}}$ as a locally cubical bicategory in this way; thus it has only identity tight 2-cells and identity 3-cells. We write $\mathfrak{Dbl}_{\mathbf{f}}$ for this locally cubical bicategory.

Example 4.2.5. By [GG09, Corollary 12], there is a locally cubical bicategory $\mathfrak{Bicat}$ defined by the following data:

- Its objects are bicategories.
- Its morphisms are functors.
- Its loose 2-cells are pseudo natural transformations.

- Its tight 2-cells are icons.
- Its 3-cells are *cubical modifications* as defined in [GG09, Definition 13].

We recall the definition of a cubical modification.

Definition 4.2.6. Let $F, G, H, K : \mathcal{D} \to \mathcal{E}$ be pseudo functors; let $\alpha : F \Rightarrow G$, $\beta : H \Rightarrow K$ be pseudo transformations; let $\gamma : F \Rightarrow H$, $\delta : G \Rightarrow K$ be icons. A **cubical modification**

$$\begin{array}{ccc} F & \overset{\alpha}{\Rightarrow} & G \\ {\scriptstyle\gamma}\Downarrow & \Downarrow\Gamma & \Downarrow{\scriptstyle\delta} \\ H & \underset{\beta}{\Rightarrow} & K \end{array}$$

is given by a family of 2-cells $\Gamma_A : \alpha_A \Rrightarrow \beta_A$ such that for every 1-cell $f : A \to B$ of $\mathcal{D}$, the following equality holds.

$$\begin{array}{ccccc} FA & \overset{Ff}{\Longrightarrow} & FB & \overset{\alpha_B}{\Longrightarrow} & GB \\ \| & & \Downarrow \alpha_f & & \| \\ FA & \overset{\alpha_A}{\Longrightarrow} & GA & \overset{Gf}{\Longrightarrow} & GB \\ \| & \Downarrow\Gamma_A & \| & \Downarrow\delta_f & \| \\ HA & \underset{\beta_A}{\Longrightarrow} & KA & \underset{Kf}{\Longrightarrow} & KB \end{array} = \begin{array}{ccccc} FA & \overset{Ff}{\Longrightarrow} & FB & \overset{\alpha_B}{\Longrightarrow} & GB \\ \| & \Downarrow \gamma_f & \| & \Downarrow \Gamma_B & \| \\ HA & \underset{Hf}{\Longrightarrow} & HB & \underset{\beta_B}{\Longrightarrow} & KB \\ \| & & \Downarrow\beta_f & & \| \\ HA & \underset{\beta_A}{\Longrightarrow} & KA & \underset{Kf}{\Longrightarrow} & KB \end{array} \tag{4.2.7}$$

The double functor $\mathrm{id}_A : * \to \mathfrak{Bicat}(A, A)$ maps the cells in the trivial bicategory $*$ to the identity cells and morphisms of $\mathfrak{Bicat}(A, A)$. The double functor $\circ$ is defined on functors of bicategories by composition. On pseudo transformations and icons it is given by the Godement product. On cubical modifications it is defined below:

$$\begin{array}{ccccc} FF'A & \overset{\alpha_{F'A}}{\Longrightarrow} & GF'A & \overset{G(\alpha'_A)}{\Longrightarrow} & GG'A \\ \| & \Downarrow\Gamma_{F'A} & \| & \Downarrow\delta_{\alpha'_A} & \| \\ HF'A & \underset{\beta_{F'A}}{\Longrightarrow} & KF'A & \underset{K(\alpha'_A)}{\Longrightarrow} & KG'A \\ \| & = & \| & \Downarrow K\Gamma'_A & \| \\ HH'A & \underset{\beta_{H'A}}{\Longrightarrow} & KH'A & \underset{K(\beta'A)}{\Longrightarrow} & KK'A \end{array}$$

Functoriality follows from naturality of the icons. Note that there are several canonical ways to define this composition on cubical modifications, by choosing different versions of the Godement product.

Now, we can similarly obtain the notion of *functor* between locally cubical bicategories from the definition of a $\mathcal{V}$-enriched functor between $\mathcal{V}$-enriched bicategories.

Definition 4.2.8. Let $\mathcal{V}$ be a monoidal 2-category. Let $\mathfrak{B}, \mathfrak{C}$ be $\mathcal{V}$-enriched bicategories. A $\mathcal{V}$-enriched functor $F : \mathfrak{B} \to \mathfrak{C}$ consists of the following data:

(i) An assignment on objects that sends each object A of $\mathfrak{B}$ to an object FA of $\mathfrak{C}$.

(ii) For each two objects A, B of $\mathfrak{B}$, a 1-cell $\mathfrak{B}(A, B) \to \mathfrak{C}(F(A), F(B))$ of $\mathcal{V}$.

(iii) For every triple of objects A, B, C of $\mathfrak{B}$, a 2-cell of $\mathcal{V}$

$$\begin{array}{ccc} & \overset{\mathfrak{B}\circ}{\frown} & \\ \mathfrak{B}(A,B) \otimes \mathfrak{B}(B,C) & \Downarrow \phi \cong & \mathfrak{C}(F(A),F(C)) \\ & \underset{\circ(F,F)}{\smile} & \end{array} \tag{4.2.9}$$

(iv) For every object A of $\mathfrak{B}$ a 2-cell of $\mathcal{V}$

$$\begin{array}{ccc} * & \xrightarrow{\mathrm{Id}_A} & \mathfrak{C}(A,A) \\ & \searrow^{\mathrm{Id}_{F(A)}} & \Downarrow \phi_u \cong \quad \downarrow F \\ & & \mathfrak{B}(F(A),F(A)) \end{array} \tag{4.2.10}$$

(v) The usual coherence diagrams, Definition 10 of [Gur13] commute.

When we apply this definition to the monoidal 2-category $\mathcal{D}bl$, we see that a **functor of locally cubical bicategories** F consists of a map of objects $A \mapsto FA$; pseudo double functors $\mathfrak{B}(A, B) \to \mathfrak{C}(F(A), F(B))$ for each two objects A, B; and tight transformations ϕ for each two objects A, B of $\mathfrak{B}$, and ϕ_u for every object A of $\mathfrak{B}$.

The following result is an extension of Theorem 4.9 of [Shu10], which shows that the trifunctor that arises from $\mathcal{L}$, is in fact a functor of locally cubical bicategories.

Theorem 4.2.11. *There is a functor of locally cubical bicategories $\mathcal{L}\colon \mathcal{D}bl_{\mathfrak{f}} \to \mathcal{B}icat$.*

Proof. Since any pseudo functor can be seen as a double functor between double categories with only identity tight 1-morphisms, each pseudo functor $\mathcal{L} : \mathcal{D}bl(\mathbb{D}, \mathbb{E}) \to \mathcal{B}icat(\mathcal{L}\mathbb{D}, \mathcal{L}\mathbb{E})$ corresponds to a pseudo double functor $\mathfrak{L} : \mathfrak{Dbl}_{\mathfrak{f}}(\mathbb{D}, \mathbb{E}) \to \mathfrak{Bicat}(\mathfrak{L}\mathbb{D}, \mathfrak{L}\mathbb{E})$. Consequently, the first two requirements in Definition 4.2.8 are satisfied by Theorems 4.2 and 4.2. The third requirement amounts to the existence of a tight transformation $\phi\colon \hat{\beta} * \hat{\alpha} \cong \widehat{\beta * \alpha}$ for every pair of transformations with loosely strong companions

$$\mathbb{C} \underset{G}{\overset{F}{\Downarrow \alpha}} \mathbb{D} \underset{K}{\overset{H}{\Downarrow \beta}} \mathbb{E}$$

such that

$$\begin{array}{ccc} 1_{\mathcal{L}H\odot\mathcal{L}F} & \longrightarrow & \hat{1}_H * \hat{1}_F \\ {\scriptstyle =}\downarrow & & \downarrow{\scriptstyle \phi} \\ 1_{\mathcal{L}(H\odot F)} & \longrightarrow & \widehat{1_H * 1_F} \end{array} \quad \text{and} \quad \begin{array}{ccc} \widehat{\gamma\alpha} * \widehat{\delta\beta} & \longrightarrow & (\hat{\gamma} * \hat{\delta}) \circ (\hat{\alpha} * \hat{\beta}) \\ {\scriptstyle \phi}\downarrow & & \downarrow{\scriptstyle \phi * \phi} \\ \widehat{\gamma\alpha * \delta\beta} & \longrightarrow & \widehat{(\gamma * \delta)} \circ \widehat{(\alpha * \beta)} \end{array} \tag{4.2.12}$$

commute. Here, we use the 'Godement product' $*$ of 2-cells in $\mathcal{D}bl$.

Now by Lemmas 4.1.30 and 4.1.31, $(\hat{\beta} * \hat{\alpha})_A = \hat{\beta}_{GA} \circ H(\hat{\alpha}_A)$ is a companion of $(\beta * \alpha)_A = \beta_{GA} \circ H(\alpha_A)$. Therefore, we take the component $(\phi_{\alpha,\beta})_A$ to be

$$\theta_{\hat{\beta}_{GA} \circ H(\hat{\alpha}_A), \widehat{\beta * \alpha}_A}.$$

As the other morphisms in the diagrams above are also θ-isomorphisms, the equations hold by uniqueness of θ-isomorphisms. For the tight transformation ϕ_u we can simply take the identity, since $\mathcal{L}$ is strictly unital. The coherence equations hold by uniqueness of θ-isomorphisms. □

Remark 4.2.13. Alternatively, one can show that, $\mathcal{L}$ lifts tight transformations with companions to oplax transformations. If their images under $\mathcal{L}$ are in fact pseudo natural transformations, $\mathcal{L}$ is a functor to the locally cubical bicategory $\mathcal{B}icat$ of bicategories, pseudo functors, pseudo natural transformations, icons and cubical modifications. For further details, see [HS19].

Our goal is to enhance this functor to act on "monoidal objects". We do so, by defining the monoidal structure of objects and higher cells in a locally cubical bicategory using the cartesian product of $\mathcal{D}bl_{\mathbf{f}}$ and $\mathcal{B}icat$, in such a way that any functor that preserves this product will preserve the monoidal structures, in a functorial way. We show that $\mathcal{L}$ preserves products and hence gives rise to a functor of the locally cubical bicategories of monoidal objects and higher monoidal cells.

In general, if $\mathcal{V}$ is a monoidal 2-category with strict 2-categorical finite products (such as $\mathcal{D}bl$), we say that a **$\mathcal{V}$-enriched bicategory B has finite products** when for each two objects $C, D \in \mathbf{B}$ there is an object $C \times D$ with projections $C \times D \to C$ and $C \times D \to D$ (i.e. morphisms $I \to \mathbf{B}(C \times D, C)$ and $I \to \mathbf{B}(C \times D, D)$ in $\mathcal{V}$) inducing an *isomorphism* in $\mathcal{V}$ (not merely an equivalence):

$$\mathbf{B}(A, C \times D) \xrightarrow{\cong} \mathbf{B}(A, C) \times \mathbf{B}(A, D) \tag{4.2.14}$$

and similarly there is a strict terminal object $*$ such that $\mathbf{B}(A, *)$ is strictly terminal in $\mathcal{V}$ for all A. This holds for $\mathcal{B}icat$ and $\mathcal{D}bl_{\mathbf{f}}$, because cartesian products of bicategories and double categories are simply componentwise, and all the morphisms in $\mathcal{B}icat$ and $\mathcal{D}bl_{\mathbf{f}}$ are defined in terms of data in their targets.

Similarly, we say that a **functor of $\mathcal{V}$-enriched bicategories preserves products** if it takes the terminal object to a terminal object and pairs of product projections $A \leftarrow A \times B \rightarrow B$ to pairs of product projections (in the above strict sense).

Theorem 4.2.15. *The functor of locally cubical bicategories $\mathcal{L} : \mathcal{D}bl_{\mathbf{f}} \rightarrow \mathcal{B}icat$ preserves products.*

Proof. Since $\mathcal{L}$ merely forgets a part of the double categories and double functors, we have simple equalities $\mathcal{L}(\mathbb{D}\times\mathbb{E}) = \mathcal{L}(\mathbb{D})\times\mathcal{L}(\mathbb{E})$, and the product projections are likewise preserved. The case of the terminal object is likewise easy. □

4.3 Monoidal Objects in Locally Cubical Bicategories

In this section, we define abstract monoidal, braided, sylleptic and symmetric objects and higher cells in a locally cubical bicategory and we prove that the symmetric, sylleptic or braided monoidal cells in a locally cubical bicategory $\mathcal{B}$ form a new locally cubical bicategory. Furthermore, we show that any functor of locally cubical bicategories that preserves finite products, preserves the monoidal structures.

The abstract definitions generalise the notions of monoidal, braided, and symmetric structure for bicategories, pseudofunctors, pseudo transformations, icons and cubical modifications [Gur13, GG09, McC00]. The monoidal constraints and coherence axioms are reformulated in equational form, instead of the explicit definitions in terms of 2-cell composites in the target bicategory. Note that certain constraint 2-cells are suppressed in [Gur13, McC00, GG09] to simplify notation. In the equational form below, this cannot be done, which leads to coherence-equations that look more intimidating, but are in fact not more complicated than their bicategorical counterparts. We give the coherence axioms for monoidal objects, 1-cells, 2-cells, icons and 3-cells explicitly, but leave the axioms for braided, symmetric and sylleptic monoidal structures as an exercise for the reader. For monoidal objects, 1-cells and 2-cells, the coherence axioms live entirely in the loose bicategory of the hom double category, since all the tight 2-cells are identities. Therefore, we write them with ordinary bicategorical pasting diagrams, leaving out the identity 2-cells.

Before we give the definitions of monoidal cells, we unfold the structure of a locally cubical bicategory and fix our notation. In addition to objects, locally cubical bicategories have 4 different elements, which together form the hom-double category. We call the objects, loose 1-cells and 2-morphisms of the hom-double category '1-cells', '2-cells' and '3-cells', respectively; the tight 1-morphisms are called 'icons', after the icons between pseudofunctors. The structure contains three types of composition. We will adopt the notation introduced for intercategories [GP14], of which locally cubical bicategories are a special case. Firstly, we have loose composition "$\bullet$" within the hom-double categories. This gives us composition of loose 2-cells along a 1-cell boundary and of 3-cells along a tight 2-cell boundary. We write this composition in the order of diagrammatic composition: $\alpha \bullet \beta$, meaning "β after α". We write Id_f and Id_α for the loose identity on a 1-cell f and a tight 2-cell α, respectively. Loose composition is weakly associative and loose identities hold up to isomorphism. We denote the associator, left and right unitor for $\bullet$ by $a^\bullet$, $r^\bullet$, $l^\bullet$, respectively. Secondly, we have tight composition "$\cdot$" in the hom-double categories. This gives us composition of tight 2-cells along a 1-cell boundary and tight composition of 3-cells along a loose 2-cell boundary, written in the

conventional order: $f \cdot g$ denoting "f after g". We write 1_f and 1_α for the tight identity on a 1-cell f and a loose 2-cell α, respectively. Tight composition is strictly associative and has strict identities. Thirdly, there is composition "$\circ$" of 1-cells, 2-cells, and 3-cells along a 0-cell boundary, given by the enriched structure. We write this composition in the conventional order: $f \circ g$ meaning "f after g". When it is clear from the context, we omit the composition symbol "$\circ$", and write the juxtaposition of 1-cells instead. The identities for this composition are denoted by "id". We denote the associator, left and right unitor for $\circ$ by $a^\circ, r^\circ, l^\circ$, respectively. We write "$\multimap$" to denote 1-cells, "$\Rightarrow$" to denote the loose 2-cells, "$\Rightarrow$" to denote the tight 2-cells and "$\Rrightarrow$" to denote 3-cells.

For readability, we will strictify the hom-double categories, as we did with the double categories in Section 4.1, except where we prove that this structure is preserved by monoidal cells. As a consequence, we omit the associativity and unit constraints for $\circ$ and $\cdot$ in various places. Furthermore, we restrict our attention to locally cubical bicategories where composition of 1-cells along 0-cells is strict, while it is weak on higher cells. This is sufficient for the cases of bicategories and double categories.

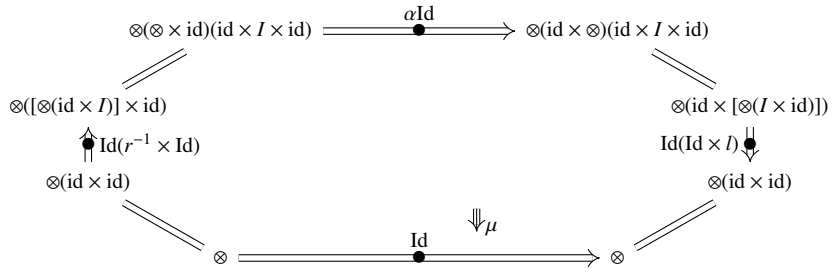
Let $\mathfrak{B}$ be a locally cubical bicategory with products and strict composition of 1-cells along 0-cells.

Definition 4.3.1. A **monoidal object** in $\mathfrak{B}$ is an object A, equipped with 1-cells $\otimes : A \times A \multimap A$ and $I_A : * \multimap A$, and 2-cells

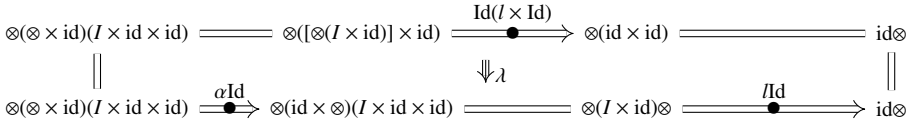
- $\alpha :\otimes (\otimes \times \mathrm{id}) \Rightarrow \otimes (\mathrm{id} \times \otimes)$
- $l :\otimes (I \times \mathrm{id})i_2 \Rightarrow \mathrm{id}$ and $r :\otimes (\mathrm{id} \times I)i_1 \Rightarrow \mathrm{id}$

where $*$ is the terminal object of $\mathcal{B}$ and $i_1 : A \to A \times *$, $i_2 : A \to * \times A$ are the embedding morphisms defining the products $A \times *$ and $* \times A$, respectively. For readability, we will omit the functions i_1 and i_2. Finally, it must be equipped with the invertible globular 3-cells π, μ, λ, ρ depicted below, which generalise the Mac Lane pentagon and the three other coherence diagrams given in Definition 4.1 of [Gur13]. The horizontally drawn equality is added for readability. These 3-cells must satisfy the three axioms B.0.1, B.0.2 B.0.3, which generalise the coherence axioms for monoidal bicategories [Gur13, Definition 4.1].

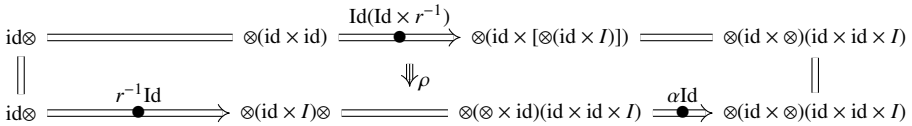
$$\begin{array}{ccccc}
\otimes(\otimes \times \mathrm{id})(\otimes \times \mathrm{id} \times \mathrm{id}) & \xRightarrow{\mathrm{Id}(\alpha \times \mathrm{Id})} & \otimes(\otimes \times \mathrm{id})(\mathrm{id} \times \otimes \times \mathrm{id}) & \xRightarrow{\alpha \mathrm{Id}} & \otimes(\mathrm{id} \times \otimes)(\mathrm{id} \times \otimes \times \mathrm{id}) \\
\| & & \Downarrow \pi & & \| \\
\otimes(\otimes \times \mathrm{id})(\otimes \times \mathrm{id} \times \mathrm{id}) & \xRightarrow{\alpha \mathrm{Id}} & \otimes(\mathrm{id} \times \otimes)(\otimes \times \mathrm{id} \times \mathrm{id}) & = & \otimes(\otimes \times \mathrm{id})(\mathrm{id} \times \mathrm{id} \times \otimes) \\
& & & & \\
\otimes(\mathrm{id} \times \otimes)(\mathrm{id} \times \otimes \times \mathrm{id}) & \xRightarrow{\mathrm{Id}(\mathrm{Id} \times \alpha)} & \otimes(\mathrm{id} \times \otimes)(\mathrm{id} \times \mathrm{id} \times \otimes) & & \\
\| & & \| & & \\
\otimes(\mathrm{id} \times \otimes)(\mathrm{id} \times \otimes \times \mathrm{id}) & \xRightarrow{\alpha \mathrm{Id}} & \otimes(\mathrm{id} \times \otimes)(\mathrm{id} \times \mathrm{id} \times \otimes) & &
\end{array} \tag{4.3.2}$$



(4.3.3)

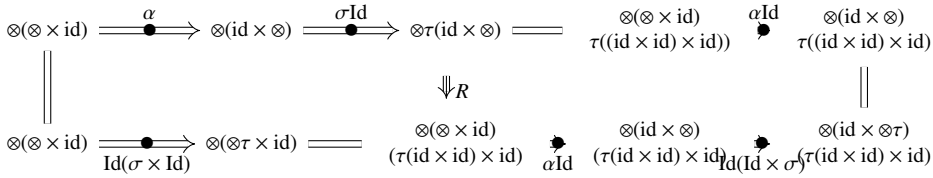


(4.3.4)

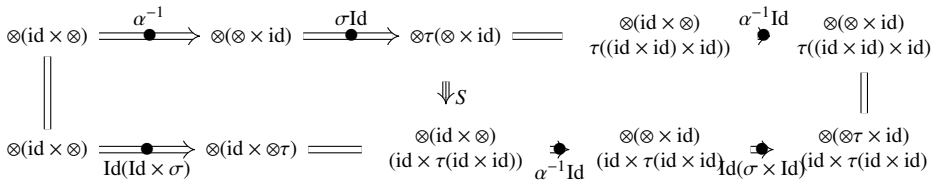


(4.3.5)

A monoidal object is **braided** if in addition it is equipped with a loose 2-cell σ_A : $\otimes \nrightarrow \otimes\tau$, where $\tau : A \times A \to A \times A$ interchanges the two copies of A; and if there are invertible globular 3-cells

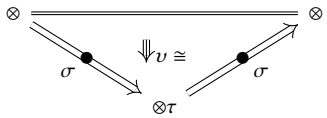


(4.3.6)



(4.3.7)

satisfying the axioms (BA1), (BA2), (BA3), and (BA4) given in [McC00, p136–139] . It is **sylleptic** when it is equipped with an additional invertible globular 3-cell



(4.3.8)

satisfying the axioms (SA1), (SA2) on [McC00, p144–145]. It is **symmetric** if in addition, it satisfies the axiom given on [McC00, p91].

Definition 4.3.9. Let A, B be monoidal objects in $\mathfrak{B}$. A 1-cell $f : A \nrightarrow B$ is **lax monoidal** when it is equipped with the following loose 2-cells:

- $\chi : \otimes(f \times f) \nrightarrow f\otimes$
- $\iota : I_B \nrightarrow fI_A$

as well as globular invertible 3-cells

$$\omega : \mathrm{Id}_\otimes(\chi \times \mathrm{Id}_f) \bullet \chi\mathrm{Id}_{\otimes\times\mathrm{id}} \bullet \mathrm{Id}_f\alpha \Rightarrow \alpha\mathrm{Id}_{f\times f\times f} \bullet \mathrm{Id}_\otimes(\mathrm{Id} \times \chi) \bullet \chi\mathrm{Id}_{\mathrm{id}\times\otimes}$$
$$\gamma : \mathrm{Id}_\otimes(\iota_f \times \mathrm{Id}_f) \bullet \chi\mathrm{Id}_{I\times\mathrm{id}} \bullet \mathrm{Id}_f l \Rightarrow l\mathrm{Id}_f$$
$$\delta : \mathrm{Id}_f r^{-1} \Rightarrow r^{-1}\mathrm{Id}_f \bullet \mathrm{Id}_\otimes(\mathrm{Id} \times \iota) \bullet \chi\mathrm{Id}_{(\mathrm{id}\times I)}$$

as in Definition 4.10 of [Gur13], which satisfy the coherence axioms B.0.4 and B.0.5.

A lax monoidal 1-cell is called **braided**, when A and B are braided and there is a globular 3-cell

$$u : \sigma_B\mathrm{Id}_{f\times f} \bullet \chi\mathrm{Id}_\tau \Rightarrow \chi \bullet (\mathrm{Id}_f\sigma_A)$$

satisfying the braiding axioms (BHA1) and (BHA2) [McC00, p141-142].

The 1-cell $f : A \nrightarrow B$ is **colax monoidal** when it is equipped with loose 2-cells $\bar{\chi}$ and $\bar{\iota}$ which go in the opposite direction of χ and ι, respectively, and with the following globular invertible 3-cells:

$$\bar{\omega} : \bar{\chi}\mathrm{Id}_{\mathrm{id}\times\otimes} \bullet \mathrm{Id}_\otimes(\mathrm{Id}_f \times \bar{\chi}) \bullet \alpha^{-1}\mathrm{Id}_{f\times f\times f} \Rightarrow \mathrm{Id}_f\alpha^{-1} \bullet \bar{\chi}\mathrm{Id}_{\otimes\times\mathrm{id}} \bullet \mathrm{Id}_\otimes(\bar{\chi} \times \mathrm{Id}_f)$$
$$\bar{\gamma} : l^{-1}\mathrm{Id}_f \Rightarrow \mathrm{Id}_f l^{-1} \bullet \bar{\chi}\mathrm{Id}_{I\times\mathrm{id}} \bullet \mathrm{Id}_\otimes(\bar{\iota}_f \times \mathrm{Id}_f)$$
$$\bar{\delta} : \bar{\chi}\mathrm{Id}_{\mathrm{id}\times I} \bullet \mathrm{Id}_\otimes(\mathrm{Id}_f \times \bar{\iota})\mathrm{Id}_{i1} \bullet r^{-1}\mathrm{Id}_f \Rightarrow \mathrm{Id}_f r^{-1}$$

satisfying analogous axioms with the cells pasted together in a different order, corresponding to the direction of $\bar{\gamma}, \bar{\delta}$, and $\bar{\omega}$.

A colax monoidal 1-cell is called **braided**, when A and B are braided and there is a globular 3-cell

$$\bar{u} : \chi\mathrm{Id}_\tau \bullet \sigma_B\mathrm{Id}_{f\times f} \Rightarrow (\mathrm{Id}_f\sigma_A) \bullet \chi$$

satisfying the braiding axioms analogous to (BHA1) and (BHA2) in [McC00, p141-142]. The 3-cells of these axioms are pasted in a different order, such that composition of their 2-cell sources and targets is well-defined.

If f is both lax and colax monoidal, the associated loose 2-cells χ and ι form adjoint equivalences with their colax counterparts, as depicted in 1.2.2, and the 3-cells correspond to their colax counterparts as mates under the adjoint equivalence structure, it is **strong monoidal**. The mate correspondences for ω, γ and δ are depicted in planar diagrams in equations B.0.6, B.0.7, and B.0.8 of Appendix B for illustration.

A monoidal 1-cell between sylleptic or symmetric objects is **sylleptic** or **symmetric**, respectively, if it is braided and the 3-cells defining the braided monoidal structure satisfy the additional axiom (SHA1) given in [McC00, p145].

By construction, monoidal objects and 1-cells in the locally cubical bicategory $\mathcal{B}icat$ correspond to monoidal bicategories and monoidal pseudo functors. In $\mathcal{D}bl$, it reduces to monoidal double categories and monoidal double functors defined in Section 4.1, since there are no non-identity 3-cells.

Definition 4.3.10. Let $f, g : A \nrightarrow B$ be lax monoidal 1-cells in $\mathfrak{B}$. A **lax monoidal 2-cell** $\beta : f \Rightarrow g$ is a loose 2-cell in $\mathfrak{B}$ that is equipped with globular 3-cells

- $\Pi : \mathrm{Id}_{\otimes}(\beta \times \beta) \bullet \chi_g \Rrightarrow \chi_f \bullet \beta\mathrm{Id}_{\otimes}$
- $M : \mathrm{Id}_I \bullet \iota_g \Rrightarrow \iota_f \bullet \beta\mathrm{Id}_{I_A}$

such that coherence equations (B.0.9), (B.0.10), and (B.0.11) in Appendix B hold. Applied to the special case of bicategories gives us equations (TA2), (TA3) and (TA4) of [GG09]. It is **colax monoidal** if it is equipped with morphisms $\bar{\Pi}, \bar{M}$, which correspond to Π and M in the opposite direction, respectively. Is is **strong monoidal**, when Π and M are isomorphisms

A monoidal 2-cell between lax monoidal 1-cells is **braided**, **sylleptic** or **symmetric** when f, g are braided, sylleptic or symmetric, and in addition the abstract coherence axiom corresponding to [McC00, (BTA1) p143] holds. This axiom corresponds to (BTA1) of [McC00, p143], when applied to the locally cubical bicategory of bicategories.

Let $f, g : A \nrightarrow B$ be colax monoidal 1-cells in $\mathfrak{B}$. A **colax monoidal 2-cell** $\beta : f \Rightarrow g$ is a loose 2-cell in $\mathfrak{B}$ that is equipped with globular 3-cells

- $\Pi : \beta\mathrm{Id}_{\otimes} \bullet \bar{\chi}_g \Rrightarrow \bar{\chi}_f \bullet \mathrm{Id}_{\otimes}(\beta \times \beta)$
- $M : \beta\mathrm{Id}_I \bullet \bar{\iota}_g \Rrightarrow \bar{\iota}_f \bullet \mathrm{Id}_I$

such that coherence equations analogous to (B.0.9), (B.0.10), and (B.0.11) hold, with the same cells pasted together in the order that makes composition of their 2-cell sources and targets well-defined.

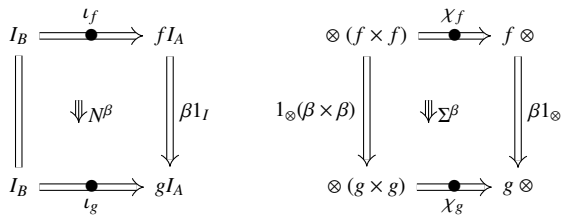
A monoidal 2-cell between colax monoidal 1-cells is **braided**, **sylleptic** or **symmetric** when f, g are braided, sylleptic or symmetric, and in addition coherence axiom analogous to [McC00, (BTA1) p143] holds. The difference comes from a different structure of the 3-cell u because of which the cells are pasted in a different order.

We call a loose 2-cell β a **strong monoidal 2-cell** when Π and M are isomorphisms.

When interpreted in $\mathcal{B}icat$, monoidal 2-cells should correspond to monoidal pseudo transformations. Such transformations are less general than tritransformations between one-object tricategories. As there is only one fixed object, the constraints Π and M are given by icons instead of adjoint equivalences, which leads to the notion of a pseudo-icon [GG09, Definition 5], from which the definition above is derived. This notion equals that of a monoidal pseudo transformation given in [SP09] up to isomorphisms $(\theta \times \mathrm{Id})(\mathrm{Id} \times \theta) \cong (\theta \times \theta)$ and $\iota \cong \mathrm{Id}\iota$ to ensure that the different instances of Π and M are of the same type.

As remarked above, we will actually construct a locally cubical bicategory of monoidal objects. The monoidal 2-cells will be the loose 2-cells therein; we now define the tight 2-morphisms.

Definition 4.3.11. Let $f, g : A \to B$ be lax monoidal 1-cells in $\mathfrak{B}$. A **monoidal icon** $\beta : f \Rightarrow g$ is a (tight) 2-morphism in $\mathfrak{B}$ that is equipped with 3-cells



(4.3.12)

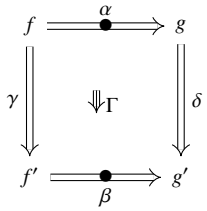
such that the coherence axioms B.0.12, B.0.13, B.0.14 in Appendix B hold. In the case of bicategories, these axioms specify to (TA2), (TA3) and (TA4) of [GG09].

If $f, g : A \to B$ are colax monoidal 1-cells the data for a monoidal icon consists of the same 2-cells between 1-cells in the opposite direction; the coherence equations analogous to B.0.12, B.0.13, and B.0.14 are derived by pasting 3-cells together in the order for which composition their 2-cell source and targets is well-defined.

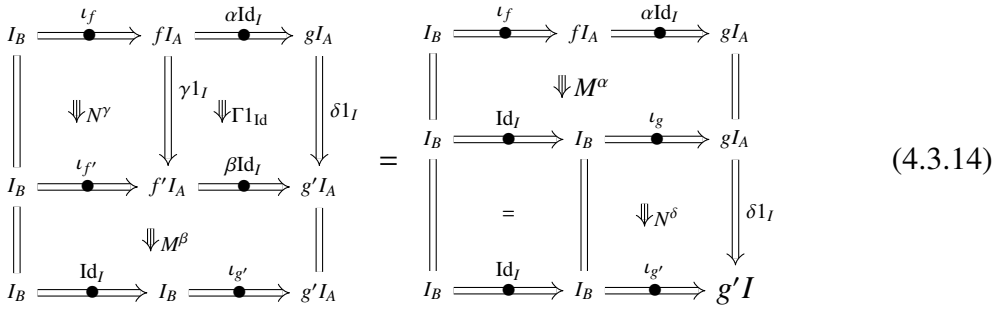
A monoidal icon is **braided**, **sylleptic** or **symetric** when f, g are braided, sylleptic or symmetric, respectively, and in addition, the coherence axiom B.0.15 holds.

Monoidal icons interpreted in $\mathcal{B}icat$ correspond to ico-icons [GG09, Definition 2]. These are doubly degenerate colax tritransformations between lax trihomomorphisms which agree on both 0-cells and 1-cells. In $\mathcal{D}bl$, they correspond to pseudo double transformations.

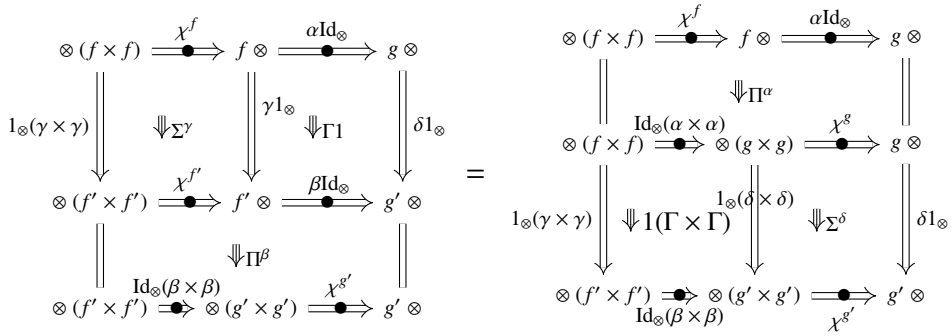
Definition 4.3.13. Let $f, g, f', g' : A \to B$ be lax monoidal 1-cells, let $\alpha : f \nrightarrow g$, $\beta : f' \nrightarrow g'$ be lax monoidal 2-cells, and let $\gamma : f \Rightarrow f'$, $\delta : g \Rightarrow g'$ be monoidal icons. A **monoidal 3-cell** is a 3-cell



such that the two equalities below hold.



(4.3.14)



(4.3.15)

If the 1-cells or 2-cells are colax, the 3-cells in the coherence equations are pasted together in a different order, such that composition of the 1-cell and 2-cell components is well-defined.

Let $f, g, f', g', \alpha, \beta, \gamma$ and $\delta : g \Rightarrow g'$ be braided, sylleptic, or symmetric monoidal 1-cells, 2-cells, and icons, respectively. A **braided, sylleptic, or symmetric monoidal 3-cell** is simply a monoidal 3-cell Γ as depicted above.

Monoidal 3-cells in $\mathcal{B}icat$ correspond to cubical pseudo-icon modifications [GG09, Definition 16]. When the icon components are identities, this reduces to a monoidal modification [SP09, Definition 2.8].

We will show that monoidal objects, lax monoidal 1-cells, lax monoidal 2-cells, monoidal icons, and monoidal 3-cells in a locally cubical bicategory $\mathfrak{B}$ form a locally cubical bicategory $\mathcal{M}on_l\mathcal{B}$. If we consider colax or strong cells instead, we ob-

tain the locally cubical bicategory $\mathcal{M}on_c\mathcal{B}$ or $\mathcal{M}on_s\mathcal{B}$, respectively. Braided, sylleptic and symmetric cells form locally cubical bicategories $\mathcal{B}r\mathcal{M}on_w\mathcal{B}$, $\mathcal{S}yl\mathcal{M}on_w\mathcal{B}$, and $\mathcal{S}ym\mathcal{M}on_w\mathcal{B}$. Here, $w \in \{l, c, s\}$ denotes whether the cells are lax, colax, or strong.

Proposition 4.3.16. *Let A, B be monoidal objects in a locally cubical bicategory with strict composition of 1-cells along 0-cells. The hom-spaces $\mathcal{M}on_w\mathcal{B}(A, B)$, $\mathcal{B}r\mathcal{M}on_w\mathcal{B}(A, B)$, $\mathcal{S}yl\mathcal{M}on_w\mathcal{B}(A, B)$, and $\mathcal{S}ym\mathcal{M}on_w\mathcal{B}(A, B)$ are double categories for $w \in \{l, c, s\}$.*

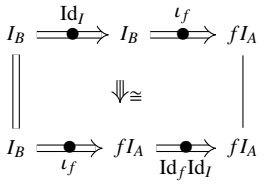
Proof. First we show that 1-cells and icons in the respective hom-spaces form a category. For each lax monoidal 1-cell $f : A \to B$, the identity icon 1_f is a lax monoidal icon with the 3-cells $N^{1_f} := 1_{\iota_f}$ and $\Sigma^{1_f} := 1_{\chi_f}$. This is well-defined, because the functor "$\circ$" preserves tight identities. The coherence equations are trivially satisfied. For each two lax monoidal 1-cells f, g and lax monoidal icons $\alpha, \beta : f \Rightarrow g$, the composite icon $\beta \cdot \alpha$ can be equipped with the lax monoidal structure given by the composites $N^{\beta\cdot\alpha} := N^\beta \cdot N^\alpha$ and $\Sigma^{\beta\cdot\alpha} := \Sigma^\beta \cdot \Sigma^\alpha$. We have a strict interchange law between $\cdot$ and $\circ$, induced by functoriality of $\circ$, so these 3-cells are well-defined. The coherence conditions (B.0.12)–(B.0.14) hold by componentwise application of the coherence equalities for $N^{\beta\cdot\alpha}$ and $\Sigma^{\beta\cdot\alpha}$. The same argument holds for colax 1-cells and icons. For strong 1-cells and icons we need to verify that the lax structure cells N^{1_f}, $N^{\beta\cdot\alpha}, \Sigma^{1_f}$, and $\Sigma^{\beta\cdot\alpha}$ are inverse in the loose direction to their colax counterparts. For N^{1_f} and Σ^{1_f}, this follows from functoriality of "$\bullet$". For $N^{\beta\cdot\alpha}$ and $\Sigma^{\beta\cdot\alpha}$, this follows from the the fact that the statement is true for their components combined with the exchange law between "$\bullet$" and "$\cdot$" and strictness of "$\cdot$". When f and g are braided, sylleptic or symmetric, the same data satisfies the coherence equation for braided monoidal icons.

We also need to show that lax monoidal 2-cells and monoidal 3-cells form a category. For every lax monoidal 2-cell $\alpha : f \nrightarrow g$, the identity 3-cell 1_α in $\mathcal{B}$ is lax monoidal. The required two equations 4.3.14 and 4.3.15 are trivially satisfied. For any two monoidal 3-cells $L : \alpha \Rrightarrow \beta$, $K : \beta \Rrightarrow \gamma$, the composition $K \cdot L$ in $\mathcal{B}$ is a monoidal 3-cell. The equations for monoidal 3-cells hold by sequential application of the respective equations for L and K. The same is true for colax monoidal 2-cells and 3-cells, and hence for strong monoidal 2-cells and 3-cells. As braided, sylleptic, and symmetric monoidal 3-cells are not required to satisfy additional data, it follows that braided, sylleptic, or symmetric monoidal 2-cells and 3-cells form a category.

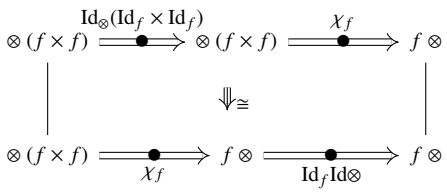
Now we describe the loose structure; we need to show that $\bullet$ and Id are well-defined as the functors which give the loose structure in the new double category. To see this, recall that $\bullet$ and Id correspond to the functors $\odot$ and U, respectively, given in Definition 4.1.1. Let f be a lax monoidal 1-cell. The loose identity 2-cell Id_f is a strong

monoidal 2-cell with monoidal structure given by the composition of coherence cells $l^\bullet$, $r^\bullet$.

$$M^{\mathrm{Id}_f} := \tag{4.3.17}$$



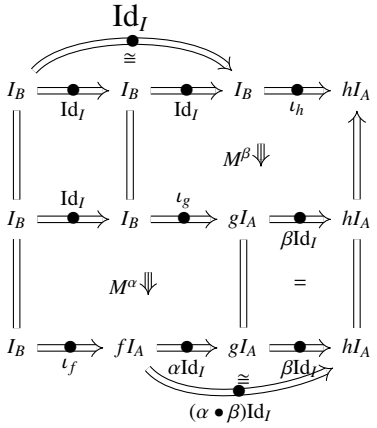
$$\Pi^{\mathrm{Id}_f} := \tag{4.3.18}$$



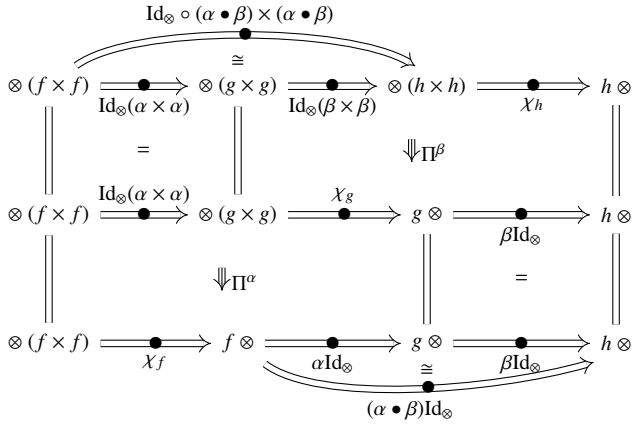
The conditions for monoidal 3-cells follow from the naturality conditions of the coherence cells $l^\bullet$ and $r^\bullet$. Let γ be a monoidal icon, one can verify that the loose identity 3-cell Id_γ is a monoidal 3-cell: The loose source and target 2-cells of Id_γ, are loose identities; hence, the coherence condition holds by naturality of $l^\bullet$ and $r^\bullet$.

Let $\alpha : f \nrightarrow g$ and $\beta : g \nrightarrow h$ be two lax monoidal 2-cells. Their composition $\alpha \bullet \beta$ is lax monoidal with the structure 3-cells given below.

$$M^{\alpha\bullet\beta} := \tag{4.3.19}$$



$\Pi^{\alpha\bullet\beta} :=$



(4.3.20)

The coherence equations are satisfied by sequential application of the respective equation for α and β, applications of the exchange law between loose and tight composition, together with simple manipulations of coherence cells.

Let Γ and Δ be monoidal 3-cells. Their composite $\Gamma \bullet \Delta$ is again monoidal. Again, the conditions for monoidal 3-cells follow directly from the conditions on the monoidal 3-cells Γ and Δ, applications of the exchange law between loose and tight composition, and simple manipulations of coherence cells. By analogous arguments, one can show that the images of $\bullet$ and Id on colax or strong cells are well-defined as colax or strong monoidal cells.

Let f be a braided, sylleptic or symmetric monoidal 1-cell. The loose identity Id_f is a braided, sylleptic or symmetric monoidal 2-cell, respectively, as the coherence equation [McC00, (BTA1) p143] merely states that the 3-cell u pasted with coherence 3-cells equals itself. Let α, β be braided, sylleptic, or symmetric monoidal 2-cells, the loose composition $\alpha \bullet \beta$ is braided, sylleptic, or symmetric monoidal, respectively. One can verify that [McC00, (BTA1) p143] holds by applying the exchange law between loose and tight composition, manipulation of coherence cells, and sequential application of the respective equations for α and β. Braided, sylleptic and symmetric monoidal 3-cells are simply monoidal 3-cells; therefore, it follows that the images of $\bullet$ and Id of braided, sylleptic, or symmetric monoidal cells are well-defined in $\mathcal{B}r\mathcal{M}on_w\mathcal{B}(A, B)$, $\mathcal{S}yl\mathcal{M}on_w\mathcal{B}(A, B)$, and $\mathcal{S}ym\mathcal{M}on_w\mathcal{B}(A, B)$, respectively.

Functoriality of $\bullet$ and Id in $\mathcal{M}on\mathcal{B}(A, B)$ follows from their functoriality in $\mathcal{B}(A, B)$. The unitality and associativity cells $a^\bullet$, $l^\bullet$, and $r^\bullet$ are monoidal 3-cells. Unfolding the constraints for monoidal 3-cells shows that the 3-cells pasted together with coherence cells need to equal themselves. It follows from coherence of the functor $\bullet$, that this is the case. Therefore, $\mathcal{M}on_w\mathcal{B}(A, B)$ is a double category for $q \in \{l, c, s\}$. Since braided, symmetric, or sylleptic monoidal 3-cells require no extra data, it follows that

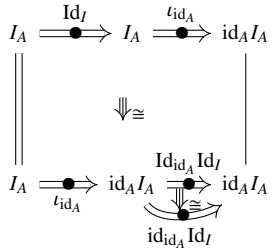
$\mathcal{B}r\mathcal{M}on_w\mathcal{B}(A,B)$, $\mathcal{S}yl\mathcal{M}on_w\mathcal{B}(A,B)$, and $\mathcal{S}ym\mathcal{M}on_w\mathcal{B}(A,B)$ are double categories for $w \in \{l, c, s\}$. □

Theorem 4.3.21. *Let $\mathfrak{B}$ be a locally cubical bicategory with strict composition of 1-cells along 0-cells. Monoidal objects, lax monoidal 1-cells, lax monoidal 2-cells, monoidal icons, and monoidal 3-cells in $\mathfrak{B}$ form a locally cubical bicategory $\mathcal{M}on_l\mathcal{B}$. If we consider colax or strong cells instead, we obtain the locally cubical bicategory $\mathcal{M}on_c\mathcal{B}$ or $\mathcal{M}on_s\mathcal{B}$, respectively. When the objects and cells are braided, sylleptic or symmetric, we obtain the locally cubical bicategories $\mathcal{B}r\mathcal{M}on_w\mathcal{B}$, $\mathcal{S}yl\mathcal{M}on_w\mathcal{B}$, and $\mathcal{S}ym\mathcal{M}on_w\mathcal{B}$, where $w \in \{l, c, s\}$ denotes whether the cells are lax, colax, or strong.*

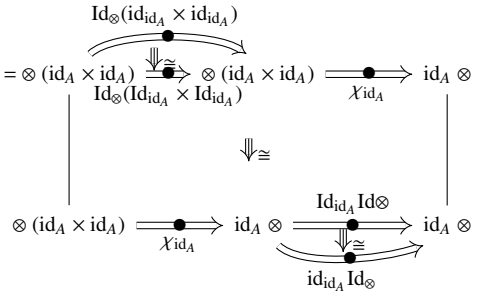
Proof. We have established in Proposition 4.3.16, that the respective homsets $\mathcal{M}on_wB(A,B)$, $\mathcal{B}r\mathcal{M}on_w\mathcal{B}$, $\mathcal{S}yl\mathcal{M}on_w\mathcal{B}$, and $\mathcal{S}ym\mathcal{M}on_w\mathcal{B}$ for $w \in \{l, c, s\}$ form double categories.

We need to check that the unit id_A is a well-defined pseudo double functor from the trivial double category to the respective hom-categories of lax, colax and strong monoidal cells, as well as braided, sylleptic and symmetric cells. The unit 1-cells id_A are monoidal for all objects $A \in \mathfrak{B}$, with the monoidal structure ξ, ι given by the unitor 2-cells, and γ, δ, and ω. This is well-defined by coherence of the double category. By functoriality of id, its image on the loose 2-cell is isomorphic to the loose identity $\mathrm{Id}_{\mathrm{id}_A}$. This isomorphism gives rise to the following lax monoidal structure on $\mathrm{id}_{\mathrm{id}_A}$:

$M^{\mathrm{id}_{\mathrm{id}_A}} :=$ (4.3.22)



$\Pi^{\mathrm{id}_{\mathrm{id}_A}} :=$ (4.3.23)



Coherence equations B.0.9, B.0.10, B.0.11, and [McC00, (BTA1) p143] hold by simple manipulations of the isomorphisms. This makes $\mathrm{id}_{\mathrm{id}_A}$ a braided, sylleptic, or symmetric monoidal 2-cell if id_A is braided, sylleptic, or symmetric, respectively. An analogous construction makes $\mathrm{id}_{\mathrm{id}_A}$ a colax monoidal 2-cell.

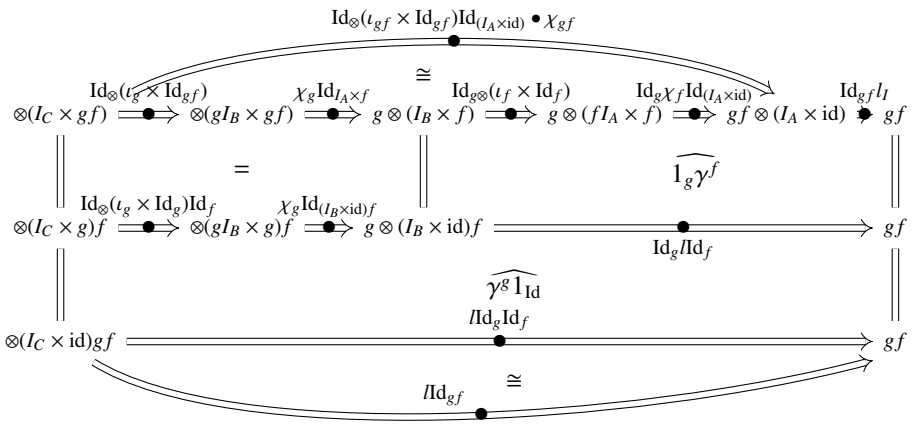
By functoriality, the image of id on the tight 2-cell and 3-cell equal 1_{id_A} and $\mathrm{Id}_{1_{\mathrm{id}_A}} = 1_{\mathrm{Id}_{\mathrm{id}_A}}$, respectively. These cells are braided, symmetric or sylleptic; lax, colax, or strong monoidal, depending on A. It follows that id_A is a well-defined functor from the trivial double category to the respective hom-categories of lax, colax and strong monoidal cells, as well as braided, sylleptic and symmetric ones.

Next, we need to show that monoidal structure is preserved by the composition along a 0-cell boundary. For any two lax monoidal 1-cells $f : A \to B$, $g : B \to C$, the composite $g \circ f$ is monoidal with $\chi^{g\circ f}$ and $\iota^{g\circ f}$ defined below.

$$\chi_{g\circ f} : \quad \otimes(gf \times gf) \overset{\chi_g \mathrm{Id}_{f\times f}}{\Rightarrow} g \otimes (f \times f) \overset{\mathrm{Id}_g \chi_f}{\Rightarrow} gf\otimes \tag{4.3.24}$$

$$\iota_{g\circ f} : \quad I_C \overset{\iota_g}{\Rightarrow} gI_B \overset{\mathrm{Id}_g \iota_f}{\Rightarrow} gfI_A \tag{4.3.25}$$

The structure 3-cell $\gamma^{g\circ f}$ for is defined below. For readability, we write "$\widehat{\ }$" to express that we have left out coherence 3-cells, needed to make the source and target of the 3-cell well defined.

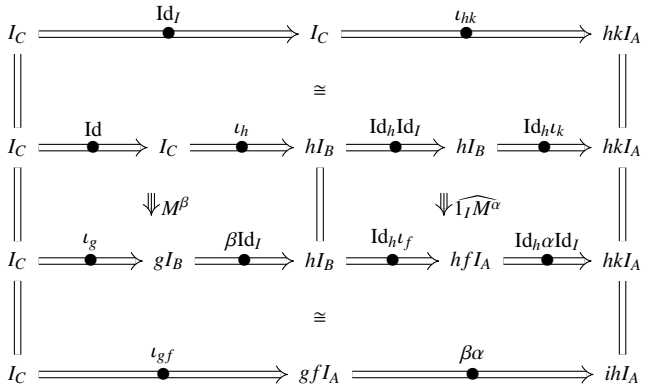


(4.3.26)

The 3-cells $\delta^{g\circ f}$ and $\omega^{g\circ f}$ are defined similarly, and so is $u^{g\circ f}$ when g, f are braided monoidal 1-cells.

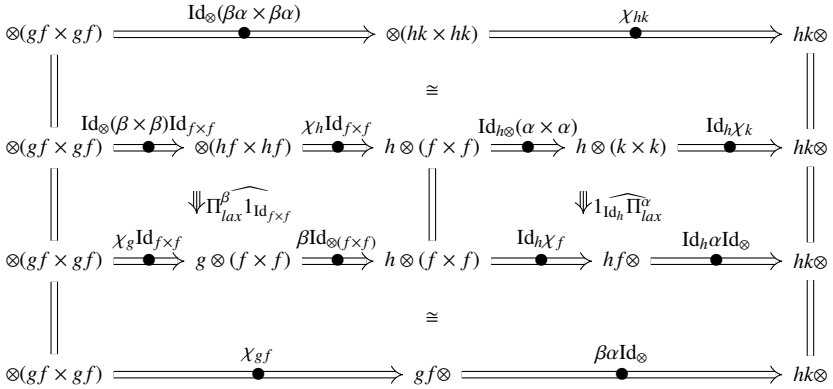
Let $f, h : A \to B$ and $g, i : B \to C$ be lax monoidal 1-cells and let $\alpha : f \to h$, $\beta : g \to i$ be lax monoidal 2-cells, the composite $\beta \circ \alpha$ is lax monoidal with the following structure 3-cells

$$M^{\beta\circ\alpha} :=$$



(4.3.27)

$$\Pi^{\beta\circ\alpha} :=$$



(4.3.28)

Colax and strong monoidal structure 2-cells are obtained in a similar way.

Let $f, h : A \to B$ and $g, i : B \to C$ be lax monoidal 1-cells and let $\alpha : f \to h$, $\beta : g \to i$ be monoidal icons, the composite $\beta \circ \alpha$ is monoidal with $N^{\beta\circ\alpha} := N^\beta \bullet \mathrm{Id}_\beta N^\alpha$ and $\Sigma^{\beta\circ\alpha} := \Sigma^\beta \mathrm{Id}_{\alpha\times\alpha} \bullet \mathrm{Id}_\beta \Sigma^\alpha$.

When g, f are strong monoidal, the maps $\chi_{g\circ f}$ and $\overline{\chi_{g\circ f}}$ are an adjoint equivalence, constructed by the enriched composition from the adjoint equivalence of the pairs $\chi_g, \overline{\chi_g}$ and $\chi_f, \overline{\chi_f}$. Similarly, $\iota_{g\circ f}$ and $\overline{\iota_{g\circ f}}$ form an adjoint equivalence. One can check that the required pairs of 3-cells correspond to each other as mates by componentwise application of the adjoint equivalences for the composites of $\iota_{g\circ f}$ and $\chi_{g\circ f}$. Let Γ and Δ be two composable monoidal 3-cells. It is easy to see that the composition $\Gamma \circ \Delta$ satisfies the two equations for monoidal 3-cells. This is a matter of applying the equations for Γ and Δ sequentially.

In all coherence equations between 3-cells for the monoidal and braided, sylleptic and symmetric structure of composition above, each 3-cell consists of a component for the first composite composed with the identity on the second composite, and a component for the second composite composed with the identity on the product of the first composite with itself. This means that the coherence equations for $g \circ f$ can be established by componentwise application of the equations for g and f. Some 3-cells also

contain coherence cells, but these equally break up in a part concerning the first, and a part concerning the second component. Manipulation of these coherence cells results in the required equalities. Note that rewriting the 1-cells and composites of loose 2-cells is necessary in several of the steps. A similar argument holds for coherence equations for braided, sylleptic and symmetric cells. □

Lemma 4.3.29. *Let $\mathcal{T} : T \to S$ be a functor of locally cubical bicategories. If F preserves products, it preserves monoidal objects, 1-cells, 2-cells, icons and 3-cells as well as any braided, sylleptic or symmetric structure on the objects, 1-cells, 2-cells, icons and 3-cells.*

Proof. Let A be a monoidal object. As the functor $\mathcal{T}$ preserves products, we have a product $\mathcal{T}(A) \times_{\mathcal{T}} \mathcal{T}(A) = \mathcal{T}(A \times A)$. As a consequence $\otimes\colon A \times A \to A$ induces 1-cells $\otimes_{\mathcal{T}} : \mathcal{T}A \times_{\mathcal{T}} \mathcal{T}A \to \mathcal{T}A$ and $I_{\mathcal{T}} := \mathcal{T}(I_A)$.

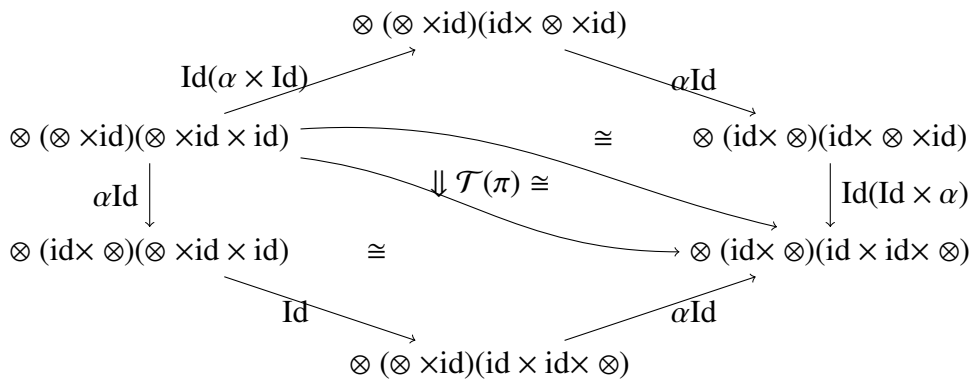
Since ϕ and ϕ_u are globular, we have an equality $\mathcal{T}(f \circ g) = \mathcal{T}(f) \circ \mathcal{T}(g)$ for all f and g and for the identity 1-cell we have an equality $\mathcal{T}(\mathrm{id}_A) = \mathrm{id}_{\mathcal{T}(A)}$. The loose associativity 2-cell of A gives rise to a loose 2-cell

$$\mathcal{T}(A) \times \mathcal{T}(A) \times \mathcal{T}(A) \;\underset{\otimes_{\mathcal{T}}(\otimes_{\mathcal{T}} \times \mathrm{Id})}{\overset{\otimes_{\mathcal{T}}(\mathrm{Id} \times \otimes_{\mathcal{T}})}{\Downarrow \alpha_{\mathcal{T}} \simeq}}\; \mathcal{T}(A)$$

which simply equals $\mathcal{T}(\alpha)$ together with the invertible 2-cells.

Likewise, the unit constraints l, r as well as the constraints for (braided) monoidal 1-cells σ induce 1-cells $l_{\mathcal{T}}, r_{\mathcal{T}}$, and $\sigma_{\mathcal{T}}$, respectively. Note that the swap functor τ is mapped by $\mathcal{T}$ to the swap functor for the product $\times_{\mathcal{T}}$, so $\sigma_{\mathcal{T}}$ is well-defined.

Furthermore, the invertible 3-cell filling the Mac Lane pentagon lifts to the invertible 3-cell of the Mac Lane Pentagon for $\mathcal{T}(A)$. Which is simply its image under $\mathcal{T}$, composed the natural transformations $\mathcal{T}_{\odot}$, ϕ,and ϕ_u ensuring that it has the right type.



Note that there may be several ways to paste these 3-cells together, but by coherence of enriched pseudo functors, the result is the same. Likewise, the isomorphic 3-cells μ, λ, ρ and the isomorphic 3-cells R, S, and ν witnessing the braiding and syllepsis, lift to the appropriate 3-cell for $\mathcal{T}(A)$. This is also the case for the isomorphic 3-cells R, S that characterise the braiding. Finally, the three equations between pasting composites of $\pi_{\mathcal{T}}, \mu_{\mathcal{T}}, \lambda_{\mathcal{T}}, \rho_{\mathcal{T}}$ hold by coherence of enriched pseudo functors.

Similarly, one can show that for a monoidal transformation f, $\mathcal{T}(f)$ is monoidal with structure loose 2-cells $\mathcal{T}(\iota_f)$ and $\mathcal{T}(\chi_f)$ and 3-cells obtained from $\mathcal{T}(\omega), \mathcal{T}(\gamma)$, and $\mathcal{T}(\delta)$ analogously to α. If f is braided, the braiding of $\mathcal{T}(f)$ is witnessed by the 3-cell obtained from $\mathcal{T}(u)$. Likewise, $\mathcal{T}$ preserves any monoidal, braided, sylleptic and symmetric structure of tight 2-morphisms, loose 2-cells and 3-cells. □

We are now ready to prove our main result.

Theorem 4.3.30. *Let $F : \mathcal{C} \to \mathcal{D}$ be a functor of locally cubical bicategories, such that the tight transformations ϕ, ϕ_u are globular. If F preserves products, then it lifts to the functors below between locally cubical bicategories, for $w \in \{l, o, s\}$.*

$$\mathcal{M}on_w F : \mathcal{M}on_w \mathcal{C} \to \mathcal{M}on_w \mathcal{D}$$
$$\mathcal{B}r\mathcal{M}on_w F : \mathcal{B}r\mathcal{M}on_w \mathcal{C} \to \mathcal{B}r\mathcal{M}on_w \mathcal{D}$$
$$\mathcal{S}yl\mathcal{M}on_w F : \mathcal{S}yl\mathcal{M}on_w \mathcal{C} \to \mathcal{S}yl\mathcal{M}on_w \mathcal{D}$$
$$\mathcal{S}ym\mathcal{M}on_w F : \mathcal{S}ym\mathcal{M}on_w \mathcal{C} \to \mathcal{S}ym\mathcal{M}on_w \mathcal{D}$$

Proof. By Lemma 4.3.29, the assignment of F on objects and higher cells is well-defined in the respective categories. We will show that the functor F gives rise to a pseudo double functor $\mathcal{M}on_l F : \mathcal{M}on_l \mathcal{C}(A, B) \to \mathcal{M}on_l \mathcal{D}(\mathcal{M}on_l F(A), \mathcal{M}on_l F(B))$. The other functors are derived in a similar way. We need to verify that $F(N^{\alpha \cdot \beta}) = F(N^{\alpha}) \cdot F(N^{\beta})$ and $F(N^{1_f}) = N^{1_{Ff}}$ in $\mathcal{M}on_l \mathcal{D}$ and likewise for Σ. This follows from functoriality of F, the fact that $N^{\alpha \cdot \beta} = N^{\alpha} \cdot N^{\beta}$ and $N^{1_f} = 1_{\iota_f}$, $F(\iota_f) = \iota_{Ff}$. The natural transformations $F_{\odot}$ and F_U are well-defined 3-cells in $\mathcal{M}onD$; the respective equations hold by coherence of the pseudo double functor F. Finally, we need to prove that ϕ and ϕ_u are well-defined tight transformations in $\mathcal{M}on(\mathcal{T}A, \mathcal{T}B)$. Since their components are globular 3-cells, we only need to check that these are monoidal. The equations hold by coherence of enriched functors after expanding the definitions of $M^{\mathcal{T}\alpha \circ \mathcal{T}\beta}, M^{\mathcal{T}(\alpha \circ \beta)}, M^{\mathcal{T}(\mathrm{Id}_f)}$, and $M^{\mathrm{Id}_{\mathcal{T}f}}$ and similarly for Π. □

We are now ready to state the main theorem of this section, which is that the functor $\mathcal{L}$ that maps double categories to their loose bicategories lifts to a functor of locally cubical bicategories. Recall that we write $\mathfrak{Dbl}_f$ for the locally cubical bicategory of double

categories, functors and transformations with loosely strong companions and $\mathfrak{Bicat}$ for the locally cubical bicategory of bicategories, functors, pseudo natural transformations, icons and cubical modifications. Furthermore, we use the prefix $\mathcal{M}on_w, \mathcal{B}r_w, \mathcal{S}yl_w$ and $\mathcal{S}ym_w$ to denote that the locally cubical bicategories of monoidal, braided, sylleptic or symmetric, double and bicategories, respectively, where $w \in \{l, c, s\}$ denotes whether the monoidal functors are lax, colax, or strong, respectively.

Theorem 4.3.31. *The functor* $\mathcal{L} : \mathfrak{Dbl}_f \to \mathfrak{Bicat}$ *lifts to the functors* $\mathcal{M}on_w\mathcal{L} : \mathcal{M}on_w\mathfrak{Dbl}_f \to \mathcal{M}on_w\mathfrak{Bicat}$, $\mathcal{B}r_w\mathcal{L} : \mathcal{B}r_w\mathfrak{Dbl}_f \to \mathcal{B}r_w\mathfrak{Bicat}$, $\mathcal{S}yl_w\mathcal{L} : \mathcal{S}yl_w\mathfrak{Dbl}_f \to \mathcal{S}yl_w\mathfrak{Bicat}$, *and* $\mathcal{S}ym_w\mathcal{L} : \mathcal{S}ym_w\mathfrak{Dbl}_f \to \mathcal{S}ym_w\mathfrak{Bicat}$ *for* $w \in \{l, o, s\}$.

Proof. Note that in the case of $\mathcal{L}$, ϕ and ϕ_u have globular components. The result then follows from Theorem 4.3.30 □

Chapter 5

Higher Categorical Models for Quantum Protocols

We discuss an abstract mathematical foundation for the diagrammatic language for quantum protocols introduced in [Vic12]. This language arises from a bicategorical description of quantum mechanics. We prove that the underlying bicategorical model has the desired properties for describing quantum protocols: being symmetric monoidal.

The formalism, which was first proposed by the author in [Wes13], is based on the algebraic approach to quantum mechanics. It extends this approach, by considering bimodules acting on C*-algebras. In the category **FHilb**, the bimodule action captures the correlation between the quantum state and a set of classical information. It turns out that quantum data types correspond to states in the model that are completely uncorrelated with the available classical information. On the other hand, classical data types are states that are maximally correlated with the available classical information. This is analogous to the case of decohered quantum systems, which exhibit a correlation between the state of the quantum system and the state of the environment, as one can see in equation A.0.1. A brief introduction to the notion of decoherence can be found in Appendix A.

In addition to classical and quantum data types, one can express protocols in their entirety, with the different probabilistic branches indexed by the classical structure.

This chapter is based on the final section of 'Constructing Symmetric Monoidal Bicategories Functorially' [HS19] and section 2 and 3 of the paper 'Mixed Quantum States in Higher Categories' [HVW14].

Related Work

The planar algebra induced by bicategories offers an intuitive tool for the description and verification of quantum protocols. In [Vic12] it is shown how various quantum

protocols such as quantum teleportation and dense coding can be expressed as a single diagram in this language. Verification of the correctness of diagrammatic protocols is often straightforward and can be automated [BKV16]. Examples are procedures for the construction of GHZ states and cluster states [RV18]. The diagrammatic language is also used to find a local hidden variable model for a subset of quantum mechanics in which a range of quantum protocols - entanglement creation, teleportation, dense coding, and secure key distribution - can be implemented [RV17].

Contribution

The symmetric monoidal structure of a bicategorical model is essential for the diagrammatic description of parallel processes. We prove the existence of this structure for a family of bicategories $\mathcal{A}lg[]$, constructed from monoidal categories. This family contains various bicategories that are relevant in the field of categorical quantum mechanics and other branches of category theory, such as the finite-dimensional versions of **2Hilb** and **2Vect** introduced in [KV94b], [BC04]. These are the bicategory of finite dimensional 2-Hilbert spaces, linear functors and natural transformations and the bicategory of finite-dimensional 2-vector spaces, linear functors and natural transformations, respectively. We show that the family gives rise to a functor from the locally cubical bicategory of monoidal categories to the locally cubical bicategory of monoidal bicategories. Hence, it provides a way of constructing a range of monoidal bicategories, pseudofunctors, transformations and modifications. Building on the theory developed in this chapter, we introduce the bicategory of mixed quantum states, which is contained in the larger structure $2[\mathrm{CP}^*[\mathbf{FHilb}]]$. This bicategory allows the description and verification of quantum teleportation and classical encryption, as shown in [HVW14]

Outline

In Section 5.1 we discuss the formalism of algebraic quantum mechanics in the more abstract form of algebras in a monoidal category. In section 5.2, we introduce the concept of bimodules on dagger Frobenius algebras in a dagger monoidal category. In Section 5.3, we establish that special dagger Frobenius algebras, dagger bimodels and bimodule homomorphisms form a weak bicategory. In section 5.4 we consider the bicategory $\mathcal{A}lg[\mathbf{C}]$ of algebras, bimodules and bimodule homomorphisms in a monoidal category $\mathbf{C}$. We apply Theorem 4.3.30 of Chapter 4 to prove that the construction $\mathcal{A}lg[-]$ gives rise to a functor of locally cubical bicategories which preserves braided and symmetric monoidal structure. We extend the result to include special dagger

Frobenius algebras in a monoidal category. Finally, in Section 5.5 we introduce the category of mixed quantum states.

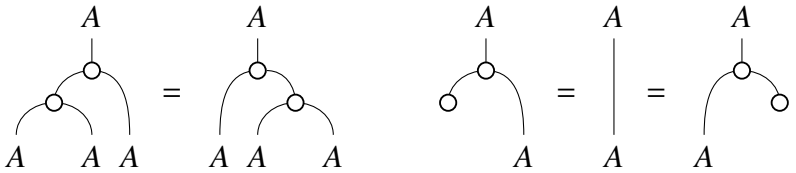
5.1 Algebraic Quantum Mechanics in Computer Science

In the field of quantum computing, the interaction of quantum information and classical information plays a key role through measurements, encoding of classical information, and controlled operations. These are essential in various important quantum protocols such as quantum teleportation, dense coding and classical encryption. As discussed in the introduction, algebraic quantum mechanics offers a suitable model for describing such interactions. This model captures classical and quantum information as two different instances of the same type of structure.

In this section we describe a framework for quantum computing based on algebraic quantum mechanics introduced in [CHK16]. The framework is a generalisation of algebraic quantum mechanics in the language of monoidal categories, based on dagger Frobenius algebras. Dagger Frobenius algebras correspond to C*-algebras in the dagger monoidal category of Hilbert spaces. The advantage of this generalisation stems from the diagrammatic language of monoidal categories, which turns complex calculations into visually intuitive procedures.

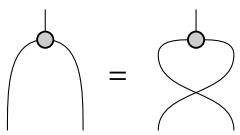
Definitions

We consider the abstract notion of an **algebra** $(A, \curlywedge, \circ)$ in a monoidal category **C**. This is also called a monoid. This is an object a, together with a multiplication morphism $\curlywedge : A \otimes A \to A$, as well as a unit morphism, $\circ : I \to A$, satisfying the associativity and unit law below.



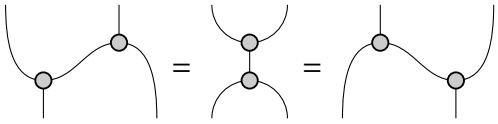
(5.1.1)

Definition 5.1.2. An algebra in a braided monoidal category **C** is called **commutative** whenever the following equation holds.



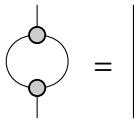
(5.1.3)

Definition 5.1.4. A **Frobenius algebra** in a monoidal category **C** is a **monoid** $(A, \curvearrowleft, \circ)$ together with a **comonoid** $(A, \curvearrowright, \circ)$ that satisfies the equations below.



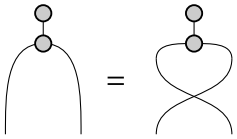
(5.1.5)

Definition 5.1.6. We call a pair of an algebra and a coalgebra **special** whenever the following equation holds.



(5.1.7)

It is called **symmetric** when the weaker condition below holds.



(5.1.8)

A Frobenius algebra in a monoidal dagger category is a **dagger Frobenius algebra** when the coalgebra is the dagger image of the algebra.

An **algebra homomorphism** $f : (A, \curvearrowleft, \circ) \to (B, \curvearrowleft, \circ)$ between two algebras is a morphism $f : A \to B$ in **C** that respects the multiplication: $f \circ \curvearrowleft = \curvearrowleft \circ (f \otimes f)$, and the unit: $\circ = f \circ \circ$.

It was shown in [Vic11, Lemma 4.1] that dagger Frobenius algebras in the monoidal dagger category of Hilbert spaces correspond to finite C*-algebras. Furthermore, commutative dagger Frobenius algebras correspond to commutative C*-algebras and algebra homomorphisms correspond to *-homomorphisms. Specifically, the unit of an n-dimensional classical structure corresponds to the sum of the basis elements of $\mathbb{C}^n$. The multiplication map is given by the inner product of states. Details are provided in [HV18]. We conclude that dagger Frobenius algebras, along with algebra homomorphisms, generalise classical states, quantum states and unitary evolutions.

Interpretation

The abstract formalism reflects some interesting characteristics of classical information. The co-multiplication associated with a commutative C*-algebra is an operator on the system which copies these states. The co-unit can be seen as a map that deletes or disregards the state. Commutativity assures that the output of the co-multiplication

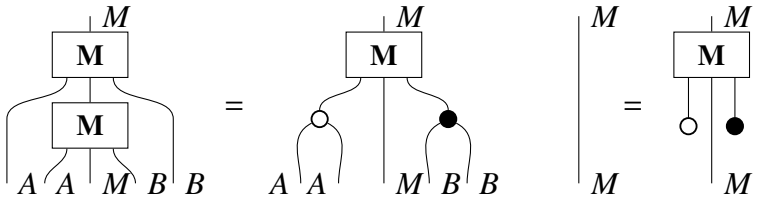
consists of two equal copies. Furthermore, the co-unit axiom guarantees that each of the copies equals the original state.

Copying of information is an essential procedure in classical computation. By the No-Cloning Theorem [Par70], quantum systems cannot be copied. Hence, this feature is unique to classical information.

5.2 Bimodules

As we have seen in the previous section, we can model classical information as commutative dagger Frobenius algebras and quantum information as non-commutative dagger Frobenius algebras in a monoidal category. Here, we take a slightly different approach. We will discuss a module-theoretic way to model quantum systems that are correlated to classical information. Classical data types arise as completely correlated systems and quantum data types arise as uncorrelated systems.

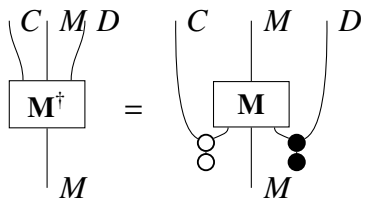
Let A and B be Frobenius algebras in a monoidal category $\mathbf{C}$. An A-B-**bimodule** in $\mathbf{C}$ is an object M together with a morphism $\mathbf{M} : A \otimes M \otimes B \to M$ in $\mathbf{C}$, satisfying the composition and unit law below.



(5.2.1)

For readability, we sometimes write A-B-bimodules $\mathbf{M}$ as ${}_A\mathbf{M}_B$ and we abbreviate the following compositions: ${}_\circ\mathbf{M} := \mathbf{M} \circ (\overset{\circ}{\downarrow} \otimes \mathrm{id})$, $\mathbf{M}_\circ := \mathbf{M} \circ (\mathrm{id} \otimes \overset{\circ}{\downarrow})$, and ${}_\circ\mathbf{M}_\circ := \mathbf{M} \circ (\overset{\circ}{\downarrow} \otimes \overset{\circ}{\downarrow})$.

A bimodule in a monoidal dagger category is called a **dagger bimodule** if the equation below holds, and the coalgebra is the dagger of the algebra and we denote $\dagger(\mathbf{M})$ by $\mathbf{M}^\dagger$.

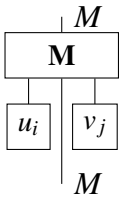


(5.2.2)

A **bimodule homomorphism** $\mathbf{f} : \mathbf{M} \to \mathbf{N}$ is a morphisms f of $\mathbf{C}$, such that $f \circ \mathbf{M} = \mathbf{N} \circ (\mathrm{id} \otimes f \otimes \mathrm{id})$.

Bimodules as Data Types

Each A-B-bimodule M on biproducts of Frobenius algebras $A = \oplus_{i=1}^{n}(A_i, m_i, u_i)$, $B = \oplus_{j=1}^{m}(B_j, n_j, v_j)$ corresponds to a decomposition $\mathbf{M} = \oplus_{i,j} P_{i,j}$ into the morphisms below.

$P_{i,j} :=$ 

(5.2.3)

One can easily verify from equations 5.2.1 and 5.2.2 that the morphisms $P_{i,j}$ are projectors. When, in addition, the category $\mathbf{C}$ has images, we can identify $\mathbf{M}$ with the direct sum of the images $\oplus_{i,j} P_{\mathbf{M}_{i,j}}(M)$. This means that each component of the classical structure corresponds to a component of the underlying object M.

In the case of Hilbert spaces, an $A-B-$bimodule on classical structures corresponds to a decomposition of the underlying Hilbert space into subspaces. The unit elements u_i, v_j are the basis elements of the classical structures A and B, respectively. Each subspace therefore corresponds to a basis element of the classical structure, which corresponds to one of the possible values of the classical structure. Each of these values restricts the possible quantum states to the corresponding subspace.

By Lemma 3.6.4 of [Wes13], any decomposition of a Hilbert space can be realised as a bimodule. When the bimodule $\mathbf{M}$ on a Hilbert space H corresponds to the decomposition $\oplus_{i=1}^{n}\mathbb{C}$, $\mathbf{M}$ corresponds to a classical data type. Conversely, when the bimodule action is trivial, we can identify $\mathbf{M}$ with H, so it is a quantum data type. Likewise, we can describe the states in different probabilistic branches of a protocol as a bimodule, where each state is indexed by the basis element of the classical structure.

5.3 The Bicategory of Algebras and Bimodules

Dagger Frobenius algebras, dagger bimodules and bimodule homomorphisms in a dagger monoidal category form a bicategory. A partial proof was given in [Wes13], which contains most data for horizontal composition, but not all. We provide the remaining details below. The material in this section is joint work with Jamie Vicary, except for Lemma 5.3.4.

Let $\mathbf{M}$ be an A-B-bimodule, and let $\mathbf{N}$ be a B-C-bimodule, the horizontal composition $\mathbf{M} \circ \mathbf{N}$ is defined by the diagram below. The pair $(c, M \circ N)$ is the coequalizer of the two morphisms $M \otimes B \otimes N \to M \otimes N$ induced by the two B-actions. As $\otimes$ preserves coequalizers, the pair $(A \otimes M \circ N \otimes C, \mathrm{id}_A \otimes c \otimes \mathrm{id}_C)$ is a coequalizer of the two morphisms

$A \otimes M \otimes B \otimes N \otimes C \to A \otimes M \otimes N \otimes C$. As the left-hand square commutes, the composite $c \circ \mathbf{M}_{\circ} \otimes {}_{\circ}\mathbf{N}$ is a cocone of the same two maps. By uniqueness of coequalizers, there is a unique map $A \otimes M_{\circ}N \otimes C \to M_{\circ}N$ making the right-hand square commute. This is the horizontal composition $\mathbf{M}_{\circ}\mathbf{N}$ of the two modules.

$$\begin{array}{ccccc} A \otimes M \otimes B \otimes N \otimes C & \overset{\mathrm{id}_A \otimes {}_{\circ}\mathbf{M} \otimes \mathrm{id}_N \otimes \mathrm{id}_C}{\underset{\mathrm{id}_A \otimes \mathrm{id}_M \otimes \mathbf{N}_{\bullet} \otimes \mathrm{id}_C}{\rightrightarrows}} & A \otimes M \otimes N \otimes C & \xrightarrow{\mathrm{id}_A \otimes c \otimes \mathrm{id}_C} & A \otimes M \circ N \otimes C \\ \downarrow{\scriptstyle \mathbf{M}_{\circ} \otimes \mathrm{id}_B \otimes {}_{\circ}\mathbf{N}} & & \downarrow{\scriptstyle \mathbf{M}_{\circ} \otimes {}_{\circ}\mathbf{N}} & & \downarrow{\scriptstyle \mathbf{M}\circ\mathbf{N}} \\ M \otimes B \otimes N & \overset{{}_{\circ}\mathbf{M}' \otimes \mathrm{id}_{N'}}{\underset{\mathrm{id}_{M'} \otimes \mathbf{N}'_{\bullet}}{\rightrightarrows}} & M \otimes N & \xrightarrow[c]{} & M \circ N \end{array} \tag{5.3.1}$$

Furthermore, $\mathbf{M}_{\circ} \otimes {}_{\circ}\mathbf{N}$ is a module. It is easy to check that $\mathbf{M}_{\circ}\mathbf{N}$ satisfies the module axioms as well, using commutativity of the diagram above and the fact that c is epic.

The horizontal composition of 2-cells $f\colon \mathbf{M} \to \mathbf{M}'$ and $g\colon \mathbf{N} \to \mathbf{N}'$ is the unique arrow making the following diagram commute:

$$\begin{array}{ccccc} M \otimes D \otimes N & \overset{{}_{\circ}\mathbf{M} \otimes \mathrm{id}[N]}{\underset{\mathrm{id}[M] \otimes \mathbf{N}_{\bullet}}{\rightrightarrows}} & M \otimes N & \xrightarrow{c} & M \circ N \\ \downarrow{\scriptstyle (f \otimes \mathrm{id}[D] \otimes g)} & & \downarrow{\scriptstyle f \otimes g} & & \downarrow{\scriptstyle f \circ g} \\ M' \otimes D \otimes N' & \overset{{}_{\circ}\mathbf{M}' \otimes \mathrm{id}[N']}{\underset{\mathrm{id}[M'] \otimes \mathbf{N}'_{\bullet}}{\rightrightarrows}} & M' \otimes N' & \xrightarrow[c']{} & M' \circ N' \end{array} \tag{5.3.2}$$

Pasting diagrams 5.3.1 and 5.3.2 together into a cube proves that $(f \circ g)$ is a bimodule homomorphism. With this additional data, we can complete the result of [Wes13].

Proposition 5.3.3. *If* $\mathbf{C}$ *is a dagger monoidal category where all coequalizers exist, then the following data defines a bicategory* $2[\mathbf{C}]$*:*

- *0-cells are special dagger Frobenius algebras in* $\mathbf{C}$*;*
- *1-cells are dagger bimodules; the identity 1-cell on* $(C, \curvearrowright, \circ)$ *is* $\curvearrowright$*;*
- *2-cells are dagger bimodule homomorphisms;*
- *horizontal composition is given by* (5.3.1) *and* (5.3.2)*;*

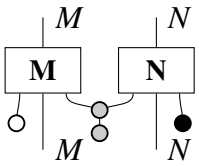
Proof. In [Wes13] is it shown that these data satisfy all coherence conditions required of a weak bicategory. □

The main example of this approach is the bicategory **2Hilb** of 2-Hilbert spaces, linear functors and natural transformations [Bae97]. It was shown in the author's MSc.

thesis [Wes13] that **2Hilb** is equivalent to the bicategory 2[**FHilb**] of special dagger Frobenius algebras, dagger bimodules and bimodule homomorphisms in **FHilb**.

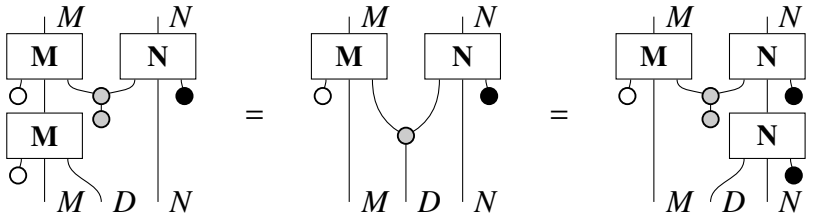
Requiring the existence of *all* coequalizers is not necessary, as we only use the existence of the specific coequalizers in 5.3.1. We give a sufficient condition for horizontal composition to be well-defined, even if not all coequalizers exist, based on *splittings* of dagger idempotents. A map $f\colon A \to A$ is a **dagger idempotent** if $f^2 = f = f^\dagger$. A dagger idempotent f **splits** when there is a map i such that $f = i \circ i^\dagger$ and $i^\dagger \circ i = \mathrm{id}$.

Lemma 5.3.4. *Let* $\mathbf{M}, \mathbf{N}$ *be dagger bimodules. The horizontal composition* $\mathbf{M}_\circ\mathbf{N}$ *is well-defined when the morphism below splits.*

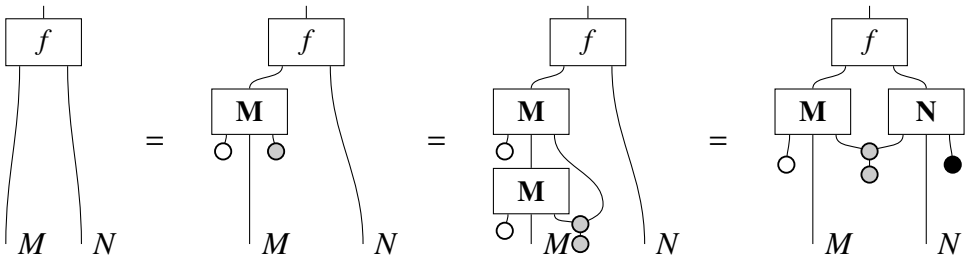


(5.3.5)

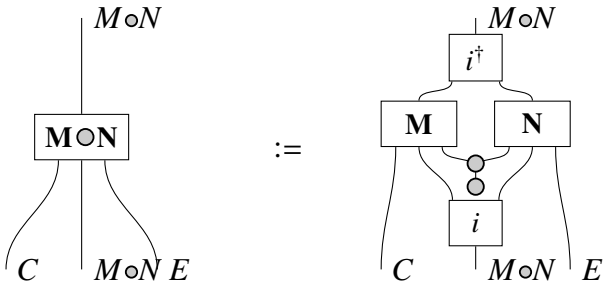
Proof. Let i be the dagger splitting of 5.3.5. The dagger $i^\dagger$ is a cocone of $({}_\circ\mathbf{M} \otimes \mathrm{id}[N])$ and $(\mathrm{id}[M] \otimes \mathbf{N}_\bullet)$ by the equalities below.



Furthermore, if $f({}_\circ\mathbf{M} \otimes \mathrm{id}[N]) = f(\mathrm{id}[M] \otimes \mathbf{N}_\bullet)$, the equations below show that f factors uniquely through $i^\dagger$. The factorization is unique: if $f = mi^\dagger$, then $m = mi^\dagger i = fi$. Hence, $i^\dagger$ is a coequalizer of the two maps.



It is easy to check that the map below makes the right-hand square of 5.3.1 commute for the coequalizer $i^\dagger$. Therefore, it is the horizontal composition of $\mathbf{M}$ and $\mathbf{N}$.

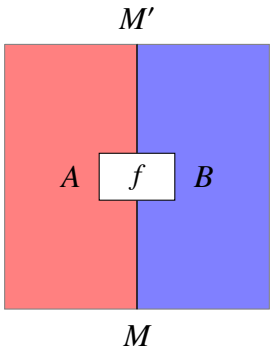


(5.3.6)

□

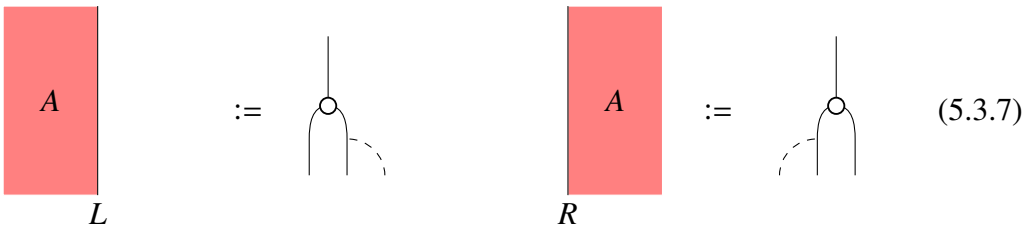
The Diagrammatic Language

The planar language for bicategories provides a way to visualise quantum protocols. The computational states are visualised as lines M, M'. These correspond to quantum systems which are correlated to classical information, visualised as the the coloured regions A, B, bordering the lines. Transformations of the computational states are bimodule homomorphisms, which are depicted as boxes.



Quantum data types correspond to modules on trivial classical regions. As there is no non-trivial interaction, the module contains no information other than the underlying object. In the case of **2Hilb**, this underlying object is a Hilbert space. Therefore, it can be interpreted as a quantum system. Such a system is in a pure quantum state.

Classical data types can be characterised diagrammatically in this language as *classical witnesses*, [Vic12, Section 2.3]. In [HVW14, Lemma 10], it was shown that special dagger Frobenius algebras indeed give rise to bimodules that satisfy the diagrammatic axioms of a classical witness. This result was implicitely derived in [Wes13]. Such classical data types are of the form $\mathbf{R}_{\circ}\mathbf{L}$, where $\mathbf{L}$ and $\mathbf{R}$ are the bimodules below, arising from a special dagger Frobenius algebra.



(5.3.7)

Similarly, measurements and controlled operations can be characterised diagrammatically as 2-cells of a certain form. As shown in [Vic12], these building blocks are sufficient to express and verify correctness of quantum teleportation, dense coding, complementary observables and quantum erasure, in purely diagrammatic terms.

5.4 The Monoidal Structure

An essential feature of a theory of physics is a procedure to combine various separate systems into one compound system. In computation, such a procedure allows one to reason about sub-procedures of an algorithm and to model parallel computations. In the Hilbert space formalism for quantum mechanics, the tensor product serves this purpose. The appropriate generalisation for categorical models is the existence of symmetric monoidal structure.

In this section we demonstrate that the bicategory of dagger Frobenius algebras, dagger bimodules and bimodule homomorphisms in a monoidal dagger category $\mathbf{C}$ is symmetric monoidal whenever $\mathbf{C}$ is symmetric monoidal.

We consider the construction $\mathcal{A}lg[]$, that maps a braided monoidal category $\mathbf{C}$ to the bicategory of algebras, bimodules and bimodule homomorphisms in $\mathbf{C}$. We apply Theorem 4.3.30 of Chapter 4 to demonstrate that the construction $\mathcal{A}lg[]$ gives rise to functors of locally cubical bicategories below. We then specialise the result to special dagger Frobenius algebras.

$$\mathcal{B}r\mathcal{M}on_s\mathcal{C}at \to \mathcal{B}r\mathcal{M}on_s\mathcal{B}icat$$
$$\mathcal{S}ym\mathcal{M}on_s\mathcal{C}at \to \mathcal{S}ym\mathcal{M}on_s\mathcal{B}icat$$

To obtain this result, we define the double category $\mathbb{A}lg[\mathbf{C}]$, whose loose bicategory corresponds to $\mathcal{A}lg[\mathbf{C}]$, and we show that $\mathbb{A}lg[\mathbf{C}]$ is fibrant and braided monoidal. This assignment gives rise to several pseudofunctors between bicategories of monoidal

categories and bicategories of fibrant monoidal double categories. Composing these functors with the functors from Theorem 4.3.30, gives the required result. This general theorem covers various categories of interest, such as **2Hilb** and **2Vect**.

The Bicategory $\mathcal{A}lg$

Let $\mathbf{C}$ be a braided monoidal category. We consider the bicategory $\mathcal{A}lg[\mathbf{C}]$ consisting of the elements listed below.

- objects are algebras in $\mathbf{C}$;
- 1-cells are bimodules; the identity 1-cell on $(C, \cap, \cup)$ is $\cap$;
- 2-cells are bimodule homomorphisms;
- horizontal composition of 1-cells is given by (5.3.1);
- horizontal composition of 2-cells is given by (5.3.2);

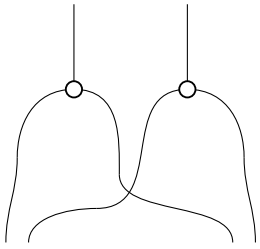
Structural data regarding this construction, such as loose composition, is as described in Section 5.3.

The Double Category $\mathbb{A}lg$

We will define a double category whose loose bicategory is the bicategory $\mathcal{A}lg[\mathbf{C}]$. The tight morphisms in this double category are algebras homomorphisms.

Lemma 5.4.1. *Let* $\mathbf{C}$ *be a braided monoidal category. The category of algebras and algebra homomorphisms in* $\mathbf{C}$ *is braided monoidal. It is symmetric whenever* $\mathbf{C}$ *is symmetric.*

Proof. The tensor product for algebras, depicted below, is inherited from the original monoidal category.



The unit object is the trivial algebra on the unit for the original monoidal structure with multiplication given by $\lambda_I = \rho_I$.

The structure isomorphisms in $\mathbf{C}$ are all algebra homomorphisms. In principle this can be shown directly, but in the diagrammatic calculus this holds trivially. Similarly, if $\mathbf{C}$ is braided monoidal, then the braiding in $\mathbf{C}$ defines a braiding on the category of algebras and algebra homomorphisms.

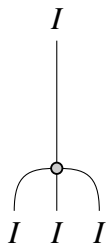
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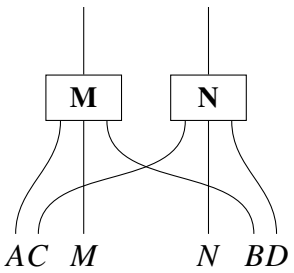
What is left is an appropriate notion of morphisms between bimodules, which map between algebra homomorphisms in the loose direction. We denote tight composition in the double category by $\circ$ and loose composition by $\odot$.

An **extended bimmodule homomorphism** $\mathbf{f} : \mathbf{M} \to \mathbf{N}$ is a triple of 2-cells $(A \xrightarrow{f_l} C, M \xrightarrow{f} N, B \xrightarrow{f_r} D)$ such that $f \circ \mathbf{M} = \mathbf{N} \circ (f_l \otimes f \otimes f_r)$. When f_l and f_r are both identities, this corresponds to the standard definition of a **bimodule homomorphism**.

Lemma 5.4.3. *Bimodules and extended bimodule homomorphisms in a braided or symmetric monoidal category* $\mathbf{C}$ *form a braided or symmetric monoidal category, respectively.*

Proof. On morphisms, the tensor product is defined as $(f_l, f, f_r) \otimes (g_l, g, g_r) := (f_l \otimes g_l, f \otimes g, f_r \otimes g_r)$. The tensor product on objects is given below, as well as the unit object. In this definition the object I is the unit object of $\mathbf{C}$.

$\mathbf{I} :=$ 

$_A\mathbf{M}_B \otimes {}_C\mathbf{N}_D :=$ 

(5.4.4)

We may draw the multiplication on the unit object symmetrically because of the associativity condition for algebras. The associator, unitor, and swap natural isomorphisms are given by the maps with the following components, where α, λ, and ρ are the structure isomorphisms of the original category.

$$\alpha_{{}_A\mathbf{M}_{B,C}\mathbf{N}_{D,E}\mathbf{P}_F} := (\alpha_{A,C,E}, \alpha_{M,N,P}, \alpha_{B,D,F}) \tag{5.4.5}$$

$$\lambda_{{}_A\mathbf{M}_B} := (\lambda_A, \lambda_M, \lambda_B) \tag{5.4.6}$$

$$\rho_{{}_A\mathbf{M}_B} := (\rho_A, \rho_M, \rho_B) \tag{5.4.7}$$

$$\sigma_{\mathbf{A}\mathbf{M}_{\mathbf{B}},\mathbf{C}\mathbf{N}_{\mathbf{D}}} := (\sigma_{A,C}, \sigma_{M,N}, \sigma_{B,D}) \tag{5.4.8}$$

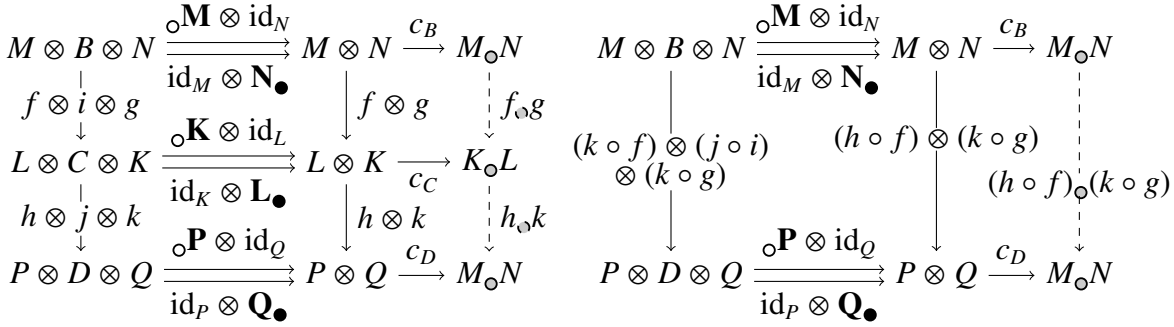
□

For clarity, we write algebras and algebra homomorphisms in normal font and we write bimodules and (extended) bimodule homomorphisms in bold. This will help distinguishing between the two categories, which together form a double category.

Proposition 5.4.9. *Let* **C** *be a monoidal category where all coequalizers exist, and where the tensor product preserves coequalizers. The category* $\mathbb{D}_0$ *of algebras and algebra homomorphisms of* **C** *and the category* $\mathbb{D}_1$ *of bimodules and extended bimodule homomorphisms of* **C** *form a double category, which we call* $\mathbb{A}lg$

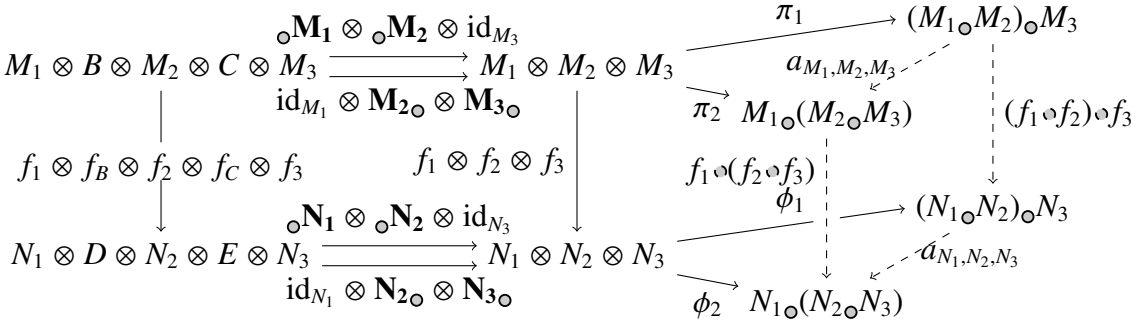
Proof. The unit functor $\mathbb{D}_0 \xrightarrow{U} \mathbb{D}_1$ is defined on objects as $U(A, \curvearrowleft, \curvearrowleft) := \curvearrowleft$; and on morphisms as $U(f) := (f, f, f)$. The source and target functors $S, T : \mathbb{D}_1 \to \mathbb{D}_0$ are defined on objects as $S({}_A\mathbf{M}_B) = A$, and $T({}_A\mathbf{M}_B) = B$, and on morphisms as $S(f_l, f, f_r) = f_l$, and $T(f_l, f, f_r) = f_r$. The functor $\odot : \mathbb{D}_1 \times_{\mathbb{D}_0} \mathbb{D}_1 \to \mathbb{D}_1$, maps objects $({}_A\mathbf{M}_B, {}_B\mathbf{N}_C)$ to ${}_A\mathbf{M} \circ \mathbf{N}_C$, and morphisms $((f_l, f, h), (h, g, g_r))$ to $(f_l, f \circ g, g_r)$, defined in 5.3.1 and 5.3.2.

It is left to verify functoriality of $\odot$. This comes down to checking that $(f \circ f') \circ (g \circ g') = (f \circ f') \circ (g \circ g')$, and $\mathrm{id}_{\mathbf{M}} \circ \mathrm{id}_{\mathbf{M}'} = \mathrm{id}_{\mathbf{M} \circ \mathbf{M}'}$. The two maps that form the first equality are the unique morphisms that make the two diagrams below commute. The outer left squares of the two diagrams are equal by the exchange law for $\otimes$ and $\circ$. As a consequence, the dashed arrows must be equal too. A similar argument shows that $\mathrm{id}_{\mathbf{M}} \circ \mathrm{id}_{\mathbf{M}'} = \mathrm{id}_{\mathbf{M} \circ \mathbf{M}'}$.



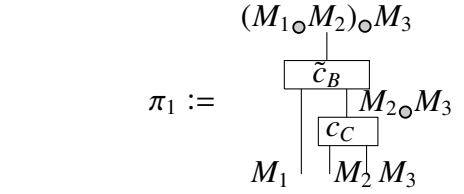
(5.4.10)

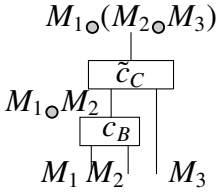
The associator $\mathbf{a} : (\mathbf{M_1} \odot \mathbf{M_2}) \odot \mathbf{M_3} \to \mathbf{M_1} \odot (\mathbf{M_2} \odot \mathbf{M_3})$ is an extended algebra homomorphism of the form $(\mathrm{id}, a, \mathrm{id})$. The components of the morphism a are defined as the unique maps that make the diagram below commute. Naturality of a follows from commutativity of the rightmost square of the diagram, which commutes because all other sub diagrams commute.



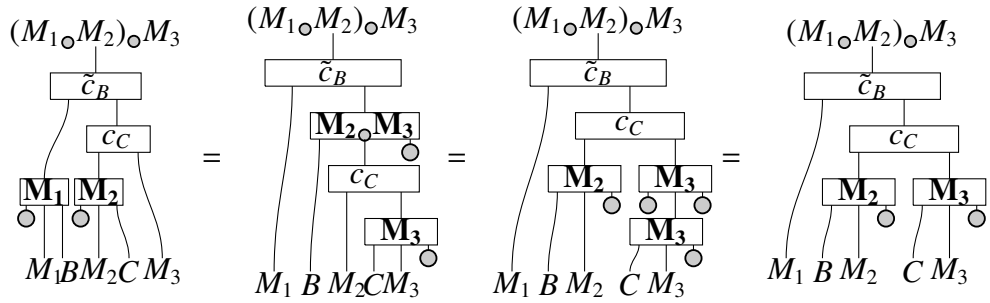
The coequalisers π_1 and π_2 correspond to the compositions of coequalisers below.

$$\pi_1 := \quad \pi_2 := \tag{5.4.11}$$

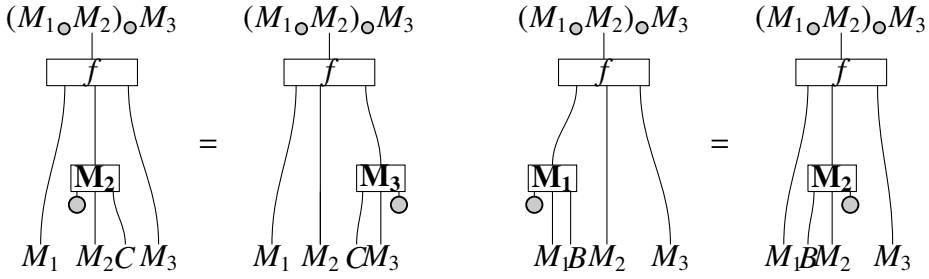




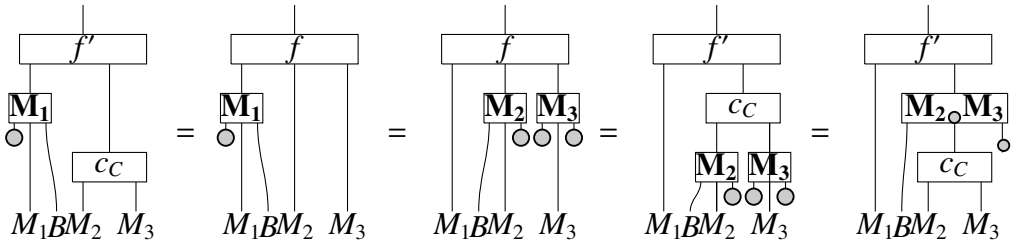
To verify that π_1 is a coequaliser we first check that it is a cocone of $_\circ\mathbf{M_1} \otimes {}_\circ\mathbf{M_2} \otimes \mathrm{id}_{M_3}$ and $\mathrm{id}_{M_1} \otimes \mathbf{M_{2\circ}} \otimes \mathbf{M_{3\circ}}$. This follows from the equalities below.



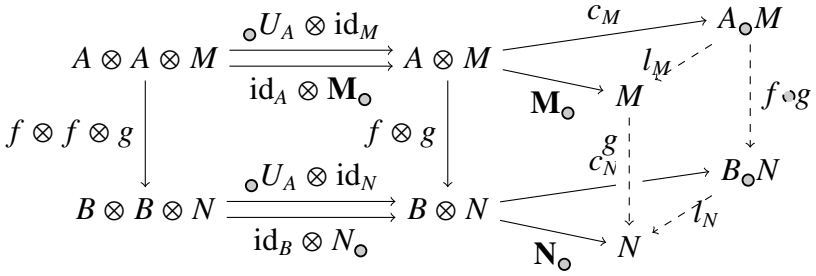
The last step to show that π_1 is a coequaliser, is to prove that if we have another cocone f, then f factorises through π_1. Let f be such a cocone. First of all, it is easy to show that the two equalities below hold, expressing that f is a cocone of the respective pairs of morphisms. One obtains this by plugging the unit on B or C, respectively, in the cocone equality for f and then applying the unit laws for modules.



It follows from the first equality that f factorises through $\mathrm{id}_{M_1} \otimes c_C$. This means that there exists a morphism f' such that $f = f' \circ (\mathrm{id}_{M_1} \otimes c_C)$. From the second statement we deduce that f' factorises through $\tilde{c}_B$, which finishes our proof. The equations below and the fact that $\mathrm{id} \otimes c_C$ is epic imply that f' is a cocone of ${}_{\circ}\mathbf{M_1} \otimes \mathrm{id}_{M_2} \otimes \mathrm{id}_{M_3}$ and $\mathrm{id}_{M_1} \otimes \mathbf{M_2}_{\circ}\mathbf{M_3}_{\circ}$. As a result, f' factorises through $\mathrm{id}_{M_1} \otimes \tilde{c}_B$. Hence, there exists a morphism f'' such that $f = f'' \circ \tilde{c}_B \circ (\mathrm{id}_{M_1} \otimes c_C) = f'' \circ \pi_1$. One can use a similar argument to show that π_2 is a coequaliser.



The components of the left unitor $l_{\mathbf{M}} : U_A \odot \mathbf{M} \to \mathbf{M}$ are given by $(\mathrm{id}, l_M, \mathrm{id})$, where l_M is defined as follows: By the module laws, $\mathbf{M}_{\circ} : A \otimes M \to M$ is a coequaliser of the maps ${}_{\circ}\mathbf{A} \otimes \mathrm{id}_M$ and $\mathrm{id}_A \ \mathbf{M}_{\circ}$. The canonical isomorphisms between $\mathbf{M}$ and $\mathbf{A}_{\circ}\mathbf{M}$ is the middle component of $l_{\mathbf{M}}$, and naturality of l follows from commutativity of the diagram below. We can define r, and prove its naturality, in a similar way.



□

The Braided Monoidal Structure of $\mathbb{A}lg$

In this section we will prove that $\mathbb{A}lg[\mathbf{C}]$ is a braided monoidal double category and that it is symmetric whenever $\mathbf{C}$ is symmetric.

Proposition 5.4.12. *Let* $\mathbf{C}$ *be a braided monoidal category where all coequalisers exist and where the tensor product preserves coequalisers. The double category* $\mathbb{A}lg[\mathbf{C}]$ *of algebras, bimodules and bimodule homomorphisms in* $\mathbf{C}$ *is braided monoidal. It is symmetric, whenever* $\mathbf{C}$ *is symmetric, respectively.*

Proof. By Lemma 5.4.1 and 5.4.3, $\mathbb{D}_0$ and $\mathbb{D}_1$ are braided or symmetric monoidal when $\mathbf{C}$ is braided or symmetric. Clearly, S and T are strict monoidal functors preserving

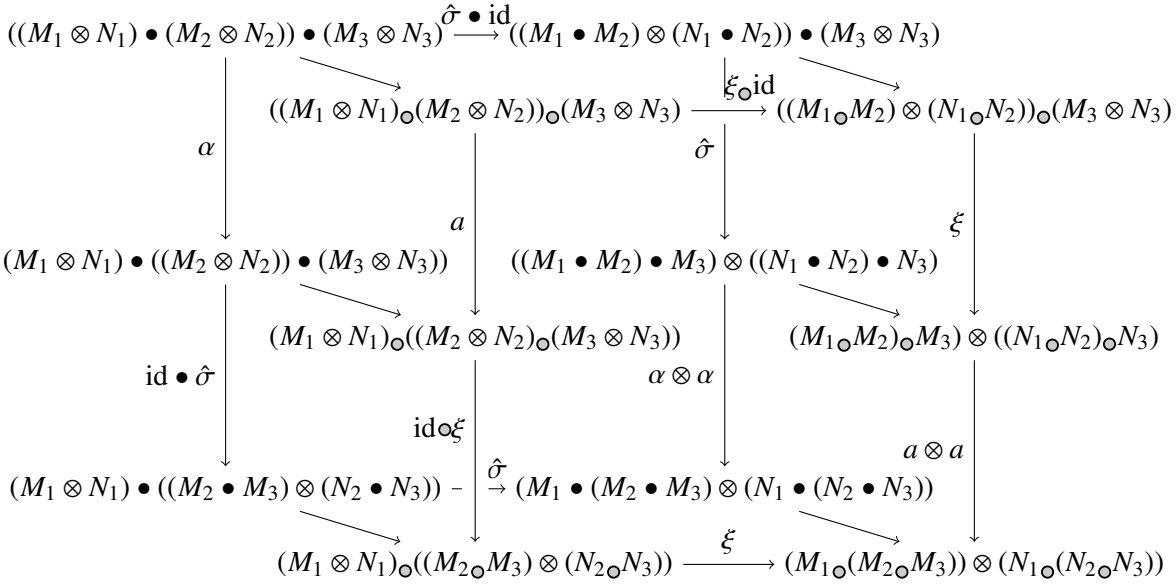
the associativity and unit constraints, and U_I is the monoidal unit of D_1, when I is the monoidal unit of D_0.

Unfolding definitions shows that the globular isomorphism $\mathfrak{u}$ from $U \circ \otimes$ to $\otimes \circ (U \times U)$ is the identity. We define the exchange law, $\mathfrak{x}$, between the functors $\odot$ and $\otimes$ as $(\mathrm{id}, \xi, \mathrm{id})$, where ξ is the unique morphism completing the commuting diagram below. In this diagram, c, c_M, and c_N are the coequalisers defining $(M_1 \otimes N_1)_{\circ}(M_2 \otimes N_2)$, $M_1{}_{\circ}M_2$, and $N_1{}_{\circ}N_2$, respectively. By a similar argument given while defining the associator $\mathbf{a}$ for the double category, one can show that $c_M \otimes c_N$ is the coequaliser of the lower two parallel maps in the diagram. The two left-most vertical morphisms are natural isomorphisms constructed from swap maps. For later use, we will denote the middle morphism by $\hat{\sigma}$.

$$
\begin{array}{ccccc}
 & & {}_{\circ}(\mathbf{M_1} \otimes \mathbf{M_2}) \otimes \mathrm{id}_{N_1 \otimes N_2} & & \\
(M_1 \otimes M_2) \otimes & \longrightarrow & & & (M_1 \otimes N_1)\circ \\
(B_1 \otimes B_2) \otimes (N_1 \otimes N_2) & \longrightarrow & (M_1 \otimes M_2) \otimes (N_1 \otimes N_2) & \xrightarrow{\mathrm{c}} & (M_2 \otimes N_2) \\
 & & \mathrm{id}_{M_1 \otimes M_2} \otimes (\mathbf{N_1} \otimes \mathbf{N_2})_{\bullet} & & \\
\cong \downarrow & & \downarrow \hat{\sigma} \cong & & \vdots\ \xi \cong \\
 & & ({}_{\circ}\mathbf{M_1} \otimes \mathrm{id}_{N_1}) \otimes ({}_{\circ}\mathbf{M_2} \otimes \mathrm{id}_{N_2}) & & \downarrow \\
(M_1 \otimes B_1 \otimes N_1)\otimes & \longrightarrow & & & (M_1 \circ M_2)\otimes \\
(M_2 \otimes B_2 \otimes N_2) & \longrightarrow & (M_1 \otimes N_1) \otimes (M_2 \otimes N_2) & \xrightarrow[c_M \otimes c_N]{} & (N_1 \circ N_2) \\
 & & (\mathrm{id}_{M_1} \otimes \mathbf{N_{1\bullet}}) \otimes (\mathrm{id}_{M_2} \otimes \mathbf{N_{2\bullet}}) & &
\end{array}
\tag{5.4.13}
$$

It is left to prove that the diagrams 4.1.8- 4.1.16 commute. Because $\mathfrak{u}$ and $\mathfrak{x}$ are globular, it suffices to verify commutativity of the diagrams for the middle component of the extended module homomorphisms.

Diagram 4.1.8 corresponds to the front square of the diagram below. The unlabelled arrows represent the coequalisers defining their target object. The back square commutes by coherence of the braided monoidal category $\mathbf{C}$. The squares on the sides commute by definition of ξ, $\mathbf{a}$ and $\circ$. It follows that the front square must commute as well, which is what we wanted to prove.



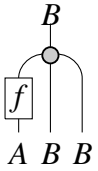
The equations 4.1.9, 4.1.10, 4.1.11, 4.1.13, 4.1.15, 4.1.17 concerning ξ are proven in the same way. It is easy to see that the other equations, 4.1.12, 4.1.14, 4.1.16, 4.1.18, concerning $\mathfrak{u}$ hold, as $\mathfrak{u}$ is the identity, and $U_{\alpha_{A,B,C}} = \alpha_{U_A,U_B,U_C}$, $U(\rho_A) = \rho_{U_A}$, $U(\lambda_A) = \lambda_{U_A}$, and $\sigma_{U_A,U_B} = U(\sigma_{A,B})$. □

Companions and Conjoints in $\mathbb{A}lg$

Finally, we will prove that $\mathbb{A}lg[\mathbf{C}]$ is fibrant. This is the last step we need to take to show that we can lift $\mathbb{A}lg[\mathbf{C}]$ to obtain the bicategory $\mathcal{A}lg[\mathbf{C}]$, which preserves any braided monoidal structure.

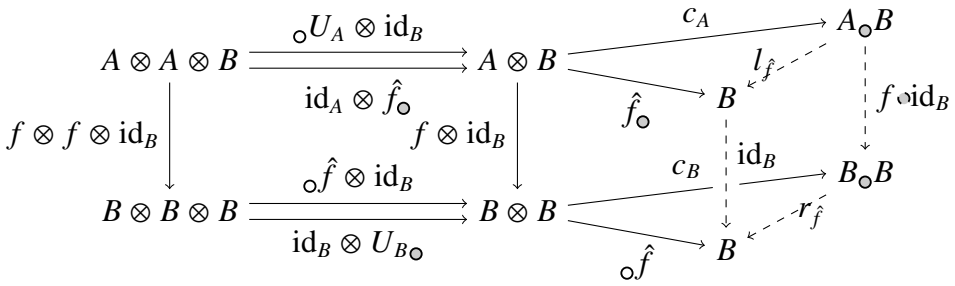
Lemma 5.4.14. *Let* $\mathbf{C}$ *be a braided monoidal category. The double category* $\mathbb{A}lg[\mathbf{C}]$ *is fibrant.*

Proof. Let f be a morphism of $\mathbb{D}_0$. The companion of f is defined by the following data:

$\hat{\mathbf{f}} :=$ 

$\eta_{\hat{\mathbf{f}}} := (id_A, f, f) \qquad \epsilon_{\hat{\mathbf{f}}} := (f, \mathrm{id}_B, \mathrm{id}_B)$ (5.4.15)

The first equation of 4.1.26 holds because $\epsilon_{\hat{\mathbf{f}}} \circ \eta_{\hat{\mathbf{f}}} = (f, f, f) = \mathbf{U}_f$. The left-hand-side of the second equation corresponds to $\eta_{\hat{\mathbf{f}}} \odot \epsilon_{\hat{\mathbf{f}}} = (id_A, f \circ \mathrm{id}_B, \mathrm{id}_B) : \mathbf{U}_A \circ \hat{\mathbf{f}} \to \hat{\mathbf{f}} \circ \mathbf{U}_B$, where $f \circ \mathrm{id}_B$: is the unique map that makes the back of the diagram below commute.



(5.4.16)

We need to show that $f \circledcirc \mathrm{id}_B \cong \mathrm{id}_B$. In this diagram, c_A and c_B are the coequalisers defining $\mathbf{U}_{A\circ}\hat{\mathbf{f}}$ and $\hat{\mathbf{f}}_\circ\mathbf{U}_B$, respectively. It is easy to check that $\hat{f}_\circ$ and ${}_\circ\hat{f}$ are coequalisers as well. The morphisms id_B, $l_{\hat{f}}$ and $r_{\hat{f}}$ are the unique morphisms that make all diagrams commute. It follows from coherence of double categories that $f \circledcirc \mathrm{id}_B \cong \mathrm{id}_B$, and thus $\eta_{\hat{f}} \odot \epsilon_{\hat{f}} \cong 1_{\hat{f}}$. This simultaneously proves that f has a conjoint, because $\mathbb{A}lg[\mathbf{C}^{h*op}] \cong \mathbb{A}lg[\mathbf{C}]$. □

Theorem 5.4.17. *Let* $\mathbf{C}$ *be a braided monoidal category where all coequalisers exist and where the tensor product preserves coequalisers. The loose bicategory* $\mathcal{A}lg(\mathbf{C})$ *is braided monoidal; it is symmetric whenever* $\mathbf{C}$ *is symmetric.*

Proof. By 5.4.9, 5.4.12, 5.4.14, $\mathbb{A}lg[\mathbf{C}]$ is braided monoidal and fibrant; and it is symmetric whenever $\mathbf{C}$ is symmetric, respectively. As a result, all constraints have loosely strong companions. Therefore we may apply Theorem 4.3.30 to finish the proof. □

Example 5.4.18. When we take $\mathbb{A}lg(\mathcal{A}B)$ of the category of Abelian groups and group homomorphisms as our symmetric monoidal category, we obtain the double category $\mathbb{M}\mathsf{od}$ of rings, ring homomorphisms, bimodules and bimodule homomorphisms. As a consequence of Lemmas 5.4.9, 5.4.12, 5.4.14, and Theorem 4.3.30, the loose bicategory $\mathcal{M}od$ of $\mathbb{M}\mathsf{od}$ is symmetric monoidal.

Monoidal Functors and Transformations

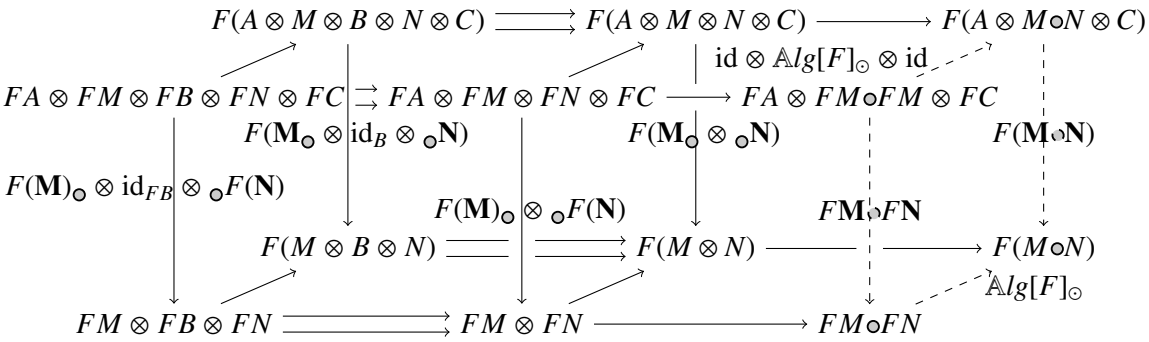
We extend $\mathbb{A}lg$ to functors and transformations and show that it gives rise to a pseudofunctor.

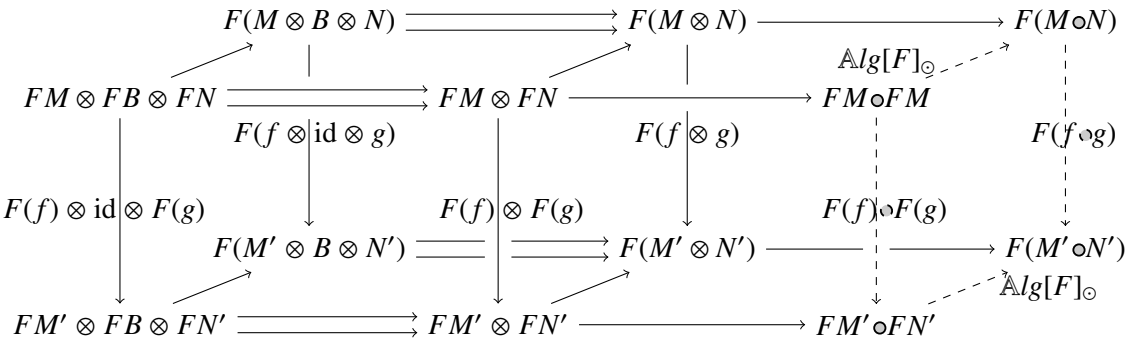
Proposition 5.4.19. *Any braided monoidal strong functor* $F : \mathbf{C} \to \mathbf{D}$ *which preserves coequalisers lifts to a braided monoidal strong double functor* $\mathbb{A}lg[F] : \mathbb{A}lg[\mathbf{C}] \to \mathbb{A}lg[\mathbf{D}]$. *The functor* $\mathbb{A}lg[F]$ *is symmetric, whenever* F *is symmetric, respectively.*

Proof. Any braided monoidal functor preserves algebras and bimodules. The functor $\mathbb{A}lg[F]_0$ maps an algebra $(A, \curvearrowleft, \circ)$ to the algebra $(FA, F(\curvearrowleft) \circ \chi, F(\circ) \circ \iota)$. The functor $\mathbb{A}lg[F]_1$ maps an A-B-bimodule $\mathbf{M}$ to $F(\mathbf{M}) \circ \chi_{A,M\otimes B} \circ (\mathrm{id} \otimes \chi_{M,B})$. On extended bimodule homomorphisms, $\mathbb{A}lg$ is defined component-wise. The pseudo double transformation $\mathbb{A}lg[F]_\odot$ is the unique morphism defined by the coequalisers below.

$$\begin{array}{ccccc}
FM \otimes FB \otimes FN & \underset{\mathrm{id}_{F(M)} \otimes F(\mathbf{N})_\bullet}{\overset{{}_\circ F(\mathbf{M}) \otimes \mathrm{id}_{F(N)}}{\rightrightarrows}} & FM \otimes FN & \xrightarrow{\mathrm{c}} & FM \circ FN \\
\cong \downarrow & & \downarrow \chi \cong & & \downarrow \mathbb{A}lg[F]_\odot \\
F(M \otimes B \otimes N) & \underset{F(\mathrm{id}_{M_1} \otimes \mathbf{N}_\bullet)}{\overset{F({}_\circ \mathbf{M} \otimes \mathrm{id}_N)}{\rightrightarrows}} & F(M \otimes N) & \xrightarrow[F(c)]{} & F(M \circ N)
\end{array} \tag{5.4.20}$$

The two commuting diagrams below show that $\mathbb{A}lg[F]_\odot$ is an extended bimodule homomorphism and that $\mathbb{A}lg[F]_\odot$ is natural in $\mathbb{A}lg[\mathbf{D}]_1$.

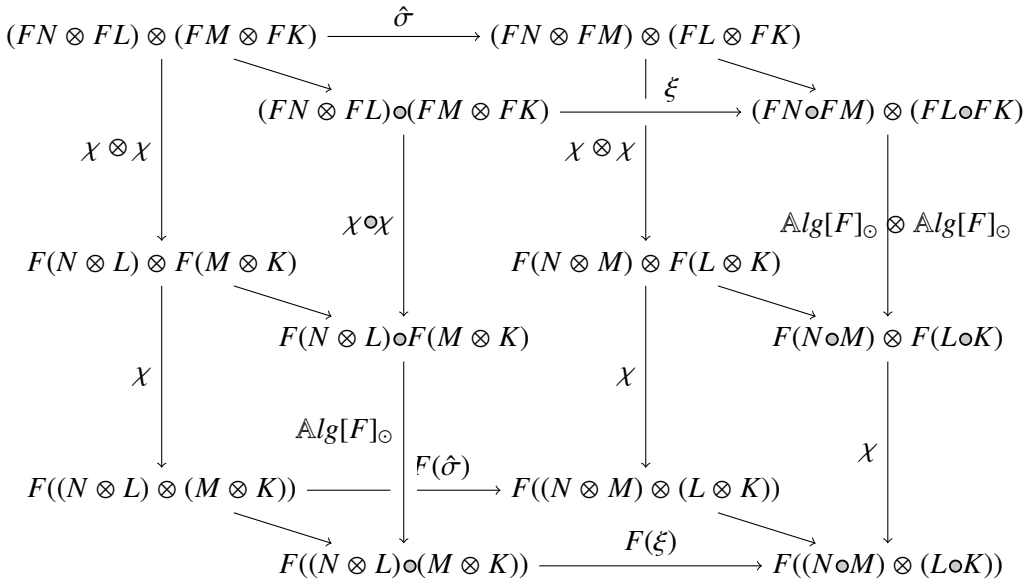




One can show with a similar commuting diagram that $\mathbb{A}lg[F]_\odot$ is a natural isomorphism in $\mathbb{A}lg[\mathbf{D}]$. The natural isomorphism $\mathbb{A}lg[F]_U : U_{F_0(A)} \to F_1(U_A)$ is a strict identity, by the definition of U, $\mathbb{A}lg[F]_0$, and $\mathbb{A}lg[F]_1$. Finally, it is straightforward that $S \circ \mathbb{A}lg[F]_1 = \mathbb{A}lg[F]_0 \circ S$ and $T \circ \mathbb{A}lg[F]_1 = \mathbb{A}lg[F]_0 \circ T$.

It is left to prove that the double functor $\mathbb{A}lg[F]$ is braided monoidal strong and that it is symmetric whenever F is symmetric. Firstly, $\mathbb{A}lg[F]_0$ and $\mathbb{A}lg[F]_1$ need to be braided monoidal strong functors, which comes down to showing that the natural transformations $\chi : \otimes(\mathbb{A}lg[F], \mathbb{A}lg[F]) \to \mathbb{A}lg[F] \otimes$ and $\iota : I_{\mathcal{D}} \to \mathbb{A}lg[F](I_C)$ give rise to tight transformations of double categories, whose components are well-defined as algebra and module homomorphisms, respectively. This follows from the naturality of χ, and the coherence and functoriality of F. Coherence of $\mathbb{A}lg[F]_0$ and $\mathbb{A}lg[F]_1$ follows from coherence of F. Similarly, the symmetric monoidal structure of F gives rise to a symmetric monoidal structure for $\mathbb{A}lg[F]_0$ and $\mathbb{A}lg[F]_1$. Secondly, we need to show that $\mathbb{A}lg[F]_0 \circ S$ equals $S \circ \mathbb{A}lg[F]_1$ as monoidal functors, and similarly, $\mathbb{A}lg[F]_0 \circ T = T \circ \mathbb{A}lg[F]_1$. The first equality amounts to $\chi^{\mathbb{A}lg[F]_0 \circ S} = \chi^{S \circ \mathbb{A}lg[F]_1}$ and $\chi^{\mathbb{A}lg[F]_0 \circ S} = \chi^{S \circ \mathbb{A}lg[F]_1}$, where we have written the functor that χ belongs to in superscript. Unfolding definitions gives us $\mathbb{A}lg[F]_0(\chi^S) \circ \chi^{\mathbb{A}lg[F]_0} = S(\chi^{\mathbb{A}lg[F]_1}) \circ \chi^S$. This holds, since χ^S is the identity. The constraints are shown to hold in a similar way.

Finally, the first of the two commuting diagrams of Definition 4.1.19 corresponds to the front square of the commuting diagram below. The unlabelled arrows represent the coequalisers defining their target object. The back square commutes by coherence of F. The squares on the sides commute by definition of ξ, $\mathbb{A}lg[F]_{\odot}$, and $\chi \circ \chi$ and by naturality of χ. It follows that the front square must commute. The second diagram can be shown to hold by a similar argument.



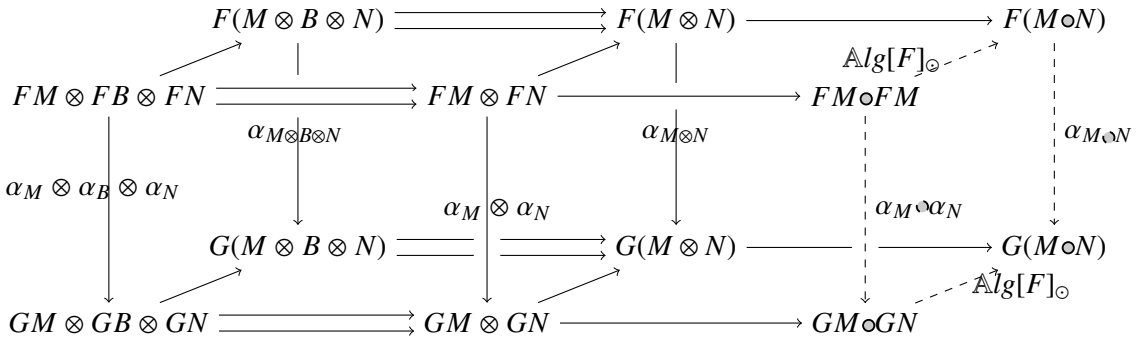
□

Note that a similar result does not hold for braided monoidal lax or colax functors, as the transformations χ and ι of $\mathbb{A}lg[F]$ may not have loosely strong companions.

Proposition 5.4.21. *Let $F, G : \mathbf{C} \to \mathbf{D}$ be braided monoidal functors that preserve coequalisers. A braided monoidal transformation $\alpha : F \Rightarrow G$ lifts to a braided monoidal double transformation $\mathbb{A}lg[\alpha] : \mathbb{A}lg[F] \Rightarrow \mathbb{A}lg[G]$. Furthermore, $\mathbb{A}lg[\alpha]$ is symmetric, whenever α is symmetric, respectively.*

Proof. The components of any monoidal transformation α are algebra homomorphisms by the two coherence equations and by naturality of α; hence, α gives rise to a natural transformation $\mathbb{A}lg[\alpha]_0 : \mathbb{A}lg[F]_0 \Rightarrow \mathbb{A}lg[G]_0$. It gives rise to a natural transformation $\mathbb{A}lg[\alpha]_1 : \mathbb{A}lg[F]_1 \Rightarrow \mathbb{A}lg[G]_1$, where the component $\mathbb{A}lg[\alpha]_{\mathbf{M}}$ of an A-B-bimodule $\mathbf{M}$ is defined as $(\alpha_A, \alpha_M, \alpha_B)$. This is well-defined by naturality of α and the coherence equations for monoidal transformations.

The first equality for tight transformations follows from the first coherence condition for monoidal transformations, as shown below. Similarly, the second equality follows from the second coherence condition for monoidal tranformations.



(5.4.22)

The coherence diagrams for monoidal transformations of double categories follow directly from the original coherence diagrams of α. □

We are now ready to prove that the $\mathbb{A}lg$ construction gives rise to the following functors of locally cubical bicategories. Recall from the previous section that the subscript s is used to denote that the 1-cells of these locally cubical bicategories are strong monoidal pseudofunctors.

Proposition 5.4.23. *The $\mathbb{A}lg$ construction gives rise to the following functors of locally cubical bicategories*

$$\mathcal{B}r\mathcal{M}on_s\mathcal{C}at \to \mathcal{B}r\mathcal{M}on\mathcal{D}bl_f$$
$$\mathcal{S}ym\mathcal{M}on_s\mathcal{C}at \to \mathcal{S}ym\mathcal{M}on\mathcal{D}bl_f$$

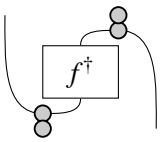
Proof. We regard $\mathcal{B}r\mathcal{M}on_s\mathcal{C}at$ and $\mathcal{S}ym\mathcal{M}on_s\mathcal{C}at$ as locally cubical bicategories with only identity tight 2-morphisms and 3-cells. The assignment on categories, functors and transformations is given in Propositions 5.4.9, 5.4.19, and 5.4.21. By Propositions 5.4.19, 5.4.14, $\mathbb{A}lg[F]$ is braided monoidal strong and $\mathbb{A}lg[\mathbf{C}]$ and $\mathbb{A}lg[\mathbf{D}]$ are fibrant. Therefore, the transformations χ and ι of $\mathbb{A}lg[F]$ have loosely strong companions. The assignment $\mathbb{A}lg$ on functors and transformations preserves horizontal composition and units strictly. It follows that the coherence equations are trivially satisfied. □

Special dagger Frobenius algebras and dagger bimodules

The result can be extended to the bicategory $2[\mathbf{C}]$ of special dagger Frobenius algebras, dagger bimodules and bimodule homomorphisms in a monoidal dagger category $\mathbf{C}$.

When a braided monoidal category $\mathbf{C}$ is equipped with a dagger functor, dagger Frobenius algebras, dagger bimodules and bimodule homomorphisms do not form a fibrant double category by the method introduced in this paper. The reason is that the bimodule defined in equation 5.4.15 as part of the data that forms a companion is not a dagger bimodule. To solve this, we restrict the categories $\mathbb{D}_0$ and $\mathbb{D}_1$ in an appropriate way to ensure that the result still holds.

Definition 5.4.24. Let A, B be Frobenius algebras and let $f : A \to B$ be an algebra homomorphism in a dagger monoidal category. The **conjugate** f_* of f is defined as

$f_* :=$ 

An algebra homomorphism f is **self-conjugate** if $f = f_*$.

We denote the double category of special dagger Frobenius algebras, self-conjugate algebra homomorphisms, dagger bimodules and extended bimodule homomorphisms (f_1, f, f_2) in $\mathbf{C}$, of which f_1 and f_2 are self-conjugate, as $\mathbb{2}[\mathbf{C}]$. The restriction to self-conjugate morphisms ensures that the 1-cell $\hat{f}$ in 5.4.15 is in fact a dagger bimodule. The double category $\mathbb{2}[\mathbf{C}]$ is a fibrant braided monoidal sub-category of $\mathbb{A}lg[\mathbf{C}]$, since

the monoidal unit is a special dagger Frobenius algebra, all structure isomorphisms are self-conjugate and the tensor product, as well as loose and tight composition, preserves all structure. We show that $\mathbb{2}$ gives rise to a functor of locally cubical bicategories. We denote $\mathcal{B}r\mathcal{M}on_s \dagger \mathcal{C}at$ as the locally cubical bicategory of braided monoidal dagger categories and strong monoidal dagger functors and $\mathcal{S}ym\mathcal{M}on_s \dagger \mathcal{C}at$ as the locally cubical bicategory of symmetric monoidal dagger categories and symmetric monoidal strong dagger functors. Both locally cubical bicategories have identity tight 2-morphisms and 3-cells.

Proposition 5.4.25. *The assignment $\mathbb{2}(-)$ gives rise to the functors of locally cubical bicategories below.*

$$\mathcal{B}r\mathcal{M}on_s \dagger \mathcal{C}at \xrightarrow{\mathbb{2}} \mathcal{B}r\mathcal{M}on_s\mathfrak{Dbl}_f$$
$$\mathcal{S}ym\mathcal{M}on_s \dagger \mathcal{C}at \xrightarrow{\mathcal{S}ym\mathbb{2}} \mathcal{S}ym\mathcal{M}on_s\mathfrak{Dbl}_f$$

Proof. Let $\mathbf{C}$ be a braided monoidal dagger category. We obtain the braided monoidal sub-double category $\mathbb{2}(\mathbf{C}) \subset \mathbb{A}lg(\mathbf{C})$. This assignment gives rise to the pseudofunctors $\mathcal{B}r\mathcal{M}on_s \dagger \mathcal{C}at \xrightarrow{\mathbb{2}} \mathcal{B}r\mathcal{M}on_s\mathfrak{Dbl}_f$ and $\mathcal{S}ym\mathcal{M}on_s \dagger \mathcal{C}at \xrightarrow{\mathcal{S}ym\mathbb{2}} \mathcal{S}ym\mathcal{M}on_s\mathfrak{Dbl}_f$. On monoidal categories, this is the assignment $\mathbf{C} \to \mathbb{2}[\mathbf{C}]$; on hom-categories, it is defined as in Prop 5.4.23. □

Now we can state out final result.

Theorem 5.4.26. *The assignment $2[-]$ gives rise to the functors of locally cubical bicategories below*

$$2[-] : \mathcal{B}r\mathcal{M}on_s \dagger \mathcal{C}at \to \mathcal{B}r\mathcal{M}on_s\mathcal{B}icat$$
$$\mathcal{S}ym2[-] : \mathcal{S}ym\mathcal{M}on_s \dagger \mathcal{C}at \to \mathcal{S}ym\mathcal{M}on_s\mathcal{B}icat$$

Proof. Theorem 4.3.31 and Proposition 5.4.25 give us the required composition of functors below.

$$\mathcal{B}r\mathcal{M}on_s \dagger \mathcal{C}at \xrightarrow{\mathbb{2}} \mathcal{B}r\mathcal{M}on_s\mathfrak{Dbl}_f \xrightarrow{\mathcal{B}r\mathcal{M}on_s\mathcal{L}} \mathcal{B}r\mathcal{M}on_s\mathfrak{Bicat}$$
$$\mathcal{S}ym\mathcal{M}on_s \dagger \mathcal{C}at \xrightarrow{\mathcal{S}ym\mathbb{2}} \mathcal{S}ym\mathcal{M}on_s\mathfrak{Dbl}_f \xrightarrow{\mathcal{S}ym\mathcal{M}on_s\mathcal{L}} \mathcal{S}ym\mathcal{M}on_s\mathfrak{Bicat}$$

□

For completeness, one could show that $\mathcal{B}r\mathcal{M}on_s\mathcal{L}$ and $\mathbb{2}$ preserve the dagger structure, which implies that $2[\mathbf{C}]$ is a symmetric monoidal dagger bicategory. We leave this for future work.

Corollary 5.4.27. *The bicategory* **2Hilb** *is symmetric monoidal.*

Proof. As shown in [Wes13, Section 3.6.3], **2Hilb** is equivalent to the subbicategory $\mathbb{2}[\mathbf{FHilb}]$ of commutative dagger Frobenius algebras, where **FHilb** is the symmetric monoidal category of finite Hilbert spaces and linear maps, which contains all coequalizers. As this subcategory is equivalent to $\mathbb{2}[\mathbf{FHilb}]$, the result follows from Theorem 5.4.26. □

Corollary 5.4.28. *The bicategory* **2Vect** *is symmetric monoidal.*

Proof. We obtain **2Vect** as $\mathcal{A}lg[\mathbf{FVect}]$ from the braided monoidal category **FVect** of finite-dimensional vector spaces and linear maps. The category **2Vect** is symmetric monoidal, contains all coequalisers and has a tensor product that preserves coequalisers. □

Corollary 5.4.29. *Let* **C** *be a braided monoidal category that contains all coequalisers and where the tensor product preserves coequalisers. The bicategory* $2[\mathbf{C}]$ *defined in [Wes13] is braided monoidal. It is symmetric monoidal whenever* **C** *is symmetric monoidal, respectively.*

Proof. The bicategory $2[\mathbf{C}]$ is the horizontal bicategory of $\mathbb{2}[\mathbf{C}]$. □

5.5 Higher Categories of Mixed States

In this section we combine the algebraic approach to quantum mechanics with the decoherence perspective on classical and quantum behaviour. We apply the $2[-]$ construction to the category of algebras and completely positive maps $\mathrm{CP}^*[\mathbf{FHilb}]$ defined in [CHK16]. The integrated approach describes the interaction of mixed quantum states with their environment. It allows a unified description of quantum teleportation and classical encryption in a single 2-category, as well as a universal security proof applicable simultaneously to both scenarios, as shown in [HVW14]. Specifically, it is shown that destroying the second half of the shared resource is equivalent to destroying the original message or state. This proof relies on the existence of a canonical 'deletion' map. Such a map, which does not exist for the state vector formalism of quantum mechanics, arises in the algebraic approach to quantum mechanics from the trace map on density matrices.

By [HVW14, Lemma 11], not all idempotents in the category CP*[**FHilb**] have a dagger splitting. Therefore, horizontal composition is not necessarily defined for all 1-cells in 2[CP*[**FHilb**]]. However, we will show that for a substructure consisting of natural numbers, matrices of finite-dimensional C*-algebras, and matrices of completely positive maps, composition is well-defined. We then proceed to show that the substructure is a symmetric monoidal bicategory.

First of all, note that for every classical structure $C = (A, \curvearrowleft, \mathrm{y})$ in **FHilb**, the morphisms $\curvearrowleft$ and y are completely positive maps of the form $I \to C$ and $C \times C \to C$. Therefore, $(C, \curvearrowleft, \mathrm{y})$ corresponds to a classical structure in CP*[**FHilb**], which we call a **classical structure over itself**. As we noted before, such a structure is just a natural number, up to isomorphism $C \cong \mathbf{C}^n$.

Lemma 5.5.1. *There is a one-to-one correspondence between dagger bimodules on classical structures over themselves in* CP*[**FHilb**]*, and matrices of finite-dimensional C*-algebras.*

Proof. First, we show that a dagger bimodule on classical structures over themselves in CP*[**FHilb**] corresponds to a matrix of finite-dimensional C*-algebras. Let $\mathbb{C}^m$-$\mathbb{C}^n$ be classical structures over themselves and let $\mathbf{M}\colon \mathbb{C}^m \otimes M \otimes \mathbb{C}^n \to M$ be a dagger bimodule in CP*[**FHilb**]. Then M is a finite-dimensional C*-algebra, and $\mathbf{M}$ is a completely positive map. By Theorem 11 of [HVW14], the units of $\mathbb{C}^m$ and $\mathbb{C}^n$ correspond to the sum over the standard basis vectors $|i\rangle$ and $|j\rangle$ of $\mathbb{C}^m$ and $\mathbb{C}^n$, respectively. By the unit law for bimodules 5.2.1, we have the equality $\mathrm{id}_M = \sum_{i,j} P_{i,j}(M)$, where $P_{ij} = (|i\rangle\langle i|) \otimes \mathrm{id}[M] \otimes (|j\rangle\langle j|)$, as in equation 5.2.3. Each $P_{i,j}$ is completely positive, as it is a composition of completely positive maps and dagger idempotent, by the first module axiom 5.2.1. Hence, its image $M_{ij} = P_{ij}(M)$ is a finite-dimensional C*-algebra by a classic theorem of Choi and Effros [CE77]; see [HKS13, Proposition 2.4]. This means that the bimodule $\mathbf{M}$ gives rise to a matrix (M_{ij}) of finite-dimensional C*-algebras.

Conversely, let (M_{ij}) be an m-by-n matrix of finite-dimensional C*-algebras. We will define the corresponding bimodule $\mathbf{M}$ in 2[CP*[**FHilb**]]. The underlying object is defined as the direct sum of the entries of the matrix $M := \bigoplus_{i,j} M_{ij}$. The module $\mathbf{M}\colon \mathbb{C}^m \otimes M \otimes \mathbb{C}^n \to M$ is defined on the basis elements $|i\rangle, |j\rangle$ of $\mathbb{C}^m$ and $\mathbb{C}^n$ as the projection onto the summand M_{ij}. This is a $*$-homomorphism, which is a completely positive map [CHK16, Lemma 3.8]. We need to check that it satisfies the bimodule equations 5.2.1, 5.2.2. The first two equalities are straightforward. For the third equality, note that $\mathbf{M}^\dagger\colon M \to \mathbb{C}^m \otimes M \otimes \mathbb{C}^n$ maps $b \in M$ to $\sum_{i,j} |i\rangle \otimes (1_{ij} b) \otimes |j\rangle$. □

Next, we show that horizontal composition is well-defined for matrices of C*-algebras.

Proposition 5.5.2. *Let* $(C, \curvearrowleft, \circ)$, $(D, \curvearrowleft, \circ)$, $(E, \curvearrowleft, \bullet)$ *be classical structures over themselves in* $\mathrm{CP}^*[\mathbf{FHilb}]$*, and let* $\mathbf{M}$ *and* $\mathbf{N}$ *be a C-D-bimodule and a D-E-bimodule. The horizontal composition* $\mathbf{M}_{\odot\mathbf{N}}$ *is well-defined.*

Proof. It is sufficient to show that the idempotent (5.3.5) splits. Let $|i\rangle$, $|j\rangle$, $|k\rangle$ be the standard bases of $\mathbb{C}^l$, $\mathbb{C}^m$, $\mathbb{C}^n$. Let $\mathbf{M}$ be a dagger $\mathbb{C}^l$-$\mathbb{C}^m$-bimodule, and let $\mathbf{N}$ be a dagger $\mathbb{C}^m$-$\mathbb{C}^n$-bimodule in $\mathrm{CP}^*[\mathbf{FHilb}]$. The idempotent (5.3.5) maps $m \otimes n$ to $\sum_{i,j,k} \mathbf{M}(|i\rangle \otimes m \otimes |j\rangle) \otimes \mathbf{N}(|j\rangle \otimes n \otimes |k\rangle)$. This morphism is a sum of orthogonal projections, and hence a projection. Again, by [CE77], its image is a C*-algebra. Therefore, it has a splitting within the subcategory. By Lemma 5.3.4, horizontal composition is well-defined. □

Lemma 5.5.3. *There is a one-to-one correspondence between homomorphisms of dagger bimodules between classical structures over themselves in* $\mathrm{CP}^*[\mathbf{FHilb}]$*, and matrices of completely positive maps between finite-dimensional C*-algebras.*

Proof. Firstly, we show that every homomorphisms of dagger bimodules between classical structures over themselves corresponds to a matrix of completely positive maps. Let $f\colon \mathbf{M} \to \mathbf{N}$ be a homomorphism of dagger $\mathbb{C}^m$-$\mathbb{C}^n$-bimodules in $\mathrm{CP}^*[\mathbf{FHilb}]$. Following the proof of Lemma 5.5.1, let $P_{ij}\colon M \to M_{ij}$ and $Q_{ij}\colon N \to N_{ij}$ be the completely positive projections, indexed by the standard bases of $\mathbb{C}^m$ and $\mathbb{C}^n$, as defined in 5.2.3. We define $f_{ij} := Q_{ij} f P_{ij}^\dagger\colon M_{ij} \to N_{ij}$ as the components of an m-by-n matrix $(f_{i,j})_{i,j}$. The components are compositions of completely positive maps; hence, they are completely positive themselves. Conversely, we show that every matrix of completely positive maps defines a bimodule homomorphism of bimodules on classical structures over themselves in $2[\mathrm{CP}^*[\mathbf{FHilb}]]$. Let (f_{ij}) be an m-by-n matrix of completely positive maps $f_{ij}\colon M_{ij} \to N_{ij}$. By Lemma 5.5.1, it suffices to define a completely positive map $f\colon M \to N$ for $M = \bigoplus_{i,j} M_{ij}$ and $N = \bigoplus_{i,j} N_{ij}$ that satisfies the bimodule homomorphims equation $f \circ \mathbf{M} = \mathbf{N} \circ (\mathrm{id} \otimes f \otimes \mathrm{id})$. We define $f := \bigoplus_{ij} f_{ij}$, which is well-defined, since $\mathrm{CP}^*[\mathbf{C}]$ has biproducts [CHK16, Theorem 3.2]. The equations below show that this satisfies the bimodule homomorphism equation for all basis elements $|i\rangle, |j\rangle$ of $\mathbb{C}^n, \mathbb{C}^m$, respectively.

$$\begin{aligned} f\mathbf{M}(|i\rangle \otimes a \otimes |j\rangle) &= \textstyle\bigoplus_{i,j} f_{ij} P_{i,j}(a) \\ &= Q_{i,j} \bigoplus_{i,j} f_{ij}(a) \\ &= \mathbf{N}(|i\rangle \otimes f(a) \otimes |j\rangle) \end{aligned}$$

□

We derive the following sub-bicategory of 2[CP*[**FHilb**]], which has sufficient coequalizers.

Theorem 2. *The following sub-structures of* 2[CP*[**FHilb**]] *form a bicategory:*

- *0-cells are natural numbers m;*
- *1-cells $m \to n$ are m-by-n matrices (M_{ij}) of finite-dimensional C*-algebras;*
- *2-cells $(M_{ij}) \to (N_{ij})$ are m-by-n matrices (f_{ij}) of completely positive maps;*
- *horizontal composition of 1-cells $\mathbf{M}$, $\mathbf{N}$, is given by $(\bigoplus_j M_{ij} \otimes N_{jk})_{i,k}$; The unit 1-cell is the matrix with all components equal to $\mathbb{C}$.*
- *horizontal composition of 2-cells f,g, is given by $(\bigoplus_j f_{ij} \otimes g_{jk})_{i,k}$;*
- *vertical composition of 2-cells f,g, is given by $(g_{ij} f_{ij})$.*

Proof. We know by Lemmas 5.5.1 and 5.5.3, that the 0-cells, 1-cells and 2-cells are well-defined elements of 2[CP*[**FHilb**]]. We apply definition 5.3.6 of horizontal composition through dagger splittings to the notions of bimodules and bimodule homomorphisms as matrices. The underlying object $M \circ N$ of 5.3.5 is the image of the map 5.3.5, which can be written explicitly as $\sum_{i,j,k} \mathbf{M}(|i\rangle \otimes [-] \otimes |j\rangle) \otimes \mathbf{N}(|j\rangle \otimes [-] \otimes |k\rangle)$. This corresponds to the biproduct $\bigoplus_{ijk} M_{ij} \otimes N_{jk}$. As a consequence, by Lemma 5.5.3, $\mathbf{M} \circ \mathbf{N}$ corresponds to the matrix $(\bigoplus_j M_{ij} \otimes N_{jk})_{i,k}$. Similarly, horizontal composition of bimodule homomorphisms $f \colon \mathbf{M} \to \mathbf{M}'$ and $g \colon \mathbf{N} \to \mathbf{N}'$ corresponds to $(\bigoplus_j f_{ij} \otimes g_{jk})$, by uniqueness of coequalizers, as this map makes the diagram 5.3.2 commute. Finally, it is easy to show that the matrices are closed under vertical composition. □

The bicategory defined above is sufficient for expressing and verifying correctness of quantum teleportation and encrypted communication, as shown in [HVW14, Section 4]. Whether 2[CP*[**FHilb**]] as a whole is well-defined remains an open problem. To solve this, we first need a characterization of its objects. A first step was made in [HVW14, Theorem 16], showing that special dagger Frobenius algebras on classical structures in CP*[**FHilb**] are isomorphic to groupoids.

Conclusions

We have explored various features that distinguish quantum mechanics from classical mechanics and assessed their respective roles in quantum computing. We have unified two prominent perspectives on contextuality and formulated necessary conditions under which contextuality provides an advantage in communication complexity. We have developed a mathematical foundation for an intuitive planar language of quantum protocols and we have introduced such a model for mixed states. Yet, there are still various open problems and our exploration leads to new interesting questions.

Contextuality of Unsharp Measurements

We have demonstrated that the sheaf-theoretic approach to contextuality is equivalent to the equivalence-based approach in scenarios where factorizability is justified. In practice, measurement results in any experiment are to some extent affected by noise. Hence, perfect predictability of measurement outcomes does not exist, which means that factorizability can generally not be assumed. The two formalisms give rise to different contextuality inequalities, [AH12], [Kun17], as a way to cope with this. The extent to which these inequalities are related remains an open question. An investigation of this issue could potentially lead to experimental ways to distinguish between the two, which may give us a clue of which assumptions about reality are justified.

Multiround Communication Complexity

We have given a unified notion of classical and quantum one-way communication complexity protocols based on the sheaf-theoretic approach to contextuality and constraint satisfaction problems. We have used this formulation to quantify the relation between the complexity advantage and the amount of contextuality available in the resource for the protocol.

While this scenario covers a number of interesting cases, one would like to account for more general scenarios where parties are allowed to send arbitrarily many rounds of messages to eachother. It was shown in [BCG$^+$16] that advantages in multiround comunication complexity imply the violation of some linear Bell inequality.

In order to give a formal account of such scenarios in sheaf-theoretic terms, one would need a notion of compositionality of empirical models. Some progress in this direction has been made in [Man18].

Communication Complexity Algorithms

The formulation of communication complexity protocols as constraint satisfaction problems provides opportunities for finding better communication complexity protocols. As constraint satisfaction is an NP-hard problem, we will not be able to use it for protocols with a large input. It may still be useful, since there are only few examples of quantum communication protocols, which all rely on a small number of qubits.

Various computational tools have been developed for calculating various aspects of contextuality. The Mathematica package [ABM16] contains two functions which are relevant for communication complexity protocols, when combined with a constraint satisfaction solver:

- Quantum empirical models from any state and any sets of compatible measurements
- Quantifying the degree of contextuality of any empirical model

To make use of these tools, one needs to determine the required quantum resources for realisations of strong non-locality scenarios. This is comparable to the work in [ABC$^+$17], and [ABCP17].

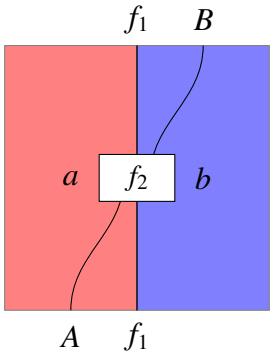
Transformations of Bicategorical Models for Quantum Protocols

We have developed machinery to construct monoidal structures of higher cells. There are various interesting functors between monoidal categories representing various types of computation, such as the embeddings CPM[C] $\hookrightarrow$ CP*[$\mathbf{C}$], described in [CHK16, Section 4] and Stoch[$\mathbf{C}$] $\hookrightarrow$ CP*[$\mathbf{C}$], described in [CHK16, Section 5]. These functors represent the embedding of classical stochastic computing and 'purely' quantum computing into the framework CP*[$\mathbf{C}$], respectively. Additionally, there is the embedding **FHilb** $\hookrightarrow$ CP*[**FHilb**] which represents the inclusion of the pure-state formalism in the algebraic framework. Bicategorical equivalents of such embeddings would provide interesting insights into the structure of 2[CP*[**FHilb**]].

Categories of Algebras and Bimodules in a Monoidal Double Category

There are interesting categories that arise from the construction $\mathcal{A}lg[-]$, when we take the base category to be a bicategory instead of a monoidal category. This generalisation captures the equivariant completion of a bicategory introduced in [CR14], which offers a way to describe topological quantum field theories.

While bicategories are hardly any more complex than monoidal categories, our machinery no longer works in those scenarios, for the following reason: We need to find a suitable notion of 1-morphism between algebras. One candidate is the algebra homomorphism, defined within the hom-categories of the bicategory. This choice is not suitable if we want the double category to be monoidal, since the structure morphisms α, ρ, and λ have source and target objects in distinct hom-categories. An alternative candidate is the **monad map**, a morphism $f : (A, \curvearrowleft, \circ) \to (B, \curvearrowleft, \circ)$ is a pair (f_1, f_2) where $f_1 : a \to b$ is a 1-cell and f_2 is a 2-cell



However, composition of monad maps is not associative nor unital, which means that algebras and monad maps do not form a category.

To solve this, one could consider algebras, bimodules and bimodule homomorphisms in a monoidal double category $\mathbb{D}$. These are defined as algebras and bimodules in the category of morphisms $\mathbb{D}$, that are coherent with the monoidal structure of the double category. Expand the results for monoidal categories to be applicable to monoidal double categories is a matter of checking that all the data is coherent. We leave this for future work. An indirect result on this is derived in [Shu08]; however, this result does not cover dagger algebras and dagger bimodules and is therefore not applicable to the equivariant completion of a bicategory.

References

[AB11a] S. Abramsky and A. Brandenburger. Axiomatizing physical theories in a sheaf-theoretic framework. *Unpublished note*, 2011.

[AB11b] S. Abramsky and A. Brandenburger. The sheaf-theoretic structure of non-locality and contextuality. *New Journal of Physics 13*, 2011.

[ABC+17] S. Abramsky, R. Soares Barbosa, G. Carù, N. de Silva, K. Kishida, and S. Mansfield. Minimum quantum resources for strong non-locality. *arXiv preprint arXiv:1705.09312*, 2017.

[ABCP17] Samson A., R. Soares Barbosa, G. Carù, and S. Perdrix. A complete characterisation of all-versus-nothing arguments for stabiliser states. *arXiv preprint arXiv:1705.08459*, 2017.

[ABdSZ] S. Abramsky, R. S. Barbosa, N. de Silva, and O. Zapata. The quantum monad on relational structures; 2017. *Submitted for publication*.

[ABM16] S. Abramsky, R. Soares Barbosa, and S. Mansfield. Quantifying contextuality via linear programming. In *Proceedings of the 13th Interational Conference on Quantum Physics and Logic (QPL 2016)*, 2016.

[ABM17] S. Abramsky, R. Soares Barbosa, and S. Mansfield. Contextual fraction as a measure of contextuality. *Physical review letters*, 119(5):050504, 2017.

[AC04] S. Abramsky and B. Coecke. A categorical semantics of quantum protocols. In *Logic in computer science, 2004. Proceedings of the 19th Annual IEEE Symposium on*, pages 415–425. IEEE, 2004.

[AE35] N. Rosen A. Einstein, B. Podolski. Can quantum-mechanical description of physical reality be considered complete? *Physical Review*, page 777780, 1935.

[AFLS15] A. Acinand, T. Fritz, A. Leverrier, and A. B. Sainz. A combinatorial approach to contextuality and non locality. *Communications in Mathematical Physics*, 334(2), 2015.

[AH12] S. Abramsky and L. Hardy. Logical Bell inequalities. *Physical Review A*, 85(6):062114, 2012.

[AH13] S. Abramsky and C. Heunen. Operational theories and categorical quantum mechanics. 2013.

[AMB11] S. Abramsky, S. Mansfield, and R. Soares Barbosa. The cohomology of non-locality and contextuality. *QPL 2011*, 2011.

[AS14] S. Abramsky and M. Sadrzadeh. Semantic unification - a sheaf theoretic approach to natural language. *Lecture Notes in Computer Science*, 8222, 2014.

[AT10] S. Abramsky and N. Tzevelekos. Introduction to categories and categorical logic. In *New structures for physics*, pages 3–94. Springer, 2010.

[Bae97] J. C. Baez. Higher-dimensional algebra ii. 2-hilbert spaces. *Advances in Mathematics*, 127(2):125–189, 1997.

[BC04] J. C. Baez and A. S. Crans. Higher-dimensional algebra vi: Lie 2-algebras. *Theory Appl. Categ*, 12(15):492–528, 2004.

[BCG+16] H. Buhrman, Ł. Czekaj, A. Grudka, M. Horodecki, P. Horodecki, M. Markiewicz, F. Speelman, and S. Strelchuk. Quantum communication complexity advantage implies violation of a bell inequality. *Proceedings of the National Academy of Sciences*, 113(12):3191–3196, 2016.

[BCVD01] H. Buhrman, R. Cleve, and W. Van Dam. Quantum entanglement and communication complexity. *SIAM Journal on Computing*, 30(6):1829–1841, 2001.

[BCW98] H. Buhrman, R. Cleve, and A. Wigderson. Quantum vs. classical communication and computation. In *Proceedings of the thirtieth annual ACM symposium on Theory of computing*, pages 63–68. ACM, 1998.

[Bel64] J. Bell. On the Einstein Podolsky Rosen paradox. *Physics 1*, 1964.

[Bel01] J. S. Bell. On the problem of hidden variables in quantum mechanics. In *John S Bell On The Foundations Of Quantum Mechanics*, pages 1–6. World Scientific, 2001.

[BKV16] K. Bar, A. Kissinger, and J. Vicary. Globular: an online proof assistant for higher-dimensional rewriting. *arXiv preprint arXiv:1612.01093*, 2016.

[Blo46] F. Bloch. Nuclear induction. *Physical review*, 70(7-8):460, 1946.

[BM99] R. Brown and G. H. Mosa. Double categories, 2-categories, thin structures and connections. *Theory Appl. Categ.*, 5:No. 7, 163–175 (electronic), 1999.

[BMS13] J. W. Barrett, C. Meusburger, and G. Schaumann. Gray categories with duals and their diagrams. 2013.

[BN96] J. C. Baez and M. Neuchl. Higher-dimensional algebra. I. Braided monoidal 2-categories. *Adv. Math.*, 121(2):196–244, 1996.

[BS76] R. Brown and C. B. Spencer. Double groupoids and crossed modules. *Cahiers Topologie Géom. Différentielle*, 17(4):343–362, 1976.

[BvDHT99] H. Buhrman, W. van Dam, P. Høyer, and A. Tapp. Multiparty quantum communication complexity. *Physical Review A*, 60(4):2737, 1999.

[CE77] M. Choi and E. G. Effros. Injectivity and operator spaces. *Journal of functional analysis*, 24(2):156–209, 1977.

[CEGA96] A. Cabello, J. M. Estebaranz, and G. García-Alcaine. Bell-Kochen-Specker theorem: A proof with 18 vectors. *Physics Letters A*, 212(4):183–187, 1996.

[CFL83] A. K. Chandra, M. L. Furst, and R. J. Lipton. Multi-party protocols. In *Proceedings of the fifteenth annual ACM symposium on Theory of computing*, pages 94–99. ACM, 1983.

[CHK16] B. Coecke, C. Heunen, and A. Kissinger. Categories of quantum and classical channels. *Quantum Information Processing*, 15(12):5179–5209, 2016.

[CHSH69] J. F Clauser, M. A Horne, A. Shimony, and R. A. Holt. Proposed experiment to test local hidden-variable theories. *Physical review letters*, 23(15):880, 1969.

[CK17] B. Coecke and A. Kissinger. *Picturing quantum processes*. Cambridge University Press, 2017.

[CP06] B. Coecke and D. Pavlovic. Quantum measurements without sums. *arXiv preprint quant-ph/0608035*, 2006.

[CR14] N. Carqueville and I. Runkel. Orbifold completion of defect bicategories. *Hamburger Beitrage zur Mathematik*, 453:304–315, 2014.

[Cra98] S. E. Crans. Generalized centers of braided and sylleptic monoidal 2-categories. *Adv. Math.*, 136(2):183–223, 1998.

[CSW14] A. Cabello, S. Severini, and A. Winter. Graph-theoretic approach to quantum correlations. 2014.

[CVDNT99] R. Cleve, W. Van Dam, M. Nielsen, and A. Tapp. Quantum entanglement and the communication complexity of the inner product function. In *Quantum Computing and Quantum Communications*, pages 61–74. Springer, 1999.

[CW18] B. Coecke and Q. Wang. Zx-rules for 2-qubit clifford+ t quantum circuits. *arXiv preprint arXiv:1804.05356*, 2018.

[dBH17] N. de Beaudrap and D. Horsman. The zx calculus is a language for surface code lattice surgery. *arXiv preprint arXiv:1704.08670*, 2017.

[DK16] E. N. Dzhafarov and J. V. Kujala. Context-content systems of random variables: The contextuality-by-default theory. *Journal of Mathematical Psychology*, 74, 2016.

[DKP07] V. Danos, E. Kashefi, and P. Panangaden. The measurement calculus. *Journal of the ACM (JACM)*, 54(2):8, 2007.

[DP10] R. Duncan and S. Perdrix. Rewriting measurement-based quantum computations with generalised flow. In *International Colloquium on Automata, Languages, and Programming*, pages 285–296. Springer, 2010.

[DPP10] R. Dawson, R. Pare, and D. A. Pronk. The span construction. *Theory Appl. Categ.*, 24:302–377 (electronic), 2010.

[DS97] B. Day and R. Street. Monoidal bicategories and Hopf algebroids. *Adv. Math.*, 129(1):99–157, 1997.

[dS15] N. de Silva. Unifying frameworks for nonlocality and contextuality. 2015.

[Fey82] R. P. Feynman. Simulating physics with computers. *International journal of theoretical physics*, 21(6-7):467–488, 1982.

[Fin82] A. Fine. Hidden variables, joint probability, and the Bell inequalities. *Physical Review Letters*, 48(5):291, 1982.

[Fio07] T. M. Fiore. Pseudo algebras and pseudo double categories. *J. Homotopy Relat. Struct.*, 2(2):119–170, 2007.

[GG09] Ri. Garner and N. Gurski. The low-dimensional structures formed by tricategories. *Math. Proc. Cambridge Philos. Soc.*, 146(3):551–589, 2009.

[GLR+13] A. S. Green, P. L. Lumsdaine, N. J. Ross, P. Selinger, and B. Valiron. Quipper: a scalable quantum programming language. In *ACM SIGPLAN Notices*, volume 48, pages 333–342. ACM, 2013.

[GP04] M. Grandis and R. Pare. Adjoints for double categories. *Cah. Topol. Géom. Différ. Catég.*, 45(3):193–240, 2004.

[GP14] M. Grandis and R. Paré. Intercategories i: The basic theory. arXiv:1412.0144, 2014.

[GPS95] R. Gordon, A. J. Power, and Ross Street. Coherence for tricategories. *Mem. Amer. Math. Soc.*, 117(558):vi+81, 1995.

[Gur] N. Gurski. Loop spaces and coherence for monoidal and braided monoidal bicategories. To appear in Adv. Math.

[Gur06] N. Gurski. *An algebraic theory of tricategories*. PhD thesis, University of Chicago, 2006.

[Gur13] N. Gurski. *Coherence in Three-Dimensional Category Theory*. Cambridge University Press, 2013.

[GVW+15] M. Giustina, M. A. M. Versteegh, S. Wengerowsky, J. Handsteiner, A. Hochrainer, K. Phelan, F. Steinlechner, J. Kofler, J. Larsson, C. Abellán, et al. Significant-loophole-free test of Bells theorem with entangled photons. *Physical review letters*, 115(25):250401, 2015.

[Har92] L. Hardy. Quantum mechanics, local realistic theories, and lorentz-invariant realistic theories. *Physical Review Letters*, 68(20):2981, 1992.

[Har93] L. Hardy. Nonlocality for two particles without inequalities for almost all entangled states. *Physical Review Letters*, 71(11):1665, 1993.

[HBD+15] B. Hensen, H. Bernien, A.E. Drau, A. Reiserer, N. Kalb, M.S. Blok, J. Ruitenberg, R.F.L. Vermeulen, R.N. Schouten, C. Abelln, W. Amaya, V. Pruneri, M. W. Mitchell, M. Markham, D.J. Twitchen, D. Elkouss, S. Wehner, T.H. Taminiau, and R. Hanson. Experimental loophole-free violation of a Bell inequality using entangled electron spins separated by 1.3 km. *Nature*, 526, 2015.

[HCLB11] M. Hoban, E. T. Campbell, K. Loukopoulos, and D. E. Browne. Non-adaptive measurement-based quantum computation and multi-party Bell inequalities. *New Journal of Physics*, 13, 2011.

[Heu17] C. Heunen. The many classical faces of quantum structures. *Entropy*, 19(4):144, 2017.

[HKS13] C. Heunen, A. Kissinger, and P. Selinger. Completely positive projections and biproducts. *arXiv preprint arXiv:1308.4557*, 2013.

[HS19] Linde Wester Hansen and Michael Shulman. Constructing symmetric monoidal bicategories functorially. *arXiv preprint arXiv:1910.09240*, 2019.

[HV18] C. Heunen and J. Vicary. *Introduction to Categorical Quantum Mechanics*. Oxford University Press, 2018. to appear.

[HVW14] C. Heunen, J. Vicary, and L. Wester. Mixed quantum states in higher categories. *EPTCS*, 172:304–315, 2014.

[HWVE14] M. Howard, J. Wallman, V. Veitch, and J. Emerson. Contextuality provides the magic for quantum computing. *Nature*, 510:351–355, 2014.

[KS67] S. Kochen and E.P. Specker. The problem of hidden variables in quantum mechanics. *Journal of Mathematics and Mechanics*, 17:59–87, 1967.

[Kun17] R. Kunjwal. Irreducible noncontextuality inequalities from the kochen-specker theorem. 2017.

[KV94a] M. Kapranov and V. Voevodsky. Braided monoidal 2-categories and Manin-Schechtman higher braid groups. *J. Pure Appl. Algebra*, 92(3):241–267, 1994.

[KV94b] M. M. Kapranov and V. A. Voevodsky. 2-categories and Zamolodchikov tetrahedra equations. In *Algebraic groups and their generalizations: quantum and infinite-dimensional methods (University Park, PA, 1991)*, volume 56 of *Proc. Sympos. Pure Math.*, pages 177–259. Amer. Math. Soc., Providence, RI, 1994.

[KZ15] A. Kissinger and V. Zamdzhiev. Quantomatic: A proof assistant for diagrammatic reasoning. In *International Conference on Automated Deduction*, pages 326–336. Springer, 2015.

[LMZ18] B. Lindenhovius, M. Mislove, and V. Zamdzhiev. Enriching a linear/nonlinear lambda calculus: A programming language for string diagrams. *arXiv preprint arXiv:1804.09822*, 2018.

[LSW11] Y. Liang, R. W. Spekkens, and H. M. Wiseman. Specker's parable of the over-protective seer: A road to contextuality, nonlocality and complementarity. *Physics Reports*, 2011. vol 506, issues 1-2, pp 1-39.

[Man80] Y. Manin. Computable and uncomputable. *Sovetskoye Radio, Moscow*, 1980.

[Man18] S. Mansfield. Sequential composition of empirical models. 2018.

[McC00] P. McCrudden. Balanced coalgebroids. *Theory Appl. Categ.*, 7:No. 6, 71–147 (electronic), 2000.

[Mer90] D. N. Mermin. Extreme quantum entanglement in a superposition of macroscopically distinct states. *Physical Review Letters*, 65(15):1838, 1990.

[MPK+16] M. D. Mazurek, M. F. Pusey, R. Kunjwal, K. J. Resch, and R. W. Spekkens. An experimental test of noncontextuality without unphysical idealizations. *Nature communications*, 7, 2016.

[Mye16] D. J. Myers. String diagrams for double categories and equipments. *arXiv preprint arXiv:1612.02762*, 2016.

[NC00] M. A. Nielsen and I. L. Chuang. *Quantum Computation and Quantum Information*. Cambridge University Press, 2000.

[Orú14] R. Orús. A practical introduction to tensor networks: Matrix product states and projected entangled pair states. *Annals of Physics*, 349:117–158, 2014.

[Par70] J. L Park. The concept of transition in quantum mechanics. *Foundations of Physics*, 1(1):23–33, 1970.

[Pri12] H. Price. Does time-symmetry imply retrocausality? how the quantum world says maybe? *Studies in History and Philosophy of Science Part B: Studies in History and Philosophy of Modern Physics*, 43(2):75–83, 2012.

[Rau13] R. Raussendorf. Contextuality in measurement-based quantum computation. *Physical Review A*, 88(2):022322, 2013.

[RK11] O. Regev and B. Klartag. Quantum one-way communication can be exponentially stronger than classical communication. In *Proceedings of the forty-third annual ACM symposium on Theory of computing*, pages 31–40. ACM, 2011.

[Rou16] F. Roumen. Cohomology of effect algebras. *Proceedings QPL 2016*, 2016.

[RV17] D. Reutter and J. Vicary. A classical groupoid model for quantum networks. *arXiv preprint arXiv:1707.00966*, 2017.

[RV18] D. Reutter and J. Vicary. Shaded tangles for the design and verification of quantum programs. *arXiv preprint arXiv:1805.01540*, 2018.

[Sel04] P. Selinger. Towards a quantum programming language. *Mathematical Structures in Computer Science*, 14(4):527–586, 2004.

[Sel09] P. Selinger. A survey of graphical languages for monoidal categories. arXiv:0908.334, 2009.

[Shu08] M. Shulman. Framed bicategories and monoidal fibrations. *Theory and Applications of Categories*, 20(18):650–738 (electronic), 2008. arXiv:0706.1286.

[Shu10] M. A. Shulman. Constructing symmetric monoidal bicategories. arXiv:1004.0993, 2010.

[Slo17] W. Slofstra. The set of quantum correlations is not closed. *arXiv preprint arXiv:1703.08618*, 2017.

[SP09] C. Schommer-Pries. *The classification of two-dimensional extended topological field theories*. PhD thesis, University of California, Berkeley, 2009.

[Spe05] R. W. Spekkens. Contextuality for preparations, transformations, and unsharp measurements. *A Physical Review*, 71, 2005.

[SU15] S. Staton and S. Uijlen. Effect algebras, presheaves, non-locality and contextuality. *International Colloquium on Automata, Languages, and Programming ICALP 2015*, proceedings part II, 2015. pp 401-413.

[Tak02] M. Takesaki. Theory of operator algebras. i. reprint of the first (1979) edition. encyclopaedia of mathematical sciences, 124. operator algebras and non-commutative geometry, 5, 2002.

[tH] G. 't Hooft. The cellular automaton interpretation of quantum mechanics.

[Vic11] J. Vicary. Categorical formulation of finite-dimensional quantum algebras. *Communications in Mathematical Physics*, 304(3):765–796, 2011.

[Vic12] J. Vicary. Higher quantum theory. *arXiv preprint arXiv:1207.4563*, 2012.

[VV18] D. Verdon and J. Vicary. Quantum teleportation with infinite reference frame uncertainty. *arXiv preprint arXiv:1802.09040*, 2018.

[Wes13] L. Wester. Categorical models for quantum computing. MSc. Thesis, 2013.

[Wes17] Linde Wester. Almost equivalent paradigms of contextuality. *arXiv preprint arXiv:1708.00843*, 2017.

[Yao79] A. C. Yao. Some complexity questions related to distributive computing (preliminary report). In *Proceedings of the eleventh annual ACM symposium on Theory of computing*, pages 209–213. ACM, 1979.

[Yao93] A. C. Yao. Quantum circuit complexity. In *Foundations of Computer Science, 1993. Proceedings., 34th Annual Symposium on*, pages 352–361. IEEE, 1993.

Appendix A

Decoherence

Quantum Systems and Their Environment

The module-theoretic approach to quantum mechanics exhibits various similarities to the dynamics of *decoherence*. While there is no formal correspondence, one may find the analogy illustrative. The study of decoherence aims to address the question of how classical behaviour can arise in a world governed by the laws of quantum mechanics. Below, we briefly set out how in an idealized scenario and under the assumption of the decoherence principle, a quantum system can exhibit classical behaviour as a result of interactions with its environment. This is also called *einselection*, which is short for environment-induced superselection.

Decoherence

We describe a quantum system and its environment as two distinct quantum systems. Let the quantum system be in the state $|\psi\rangle$ and the environment be in the state $|e\rangle$. For some orthonormal basis $\{|i\rangle\}$ and $\psi_i := \langle i|\psi\rangle$, we can write $|\psi\rangle = \sum_i \psi_i |i\rangle$. In this notation, the joint state is given by $\sum_i |i\rangle |e\rangle \langle i|\psi\rangle$.

Now, suppose there is an interaction between the system and the environment, described by a unitary operation U, which does not disturb the state of the system. In practice, we cannot achieve a perfect realisation of such an interaction, as any interaction will cause some disturbance to the system. Nevertheless, it is worth considering such a scenario, as we will see below. The operation U acts on each component as $|i\rangle |e\rangle \mapsto |i\rangle |e_i\rangle$. Hence, it sends the state $|\psi\rangle$ to

$$\sum_i \psi_i |i\rangle |e_i\rangle \tag{A.0.1}$$

By the **decoherence principle**, there exists a basis $\{|i\rangle\}$, called the **einselected basis**, for which the equality $\langle e_i|e_j\rangle = \delta_{i,j}$ holds approximately. This approximation is better

when the environment has higher degrees of freedom. In other words, the environmental states $\{e_i\}$ form a near-orthonormal basis. In terms of density matrices, the quantum state before decoherence corresponds to the state below.

$$|\psi\rangle\langle\psi| = \sum_{i,j} \psi_i^* \psi_j |i\rangle\langle j|$$

The probability of measuring the state $\langle\phi|$ is obtained by the Born rule.

$$\begin{aligned}\langle\phi| \left(\sum_{i,j} \psi_i^* \psi_j |i\rangle\langle j| \right) |\phi\rangle &= \sum_{i,j} \psi_i^* \psi_j \langle\phi|i\rangle\langle j|\phi\rangle \\ &= \sum_{i,j} \psi_i^* \psi_j \phi_i^* \phi_j\end{aligned}$$

Here, $\phi_i := \langle i|\phi\rangle$. The quantum state after decoherence is obtained by tracing out the environment. This results in the maximally mixed state below.

$$\begin{aligned}\mathrm{Tr}_2 \left(\sum_{i,j} \psi_i^* \psi_j |ie_i\rangle\langle je_j| \right) &= \sum_{i,j} \psi_i^* \psi_j |i\rangle\langle j|\langle e_i|e_j\rangle \\ &\approx \sum_{i,j} \psi_i^* \psi_j |i\rangle\langle j| \delta_{i,j} \\ &\approx \sum_{i} \psi_i^* \psi_i |i\rangle\langle i|\end{aligned}$$

Applying the Born rule gives the following probability for measuring $|\phi\rangle$:

$$\langle\phi| \left(\sum_{i} \psi_i^* \psi_i |i\rangle\langle i| \right) |\phi\rangle = \sum_{i} \left|\phi_i\right|^2$$

The probability of each outcome $|\phi\rangle$ for this state is the weighted sum over the probabilities of obtaining outcome $|\phi\rangle$ for each of the components $|i\rangle\langle i|$. In other words, the outcome probabilities for the basis elements $\{|i\rangle\}$ are **additive**, just like probabilities of mutually exclusive events in classical physics.

In comparison, if we measure a state before decoherence there is an additional component $\sum_i \psi_i^* \psi_i \phi_i^* \phi_i$, which causes the probability to be smaller or larger than the sum of the probabilities for each of the components. This effect is called **quantum coherence**.

Environmental Interactions in the Semantics of Quantum Protocols

The semantics for quantum protocols introduced in Chapter 5 exhibits similarities to the principle of decoherence. In the decohered quantum state, equation A.0.1, there is a correlation between the quantum state and the state of the environment. More specifically, this is a correlation between the basis states of the quantum system and the basis

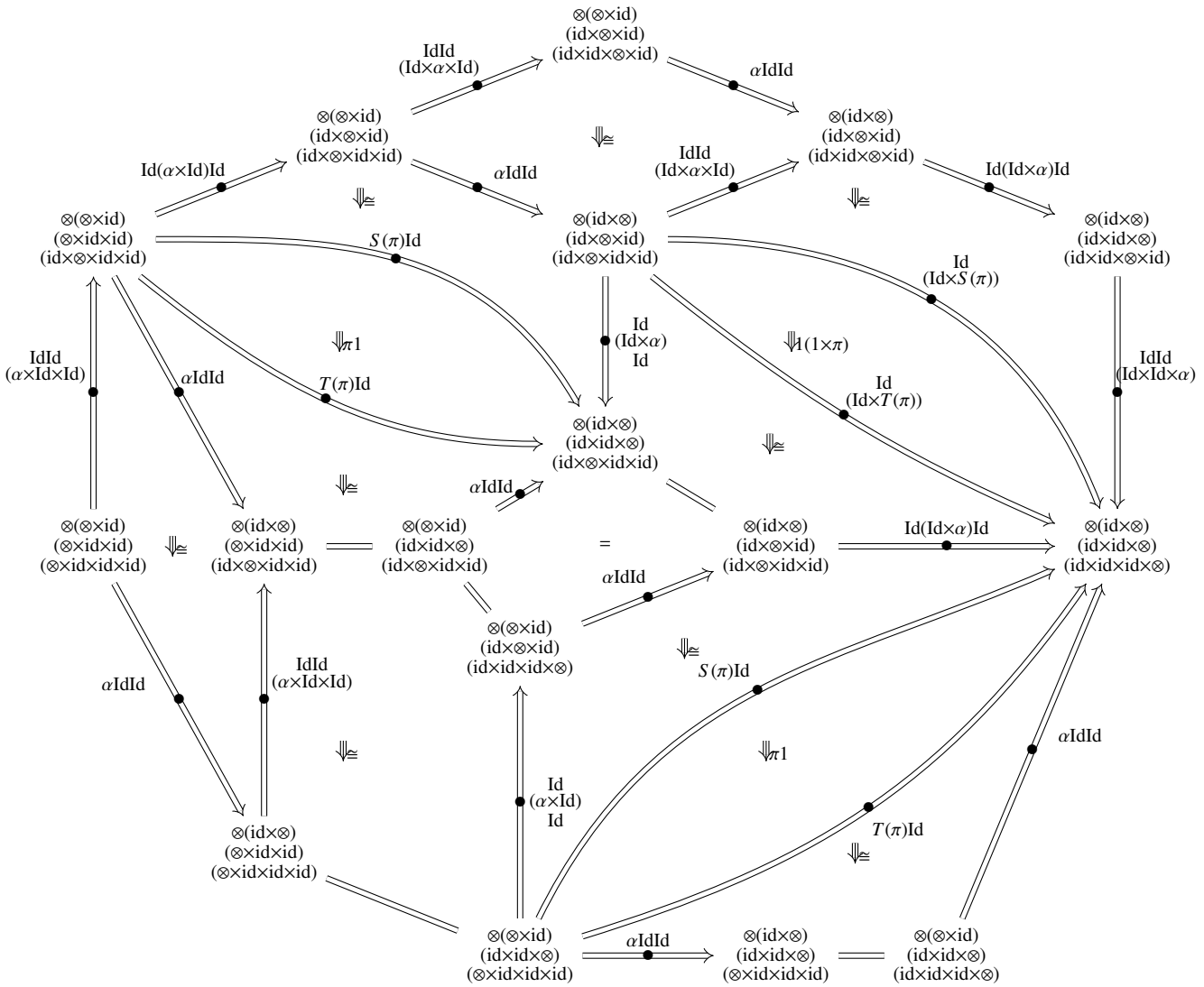
states of the environment. One could therefore consider the basis of the environment as classical information about the quantum system. One could extend the analogy, by interpreting the bimodule action as an interaction between the quantum system and the environment through which information about the quantum system is 'leaked' into the environment. In support of this interpretation, in [CP06], quantum measurements are characterized exactly as dagger modules. This 'leaking' of information into the environment causes the system to exhibit classical features. As in the case of decoherence, classical datatypes arise when the environment captures *all* quantum information about the system. Quantum states are preserved when all interactions are trivial, which means that the system is completely isolated.

Appendix B

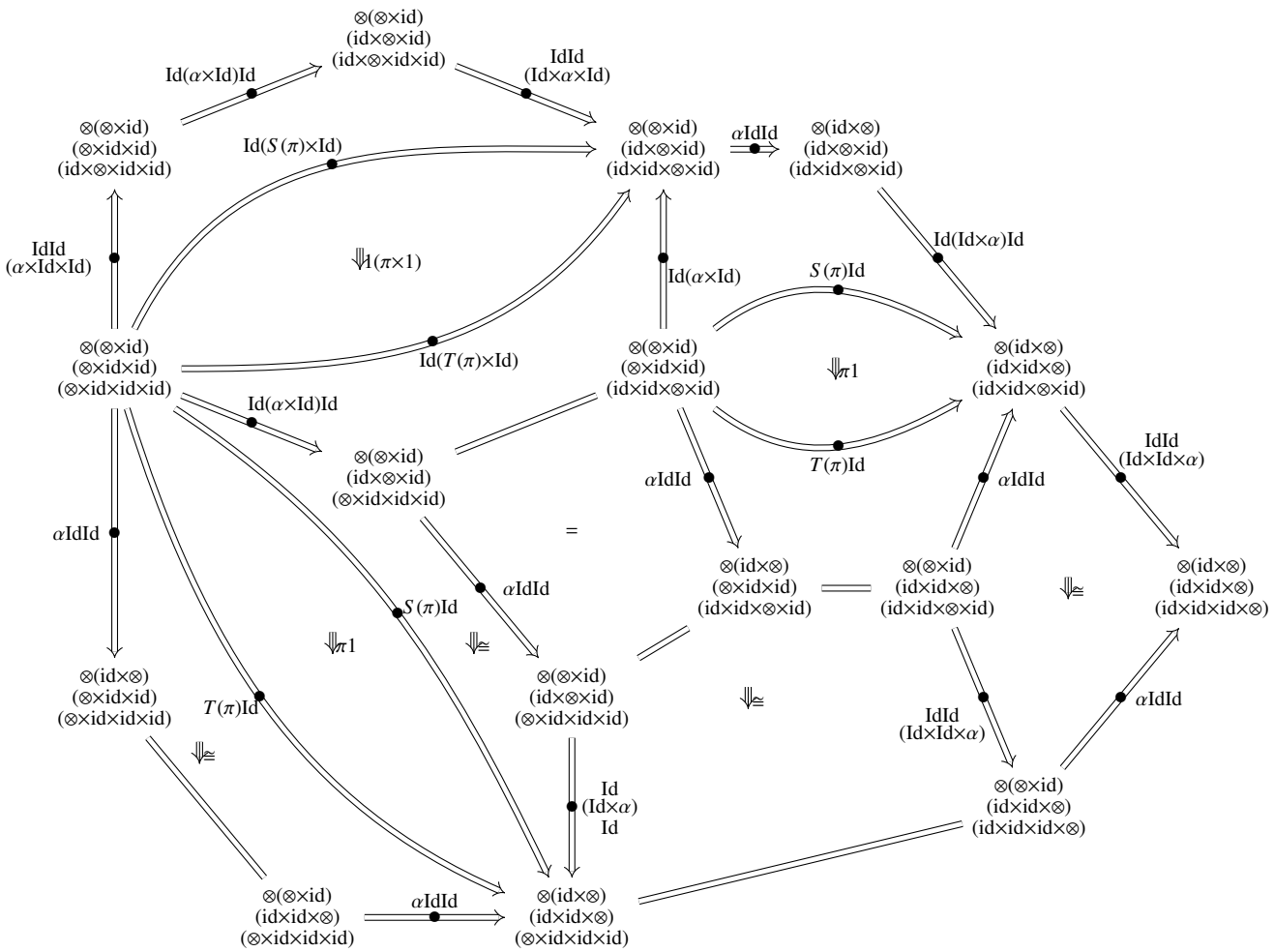
Coherence Diagrams

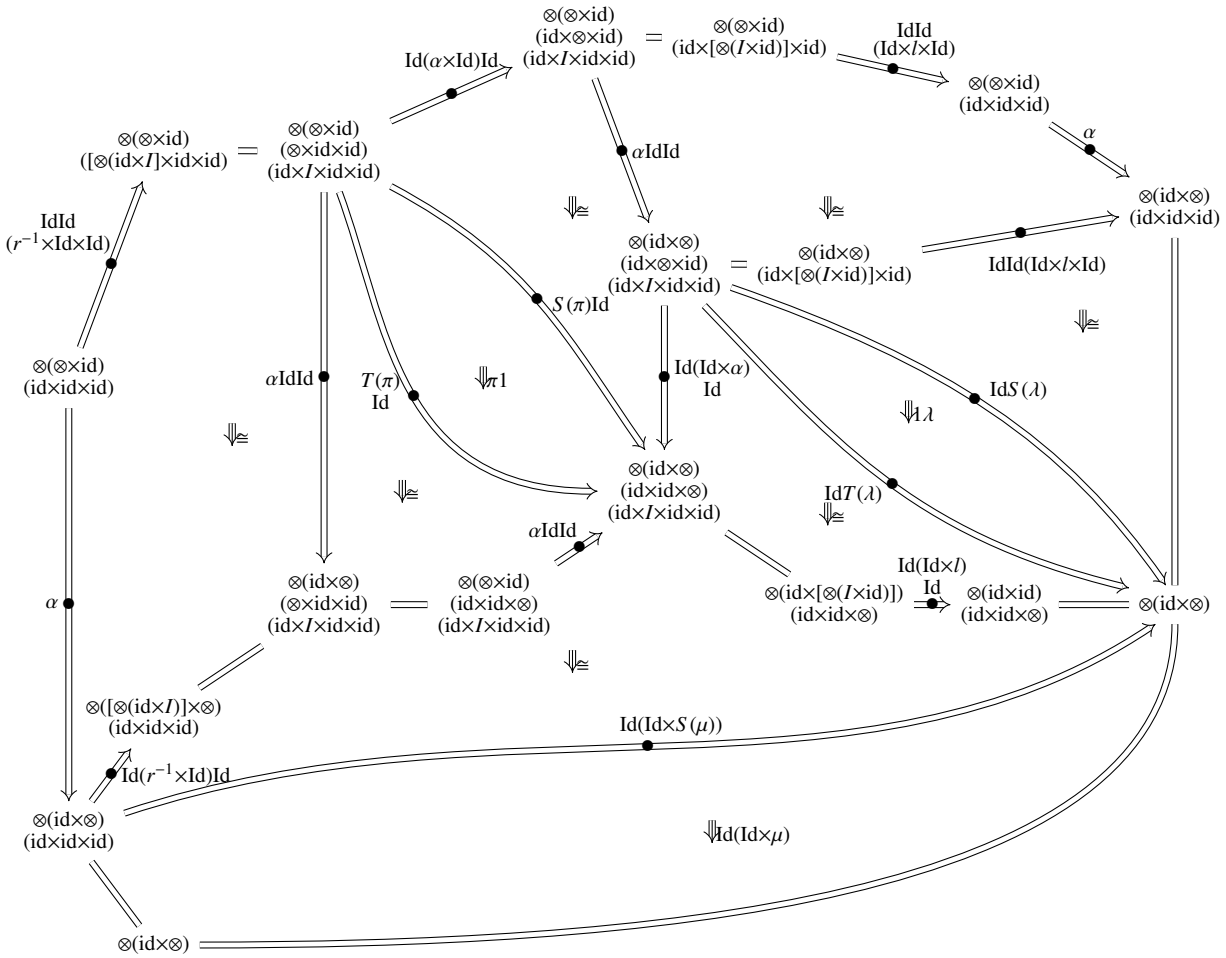
We give the coherence diagrams for monoidal objects, 1-cells, 2-cells and icons in a locally cubical bicategory, defined in Section 4.3. For readability, we sometimes write $S(\alpha)$ and $T(\alpha)$ for the composite 2-cells that form the source and target, respectively, of a 3-cell α. Furthermore, we simplify notation for coherence constraints for double categories, by writing $\cong$ to indicate composites of such coherence cells.

Monoidal Object



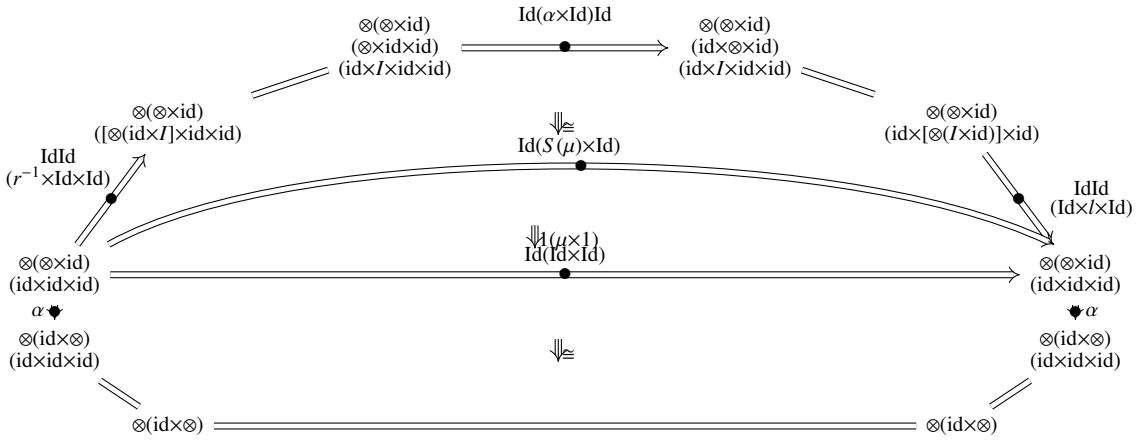
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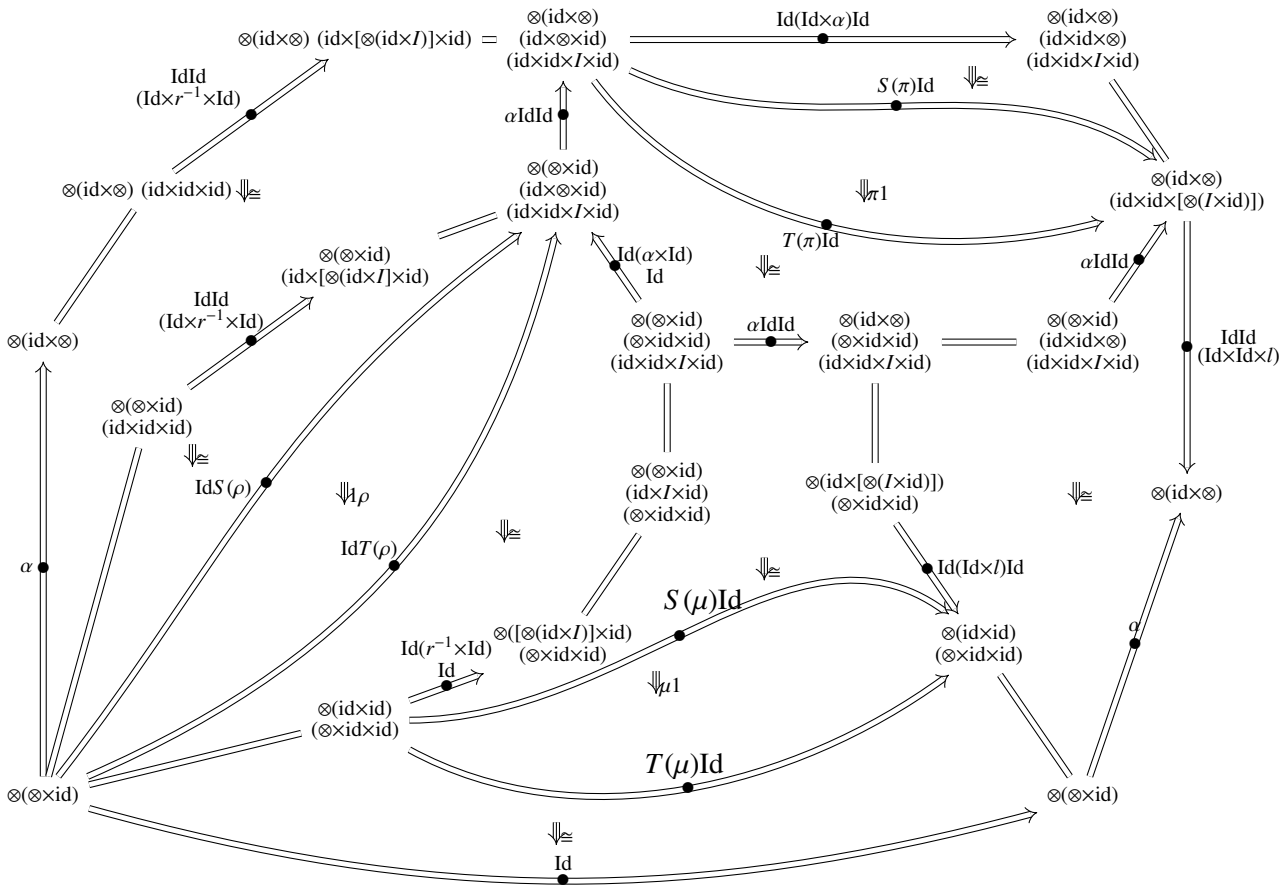

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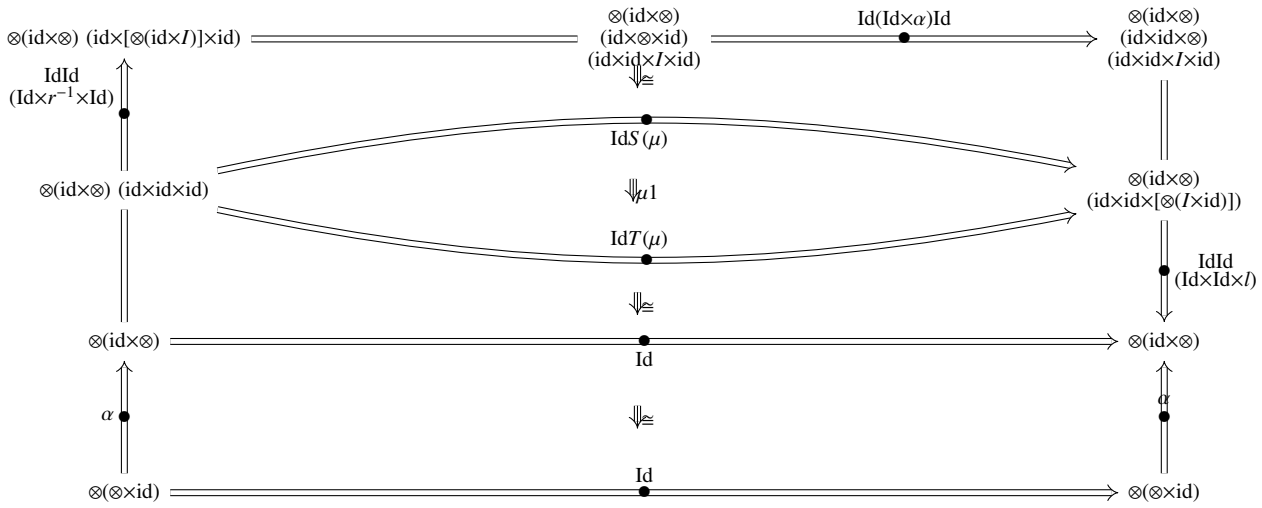
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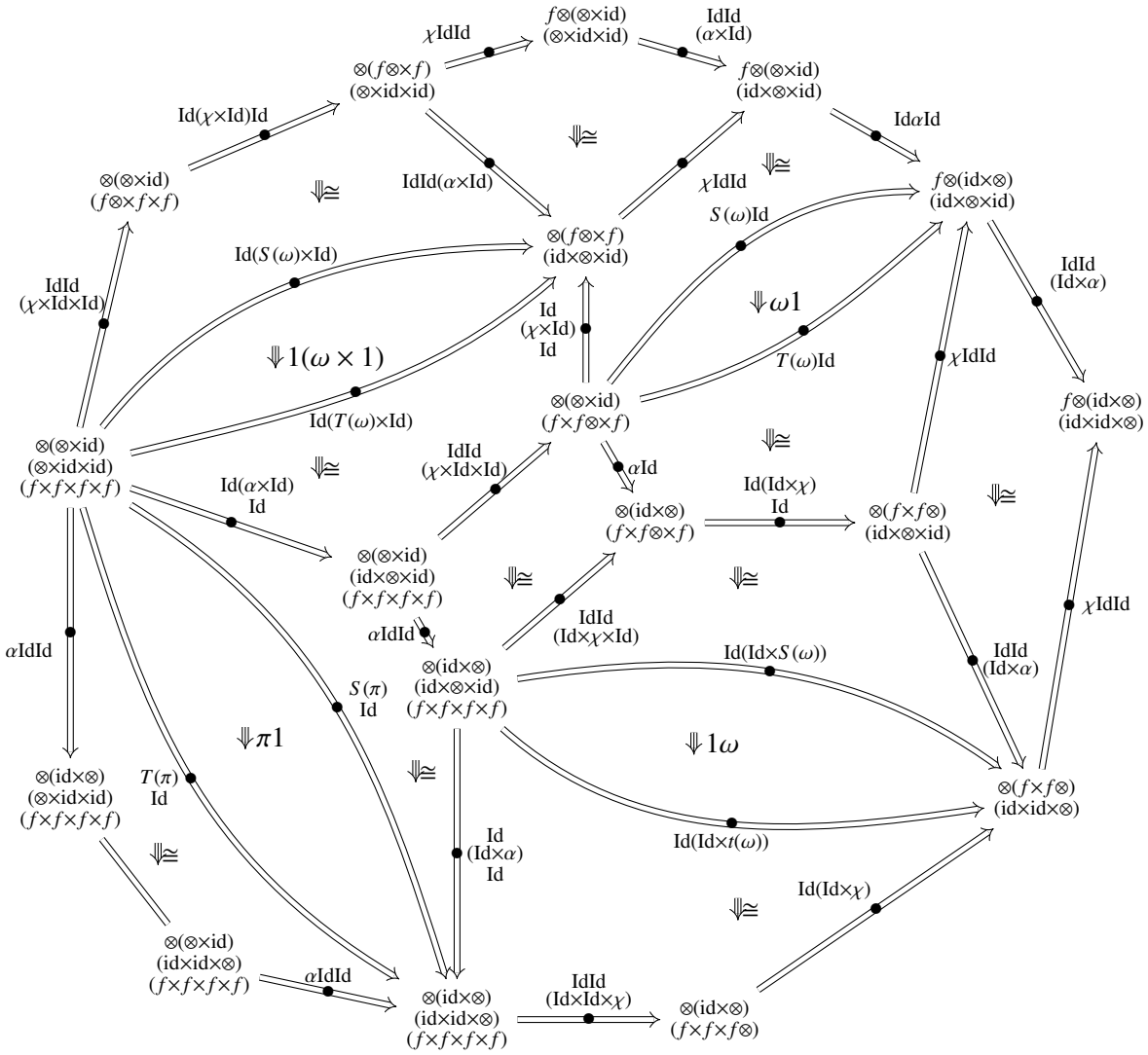

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IdId (Id×r⁻¹×Id)
S(π)Id
αIdId
⊗(⊗×id) (id×⊗×id) (id×id×I×id)
⊗(id×⊗) (id×id×[⊗(I×id)])
⊗(id×⊗) (id×id×⊗)
⊗(id×⊗) (id×id×id)
T(π)Id
⊗(⊗×id) (id×[⊗(id×I)]×id)
Id(α×Id) Id
IdId (Id×r⁻¹×Id)
⊗(⊗×id) (⊗×id×id) (id×id×I×id)
αIdId
⊗(id×⊗) (⊗×id×id) (id×id×I×id)
⊗(⊗×id) (id×id×⊗) (id×id×I×id)
IdId (Id×Id×l)
⊗(⊗×id) (id×id×id)
IdS(ρ)
⊗(⊗×id) (id×I×id) (⊗×id×id)
⊗(id×[⊗(I×id)]) (⊗×id×id)
⊗(id×⊗)
IdT(ρ)
α
Id(Id×l)Id
S(μ)Id
⊗([⊗(id×I)]×id) (⊗×id×id)
Id(r⁻¹×Id) Id
⊗(id×id) (⊗×id×id)
⊗(id×id) (⊗×id×id)
α
T(μ)Id
⊗(⊗×id)
⊗(⊗×id)
Id

= (B.0.3)

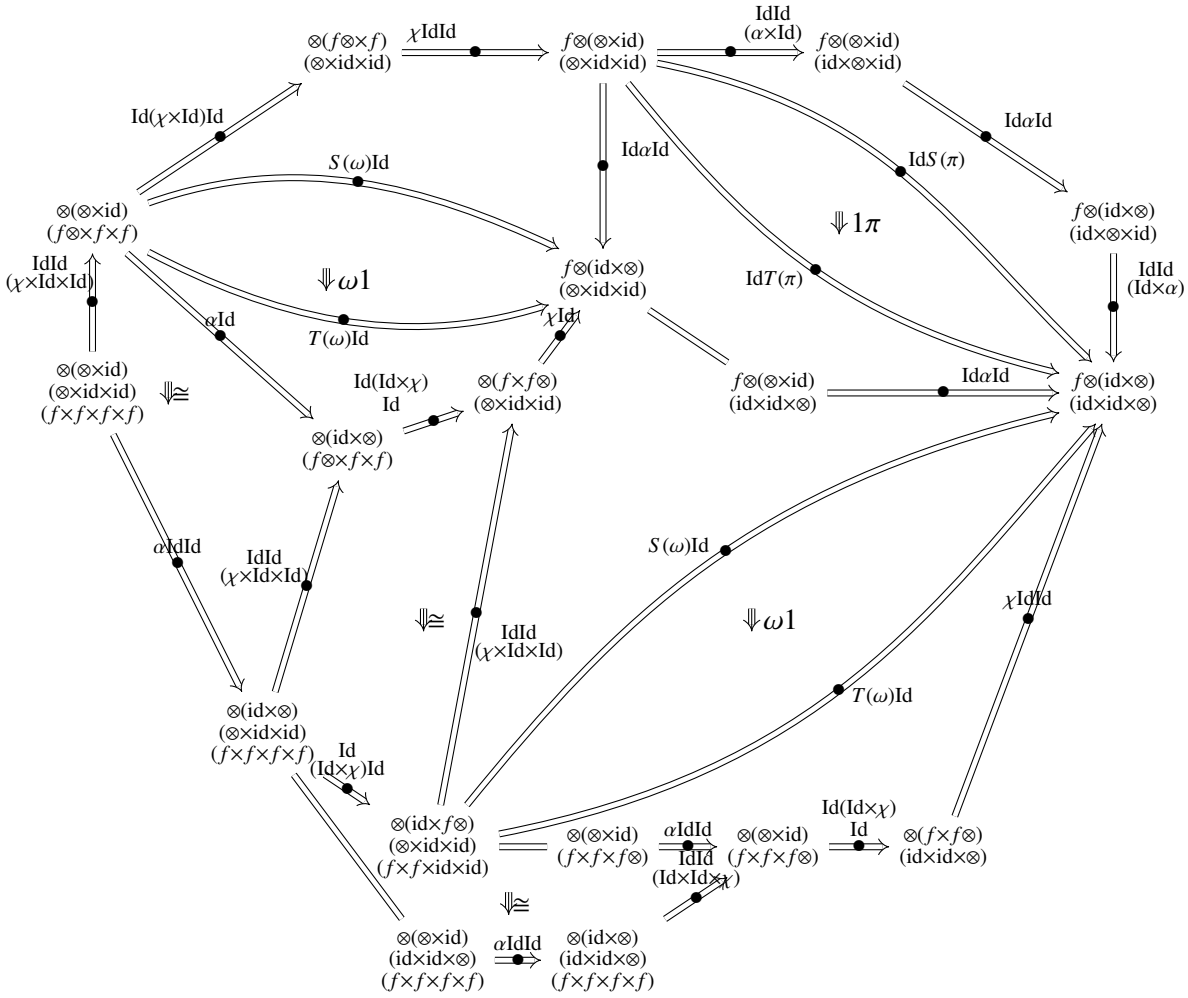

⊗(id×⊗) (id×[⊗(id×I)]×id)
⊗(id×⊗) (id×⊗×id) (id×id×I×id)
Id(Id×α)Id
⊗(id×⊗) (id×id×⊗) (id×id×I×id)
IdId (Id×r⁻¹×Id)
IdS(μ)
⊗(id×⊗) (id×id×id)
⊗(id×⊗) (id×id×[⊗(I×id)])
IdT(μ)
IdId (Id×Id×l)
⊗(id×⊗)
Id
⊗(id×⊗)
α
α
⊗(⊗×id)
Id
⊗(⊗×id)

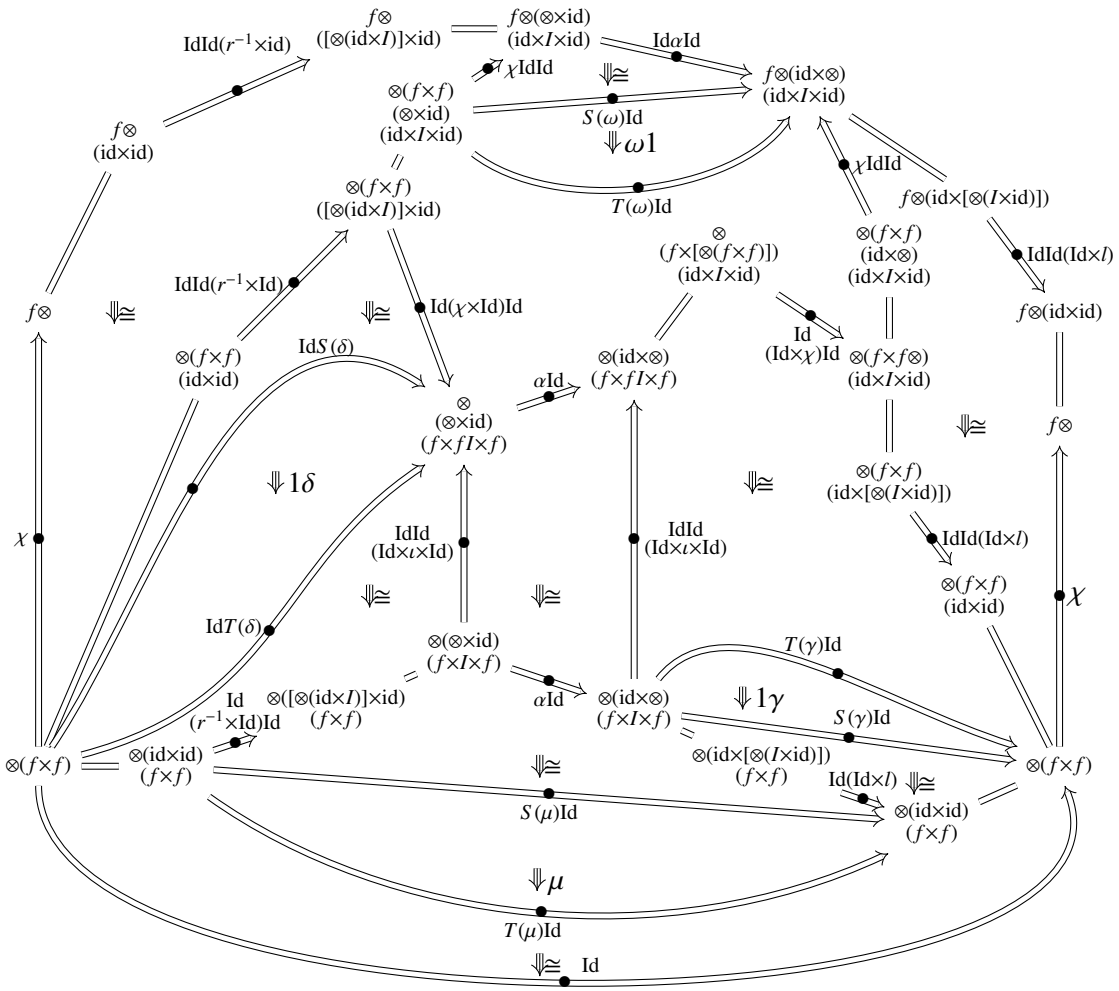
Lax Monoidal 1-cell



=

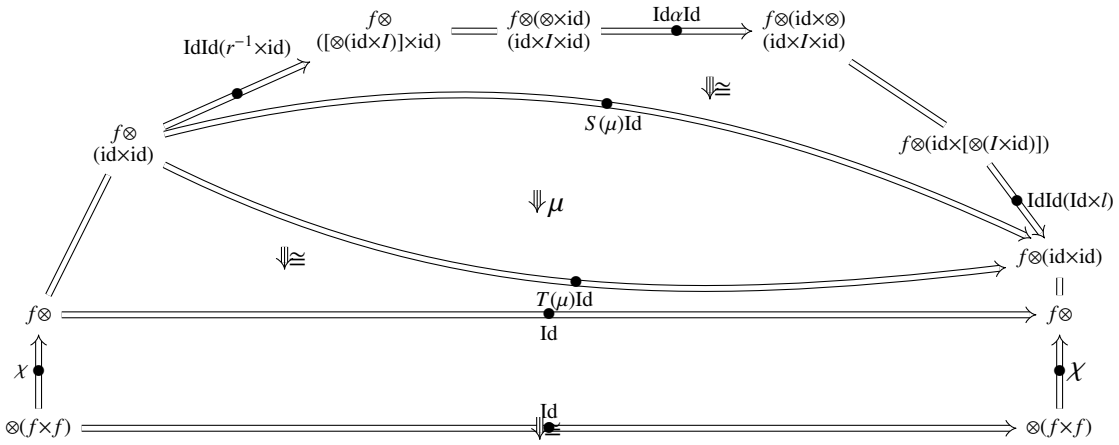
(B.0.4)

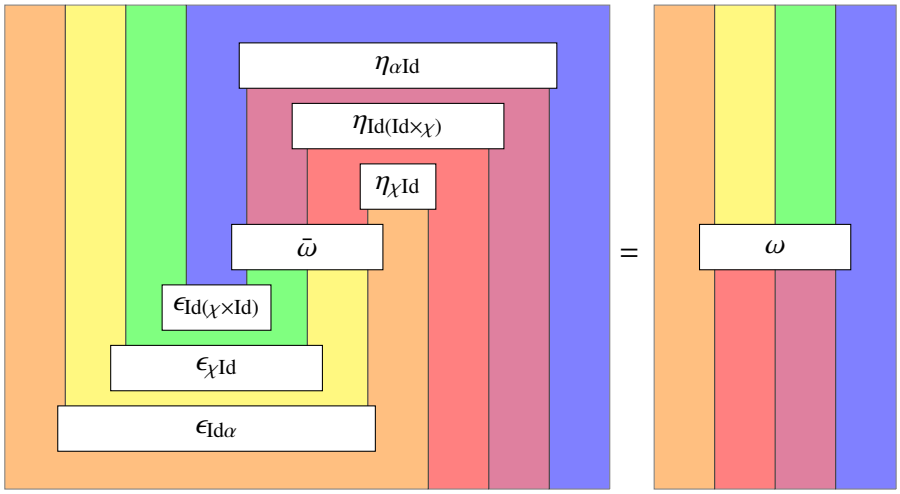

⊗(f⊗×f)
(⊗×id×id)
χIdId
f⊗(⊗×id)
(⊗×id×id)
IdId
(α×Id)
f⊗(⊗×id)
(id×⊗×id)
Id(χ×Id)Id
S(ω)Id
IdαId
IdS(π)
IdαId
f⊗(id×⊗)
(id×⊗×id)
⊗(⊗×id)
(f⊗×f×f)
⇓1π
IdId
(χ×Id×Id)
⇓ω1
f⊗(id×⊗)
(⊗×id×id)
IdT(π)
IdId
(Id×α)
αId
T(ω)Id
χId
⊗(⊗×id)
(⊗×id×id)
(f×f×f×f)
⇓≅
Id(Id×χ)
Id
⊗(f×f⊗)
(⊗×id×id)
f⊗(⊗×id)
(id×id×⊗)
IdαId
f⊗(id×⊗)
(id×id×⊗)
⊗(id×⊗)
(f⊗×f×f)
αIdId
IdId
(χ×Id×Id)
S(ω)Id
⇓≅
IdId
(χ×Id×Id)
⇓ω1
χIdId
T(ω)Id
⊗(id×⊗)
(⊗×id×id)
(f×f×f×f)
Id
(Id×χ)Id
⊗(id×f⊗)
(⊗×id×id)
(f×f×id×id)
⊗(⊗×id)
(f×f×f⊗)
αIdId
IdId
(Id×Id×χ)
⊗(⊗×id)
(f×f×f⊗)
Id(Id×χ)
Id
⊗(f×f⊗)
(id×id×⊗)
⇓≅
⊗(⊗×id)
(id×id×⊗)
(f×f×f×f)
αIdId
⊗(id×⊗)
(id×id×⊗)
(f×f×f×f)


f⊗ ([⊗(id×I)]×id)
f⊗(⊗×id) (id×I×id)
IdId(r⁻¹×id)
IdαId
χIdId
f⊗(id×⊗) (id×I×id)
⊗(f×f) (⊗×id) (id×I×id)
S(ω)Id
ω1
T(ω)Id
f⊗ (id×id)
⊗(f×f) ([⊗(id×I)]×id)
χIdId
f⊗(id×[⊗(I×id)])
⊗ (f×[⊗(f×f)]) (id×I×id)
⊗(f×f) (id×⊗) (id×I×id)
IdId(Id×l)
IdId(r⁻¹×Id)
Id(χ×Id)Id
f⊗
f⊗(id×id)
⊗(f×f) (id×id)
IdS(δ)
⊗(id×⊗) (f×fI×f)
Id (Id×χ)Id
⊗(f×f⊗) (id×I×id)
αId
⊗ (⊗×id) (f×fI×f)
f⊗
1δ
⊗(f×f) (id×[⊗(I×id)])
IdId (Id×ι×Id)
IdId (Id×ι×Id)
IdId(Id×l)
⊗(f×f) (id×id)
χ
χ
IdT(δ)
⊗(⊗×id) (f×I×f)
T(γ)Id
Id (r⁻¹×Id)Id
⊗([⊗(id×I)]×id) (f×f)
αId
⊗(id×⊗) (f×I×f)
1γ
S(γ)Id
⊗(id×[⊗(I×id)]) (f×f)
⊗(f×f)
⊗(f×f)
⊗(id×id) (f×f)
Id(Id×l)
⊗(id×id) (f×f)
S(μ)Id
μ
T(μ)Id
Id

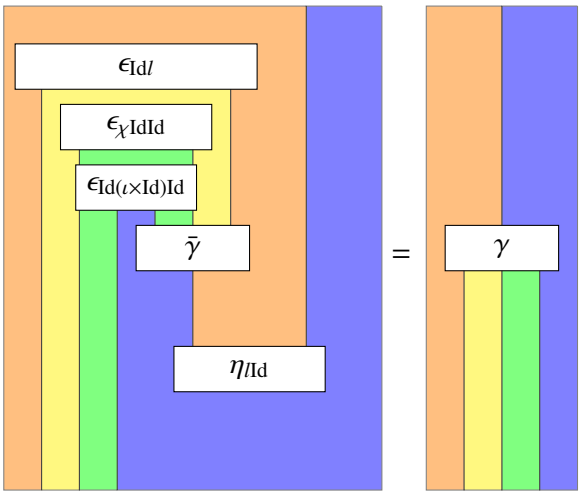
(B.0.5)

=

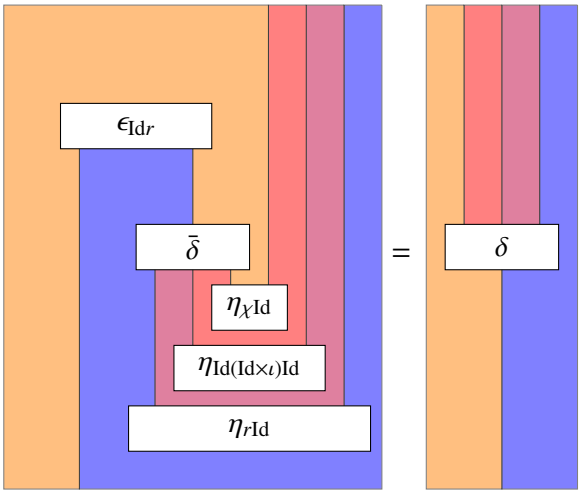

f⊗ ([⊗(id×I)]×id)
f⊗(⊗×id) (id×I×id)
IdId(r⁻¹×id)
IdαId
f⊗(id×⊗) (id×I×id)
S(μ)Id
f⊗ (id×id)
f⊗(id×[⊗(I×id)])
μ
IdId(Id×l)
f⊗(id×id)
T(μ)Id
f⊗
Id
f⊗
χ
χ
Id
⊗(f×f)
⊗(f×f)


$\eta_{\alpha \mathrm{Id}}$
$\eta_{\mathrm{Id}(\mathrm{Id}\times\chi)}$
$\eta_{\chi \mathrm{Id}}$
$\bar{\omega}$
$\epsilon_{\mathrm{Id}(\chi\times\mathrm{Id})}$
$\epsilon_{\chi \mathrm{Id}}$
$\epsilon_{\mathrm{Id}\alpha}$
=
ω

(B.0.6)

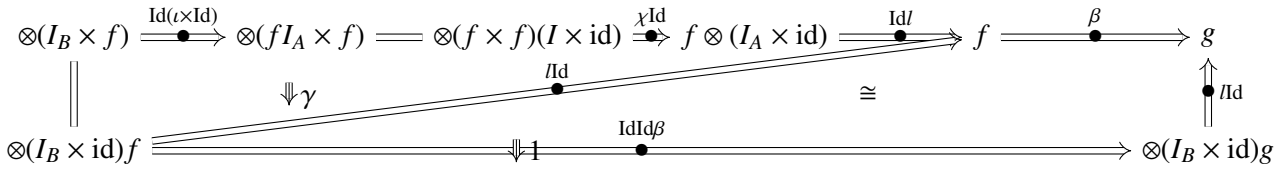

$\epsilon_{\mathrm{Id}l}$
$\epsilon_{\chi \mathrm{Id}\mathrm{Id}}$
$\epsilon_{\mathrm{Id}(\iota\times\mathrm{Id})\mathrm{Id}}$
$\bar{\gamma}$
$\eta_{l\mathrm{Id}}$
=
γ

(B.0.7)


$\epsilon_{\mathrm{Id}r}$
$\bar{\delta}$
$\eta_{\chi \mathrm{Id}}$
$\eta_{\mathrm{Id}(\mathrm{Id}\times\iota)\mathrm{Id}}$
$\eta_{r\mathrm{Id}}$
=
δ

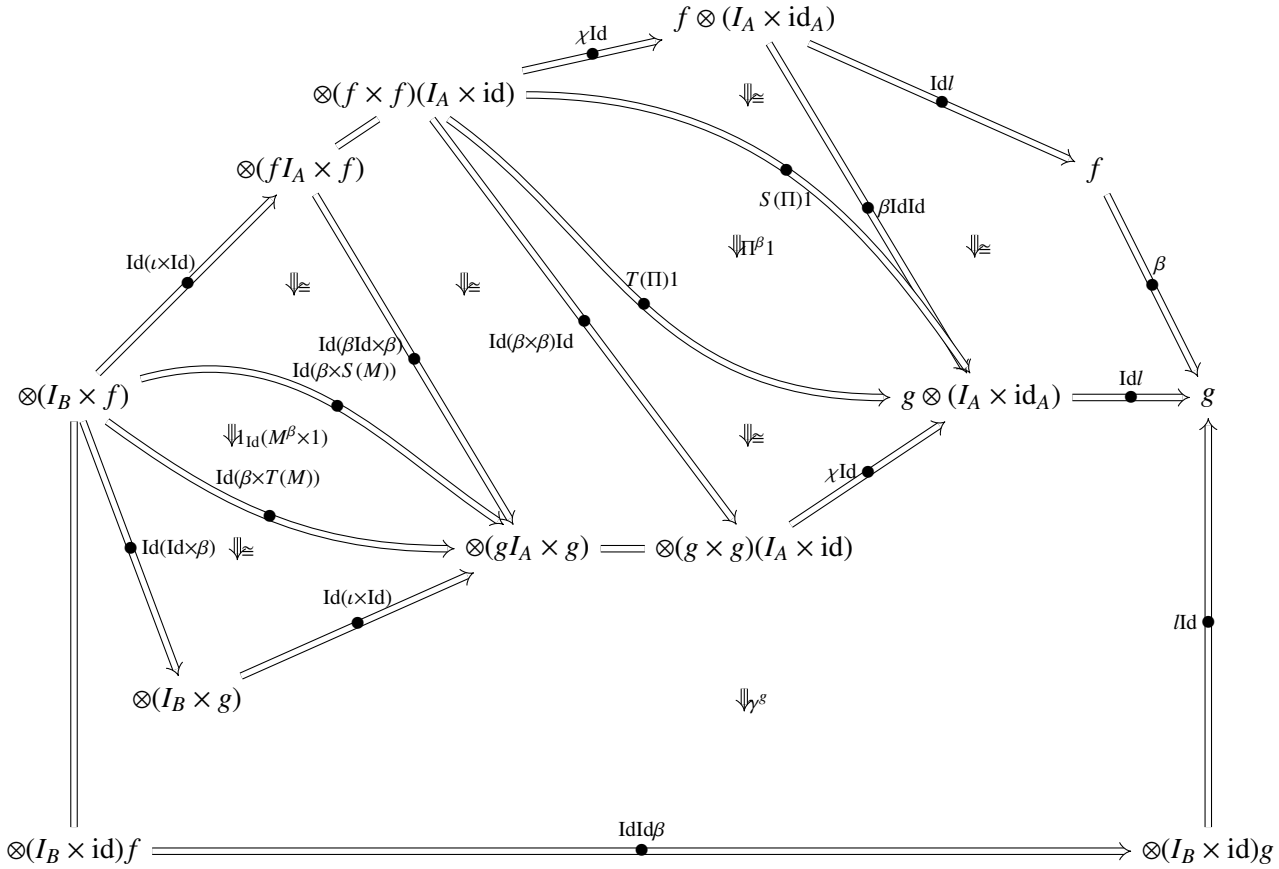
(B.0.8)

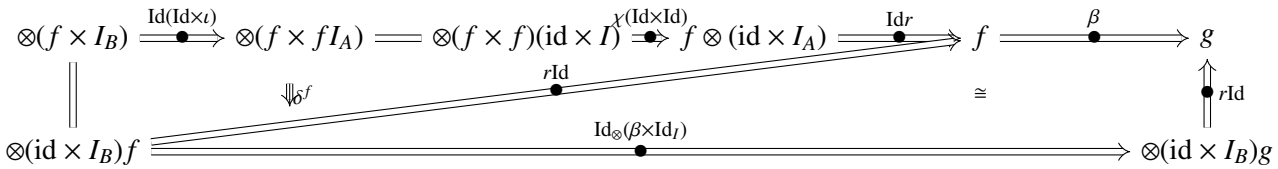
Lax Monoidal 2-cell



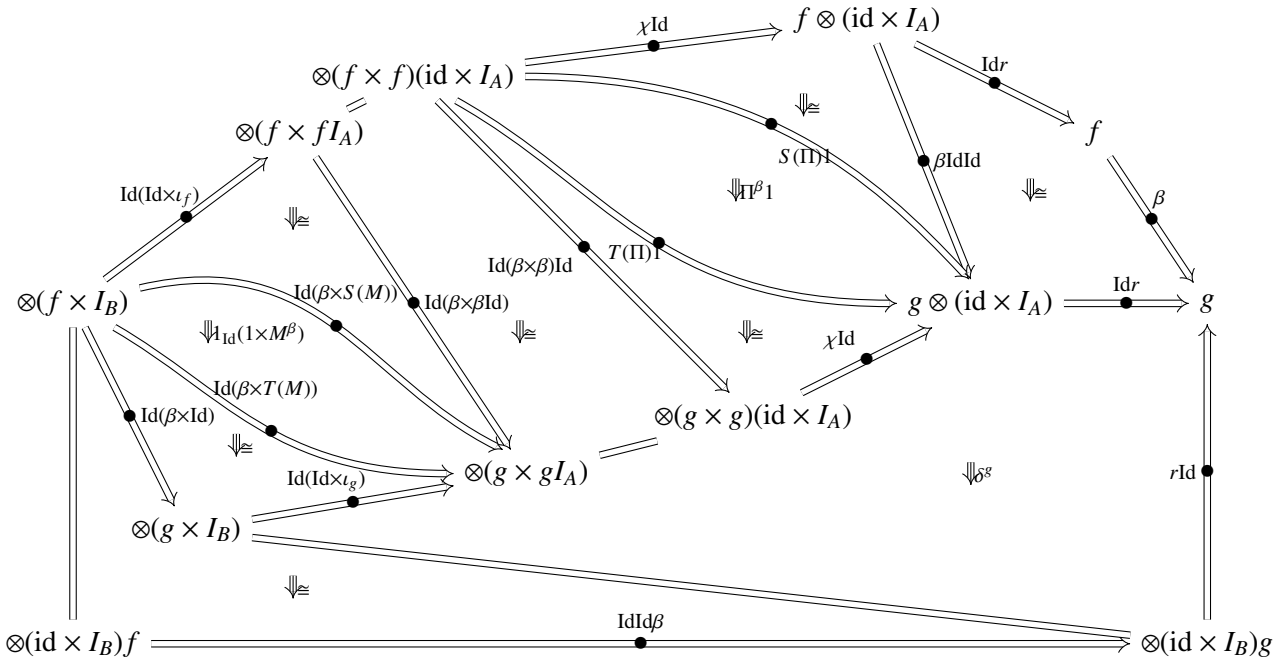
=

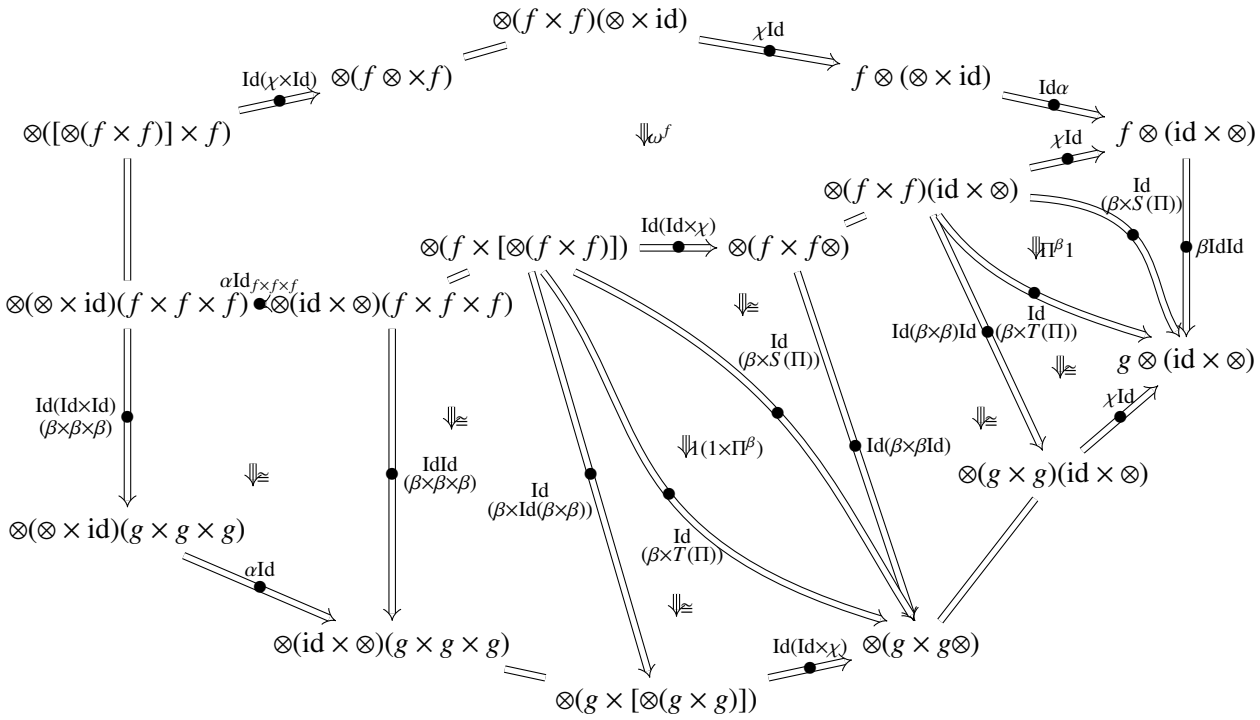
(B.0.9)



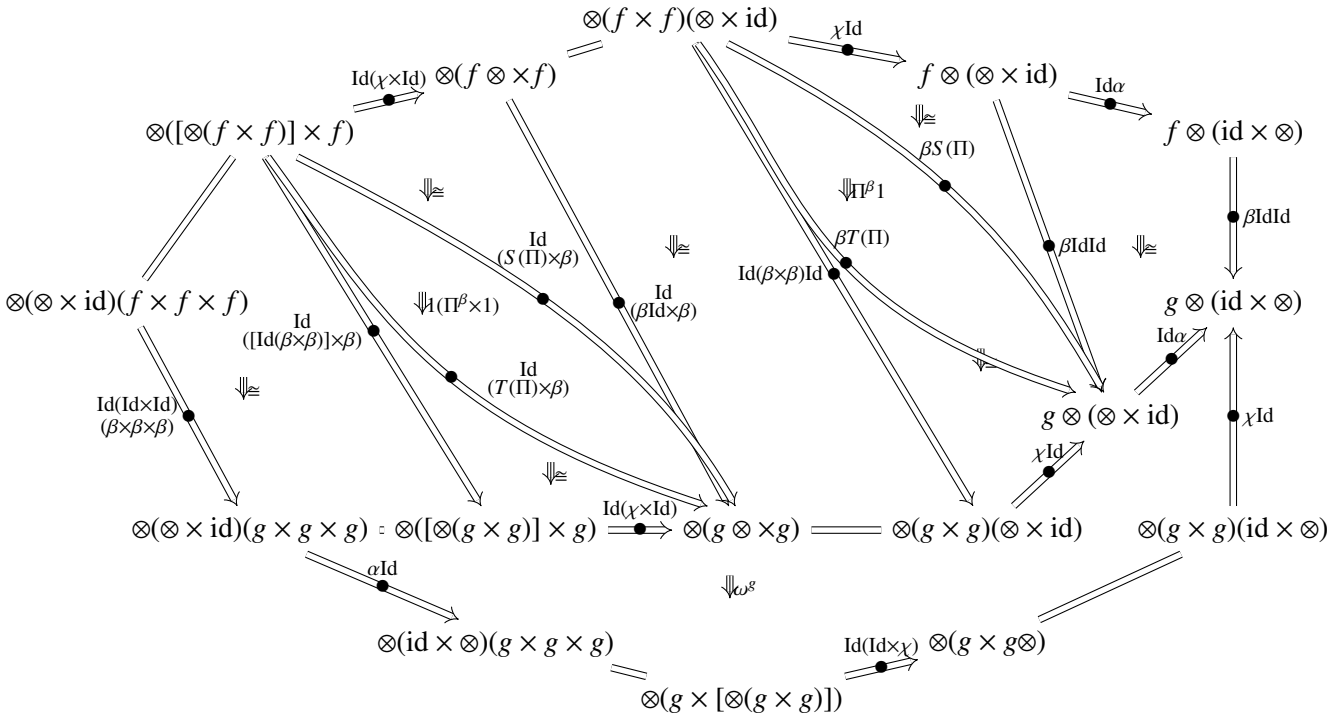

$\otimes(f \times I_B)$
$\mathrm{Id}(\mathrm{Id}\times\iota)$
$\otimes(f \times fI_A)$
$\otimes(f \times f)(\mathrm{id} \times I)$
$\chi(\mathrm{Id}\times\mathrm{Id})$
$f \otimes (\mathrm{id} \times I_A)$
$\mathrm{Id}r$
f
β
g
δ^f
$r\mathrm{Id}$
$\cong$
$r\mathrm{Id}$
$\otimes(\mathrm{id} \times I_B)f$
$\mathrm{Id}_\otimes(\beta\times\mathrm{Id}_I)$
$\otimes(\mathrm{id} \times I_B)g$

$=$ (B.0.10)

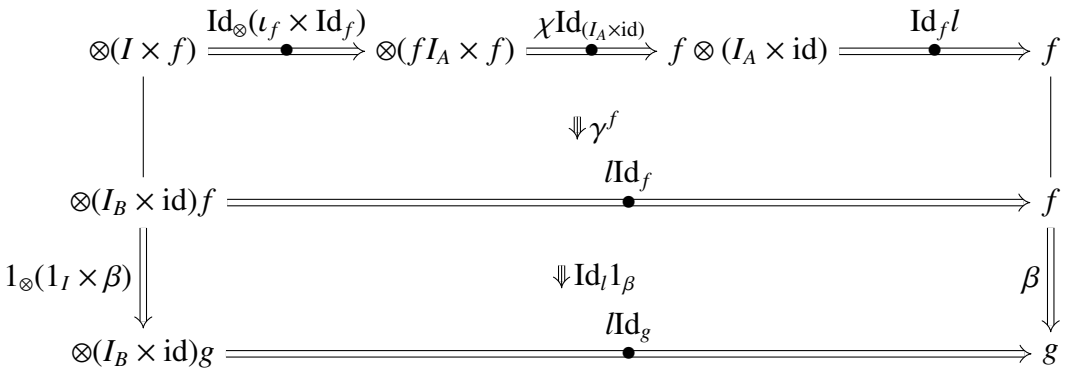

$\chi\mathrm{Id}$
$f \otimes (\mathrm{id} \times I_A)$
$\otimes(f \times f)(\mathrm{id} \times I_A)$
$\mathrm{Id}r$
$\otimes(f \times fI_A)$
f
$S(\Pi)1$
$\beta\mathrm{IdId}$
$\Pi^\beta 1$
$\mathrm{Id}(\mathrm{Id}\times\iota_f)$
β
$\mathrm{Id}(\beta\times\beta)\mathrm{Id}$
$T(\Pi)1$
$\otimes(f \times I_B)$
$\mathrm{Id}(\beta\times S(M))$
$\mathrm{Id}(\beta\times\beta\mathrm{Id})$
$g \otimes (\mathrm{id} \times I_A)$
$\mathrm{Id}r$
g
$\mathrm{Id}_{\mathrm{Id}}(1\times M^\beta)$
$\chi\mathrm{Id}$
$\mathrm{Id}(\beta\times T(M))$
$\mathrm{Id}(\beta\times\mathrm{Id})$
$\otimes(g \times g)(\mathrm{id} \times I_A)$
$\mathrm{Id}(\mathrm{Id}\times\iota_g)$
$\otimes(g \times gI_A)$
δ^g
$r\mathrm{Id}$
$\otimes(g \times I_B)$
$\otimes(\mathrm{id} \times I_B)f$
$\mathrm{IdId}\beta$
$\otimes(\mathrm{id} \times I_B)g$


⊗(f × f)(⊗ × id)
χId
Id(χ×Id)
⊗(f ⊗ ×f)
f ⊗ (⊗ × id)
Idα
⊗([⊗(f × f)] × f)
ωf
χId
f ⊗ (id × ⊗)
⊗(f × f)(id × ⊗)
Id (β×S(Π))
Id(Id×χ)
⊗(f × [⊗(f × f)])
⊗(f × f⊗)
Π^β 1
βIdId
αId f×f×f
⊗(⊗ × id)(f × f × f)
⊗(id × ⊗)(f × f × f)
Id (β×S(Π))
Id (β×T(Π))
Id(β×β)Id
g ⊗ (id × ⊗)
Id(Id×Id) (β×β×β)
IdId (β×β×β)
1(1×Π^β)
Id(β×βId)
χId
⊗(g × g)(id × ⊗)
Id (β×Id(β×β))
Id (β×T(Π))
⊗(⊗ × id)(g × g × g)
αId
⊗(id × ⊗)(g × g × g)
Id(Id×χ)
⊗(g × g⊗)
⊗(g × [⊗(g × g)])

= (B.0.11)

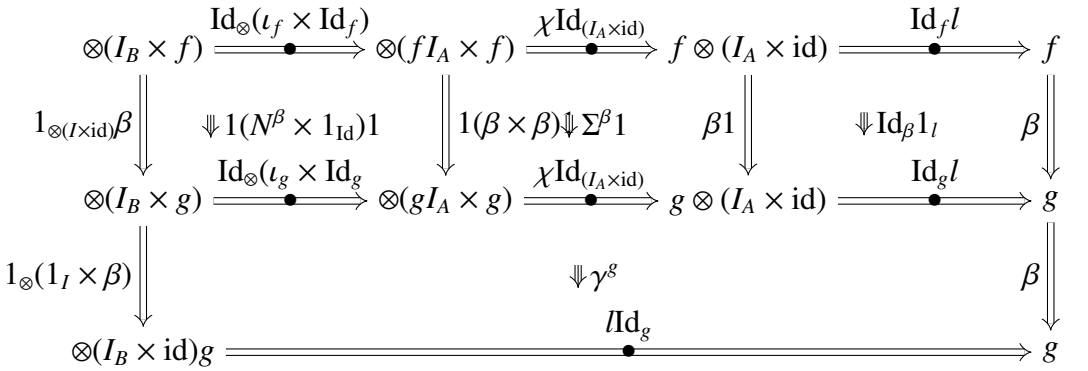

⊗(f × f)(⊗ × id)
χId
Id(χ×Id)
⊗(f ⊗ ×f)
f ⊗ (⊗ × id)
Idα
⊗([⊗(f × f)] × f)
βS(Π)
f ⊗ (id × ⊗)
Π^β 1
βIdId
βT(Π)
Id (S(Π)×β)
Id(β×β)Id
βIdId
⊗(⊗ × id)(f × f × f)
1(Π^β×1)
Id (βId×β)
g ⊗ (id × ⊗)
Id ([Id(β×β)]×β)
Idα
Id (T(Π)×β)
g ⊗ (⊗ × id)
Id(Id×Id) (β×β×β)
χId
χId
⊗(⊗ × id)(g × g × g)
⊗([⊗(g × g)] × g)
Id(χ×Id)
⊗(g ⊗ ×g)
⊗(g × g)(⊗ × id)
⊗(g × g)(id × ⊗)
αId
ωg
⊗(id × ⊗)(g × g × g)
Id(Id×χ)
⊗(g × g⊗)
⊗(g × [⊗(g × g)])

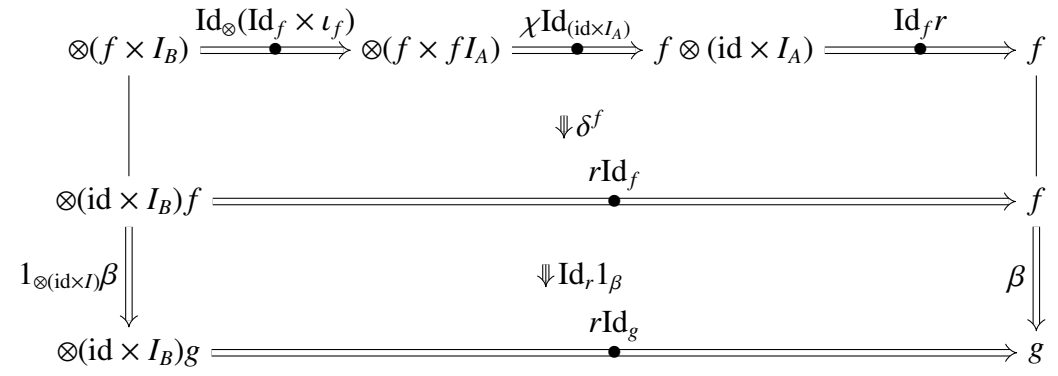
Monoidal Icon



(B.0.12)

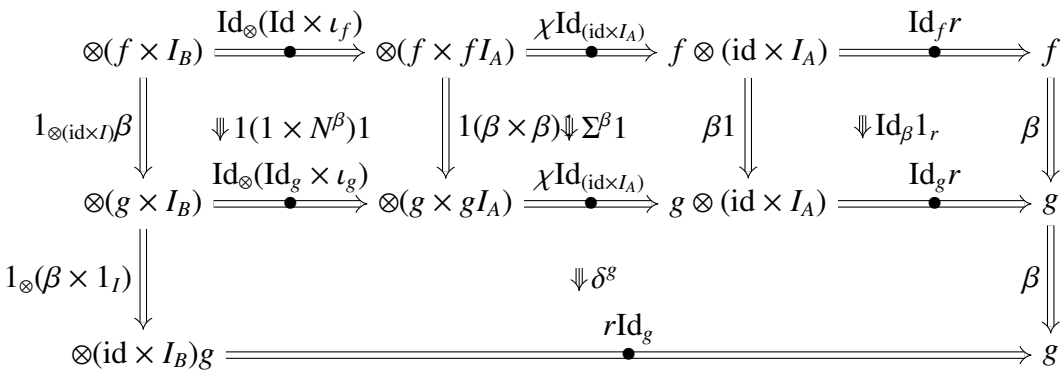
=

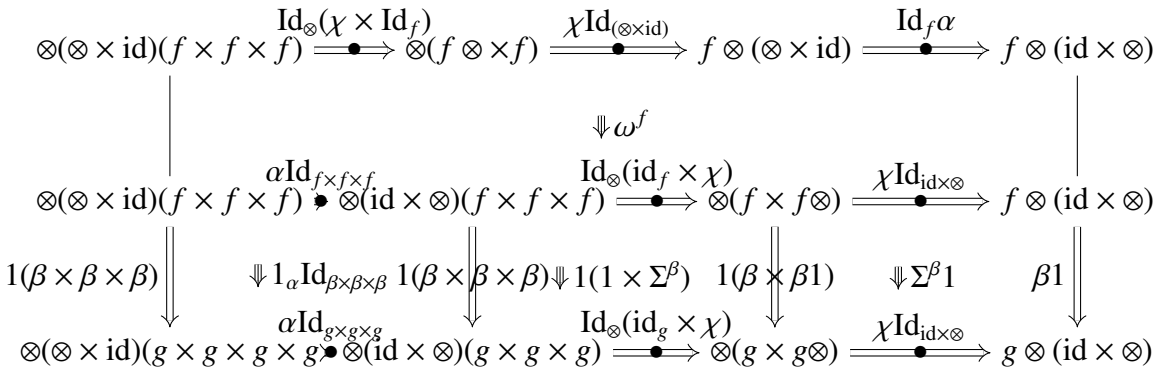



$\otimes(f \times I_B)$
$\mathrm{Id}_{\otimes}(\mathrm{Id}_f \times \iota_f)$
$\otimes(f \times fI_A)$
$\chi \mathrm{Id}_{(\mathrm{id} \times I_A)}$
$f \otimes (\mathrm{id} \times I_A)$
$\mathrm{Id}_f r$
f
$\Downarrow \delta^f$
$r\mathrm{Id}_f$
$\otimes(\mathrm{id} \times I_B)f$
f
$1_{\otimes(\mathrm{id} \times I)}\beta$
$\Downarrow \mathrm{Id}_r 1_\beta$
β
$r\mathrm{Id}_g$
$\otimes(\mathrm{id} \times I_B)g$
g

(B.0.13)

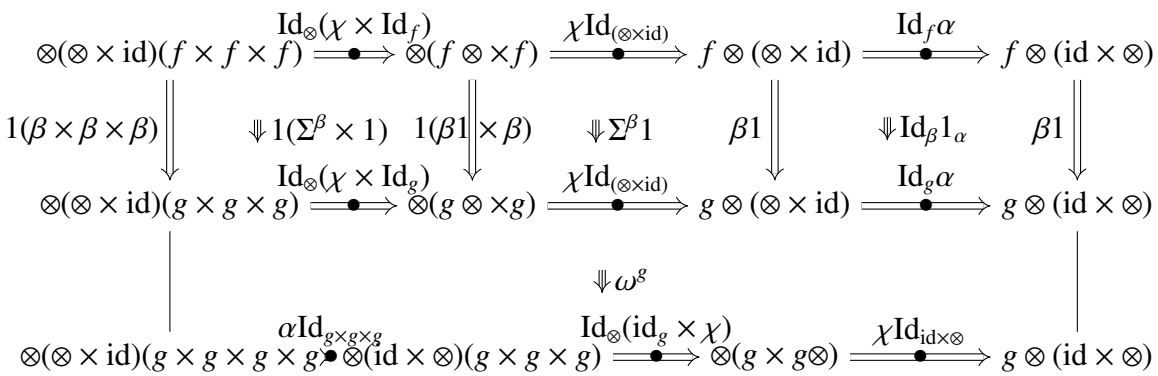
=


$\otimes(f \times I_B)$
$\mathrm{Id}_{\otimes}(\mathrm{Id} \times \iota_f)$
$\otimes(f \times fI_A)$
$\chi \mathrm{Id}_{(\mathrm{id} \times I_A)}$
$f \otimes (\mathrm{id} \times I_A)$
$\mathrm{Id}_f r$
f
$1_{\otimes(\mathrm{id} \times I)}\beta$
$\Downarrow 1(1 \times N^\beta)1$
$1(\beta \times \beta)\Downarrow \Sigma^\beta 1$
$\beta 1$
$\Downarrow \mathrm{Id}_\beta 1_r$
β
$\otimes(g \times I_B)$
$\mathrm{Id}_{\otimes}(\mathrm{Id}_g \times \iota_g)$
$\otimes(g \times gI_A)$
$\chi \mathrm{Id}_{(\mathrm{id} \times I_A)}$
$g \otimes (\mathrm{id} \times I_A)$
$\mathrm{Id}_g r$
g
$1_{\otimes}(\beta \times 1_I)$
$\Downarrow \delta^g$
β
$r\mathrm{Id}_g$
$\otimes(\mathrm{id} \times I_B)g$
g

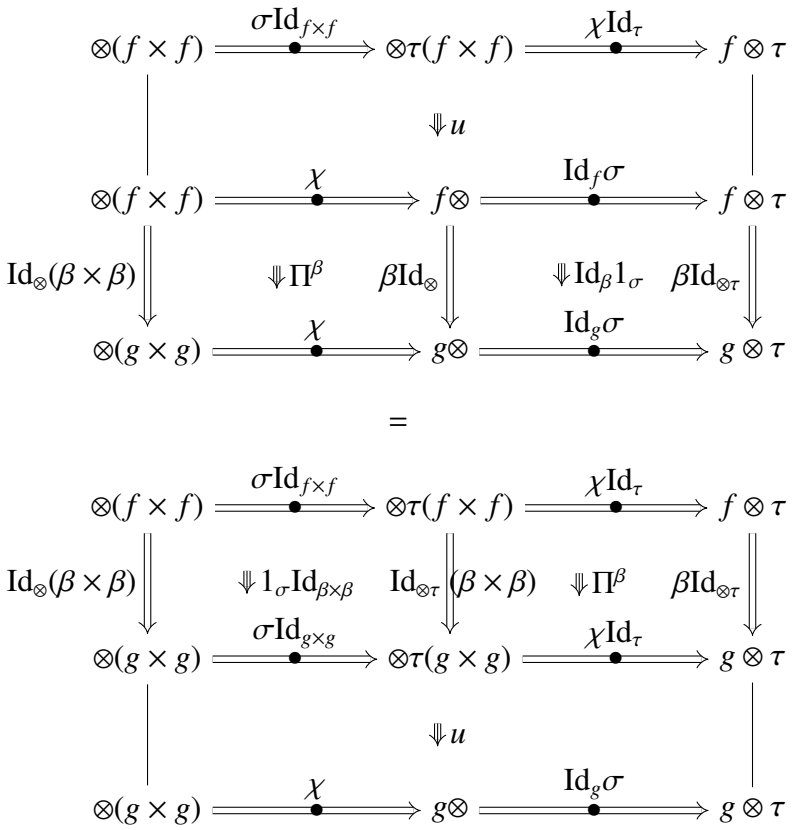

⊗(⊗ × id)(f × f × f)
⊗(f ⊗ ×f)
f ⊗ (⊗ × id)
f ⊗ (id × ⊗)
⊗(id × ⊗)(f × f × f)
⊗(f × f⊗)
⊗(⊗ × id)(g × g × g)
⊗(id × ⊗)(g × g × g)
⊗(g × g⊗)
g ⊗ (id × ⊗)
⊗(g ⊗ ×g)
g ⊗ (⊗ × id)

(B.0.14)

=


⊗(⊗ × id)(f × f × f)
⊗(f ⊗ ×f)
f ⊗ (⊗ × id)
f ⊗ (id × ⊗)
⊗(⊗ × id)(g × g × g)
⊗(g ⊗ ×g)
g ⊗ (⊗ × id)
g ⊗ (id × ⊗)
⊗(id × ⊗)(f × f × f)
⊗(f × f⊗)
⊗(id × ⊗)(g × g × g)
⊗(g × g⊗)

Braided Monoidal Icon



(B.0.15)

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