Graphical Reasoning in Compact Closed Categories for Quantum Computation

Lucas Dixon\textsuperscript{*} \hspace{1cm} Ross Duncan\textsuperscript{†}
University of Edinburgh \hspace{1cm} University of Oxford

February 3, 2009

Abstract

Compact closed categories provide a foundational formalism for a variety of important domains, including quantum computation. These categories have a natural visualisation as a form of graphs. We present a formalism for equational reasoning about such graphs and develop this into a generic proof system with a fixed logical kernel for equational reasoning about compact closed categories. Automating this reasoning process is motivated by the slow and error prone nature of manual graph manipulation. A salient feature of our system is that it provides a formal and declarative account of derived results that can include ‘ellipses’-style notation. We illustrate the framework by instantiating it for a graphical language of quantum computation and show how this can be used to perform symbolic computation.

Keywords: graph rewriting, quantum computing, categorical logic, interactive theorem proving, graphical calculi, ellipses notation.

1 Introduction

Recent work in quantum computation has emphasised the use of graphical languages motivated by the underlying logical structure of quantum mechanics itself [1,19,4,6,7]. These techniques have a number of advantages over the conventional matrix-based approach to quantum mechanics:

- The visual representation abstracts over the values in the matrices. This removes detail that is difficult or tedious for a human to interpret.
- Many properties have a natural graphical representation. For example, separability of quantum states can be inferred from disjoint subgraphs.
The algebra of graphs generalises to domains other than vector spaces: it provides a representation for compact closed categories [11].

A major problem with these graphical representations is the lack of machinery for automating their manipulation. The main contribution of this paper is a graph-based formalism that is suitable for representing and reasoning about compact closed categories with additional equational structure. This has a wide variety applications including reasoning about relations, stochastic processes, and synchronous processes. In this paper we introduce the representation, develop it into a formal proof system, and highlight its application for symbolic reasoning about quantum computation.

We begin by presenting a graphical model of quantum computation. This model displays the typical features of a graphical calculi: quantum processes are represented by graphs built up from basic elements. Non-structural equivalences are captured by equations between graphs. An important result in this calculus is the Spider Theorem which takes the form of an equation between graphs involving informal ellipses notation (see \S 2).

The formalisation, in a graphical form, of rules containing ellipses notation and the corresponding reasoning with such rules requires an extension of the graphical calculus that eventually forms graph patterns. We develop this by first defining a formalism for graphs, their transformations, and an appropriate subgraph relation. An important difference between this approach and standard texts on graph theory lies in the notion of subgraph. We view vertices as operations which have types corresponding to their incident edges and thus we do not allow additional edges in a subgraph. We introduce a general form of graph combination, called plugging, which includes both parallel and sequential composition as special cases. Since redexes are preserved by plugging, this gives a compositional account of equational reasoning for compact closed categories. We prove that our graph-based formalism is a faithful representation the of free compact closed category generated from its basic elements. We also introduce a general formalism for ellipses notation in graphs which forms !-box graphs. By combining !-box graphs with our compositional graph formalism, we provide a suitable representation for graph patterns that can formally represent and reason with rules derived from the Spider Theorem.

Using our graph-based formalism as the representational foundation, we develop a simple logical framework for manipulating models of compact closed categories. This has a suitable rewriting mechanism where the axioms of the underlying object-formalism are expressed as equations between graphs. We then present a short case study that illustrates the framework by instantiating it for the introduced model of quantum computation. This shows how the framework can be used to symbolically perform simplifications of quantum programs as well as simulate computations.
2 Quantum Computations as Graphs

In this section we will describe a set of generators and equations used to reason about quantum computation, and show how some of its formal properties lead to particular issues for the development of reasoning machinery.

Initiated in [1], a substantial strand of work in quantum informatics has involved the development of high-level models of quantum processes based on compact closed categories. In these formalisms, quantum processes—such as quantum logic gates, or the measurement of a qubit—correspond to arrows in the category, while the different quantum data types, usually just arrays of qubits, are the objects.

In terms of the graphical language, a recent account is described by Coecke and Duncan [5]. This is based on providing a graphical language for compact closed categories, described in §5. This account allows edges to represent qubits and, in particular, the domain and codomain edges represent the inputs and outputs respectively of a quantum process. Internally, several edges may represent the same physical qubit at different times. An edge may even represent a “virtual” qubit which stands for a correlation between different parts of the system. Coloured nodes (a light green and a darker red) are used to denote two families of operations on qubits, expressed graphically as the following generators:

\[
\begin{align*}
\epsilon_Z &= \quad & \delta_Z &= \quad & \epsilon_Z^\dagger &= \quad & \delta_Z^\dagger &= \quad & \alpha_Z &= \\
\epsilon_X &= \quad & \delta_X &= \quad & \epsilon_X^\dagger &= \quad & \delta_X^\dagger &= \quad & \alpha_X &=
\end{align*}
\]

where \( \alpha \in [0, 2\pi) \). The \( \delta_Z \) and \( \epsilon_Z \) represent quantum operations which respectively copy and delete the eigenstates of the Pauli \( Z \) operator. In addition, we have \( \epsilon_X \) which represents a Hadamard gate. Notice that \( \delta_Z \) has one edge in its domain for the qubit to be copied, and two edges in its codomain for the two copies it produces. Similarly, \( \epsilon_Z \) has one qubit as input and no outputs. The adjoints \( \delta_Z^\dagger \) and \( \epsilon_Z^\dagger \) correspond to an operation known as fusion, and to the operation of preparing a fresh qubit in a certain state. The \( \alpha_Z \) corresponds to phase shift of angle \( \alpha \) in the \( Z \) direction. The family of maps indexed by \( X \) are defined in exactly the same way, but relative to the Pauli \( X \) operator rather than the \( Z \).

The free compact closed category is then given by all graphs formed by composing and tensoring these basic graphs. All quantum operations may be defined by combining these simple operations—which are essentially classical—on two complementary observables.

We emphasise that this is a notation for representing quantum processes, not just quantum states. In this setting a state is simply a process with no

---

1 In this account, no interpretation of edge direction is needed as objects in the underlying categorical model are self dual.

2 Uniform copying operations are forbidden by the no-cloning theorem [23], but such operations are possible if we demand only the eigenstates of some self-adjoint operator to be copied. Other states will not not copied. The same remarks hold true for erasing [13].
inputs; that is, a concrete graph with empty domain. Since our formalism is based on the underlying mathematical structure rather than any particular model of quantum computation, it is capable of representing quantum circuits, measurement-based quantum computations, as well as other models. Indeed, an important application of this work is to show that states or computations implemented differently are equivalent.

The beauty of graphical calculi for compact closed categories is that equations which hold for general algebraic reasons are absorbed into the notation. However, in order to represent quantum computation, generic structure will not suffice: we need additional equations between graphs. In the system we present here, these describe the interaction between complementary observables and allow equivalent computations to be proved equivalent. The equations are discussed in detail in [5] and are presented here graphically in Figure 1.

The equations from Figure 1, which involve only one colour, allow the remarkable spider theorem, first noted in [7], to be proved:

**Theorem 1 (Spider Theorem).** Let $G$ be a connected graph generated from $\delta_Z$, $\epsilon_Z$, $\alpha_Z$ and their adjoints; then $G$ is totally determined by the number of inputs, the number of outputs, and the sum modulo $2\pi$ of the $\alpha$s which occur in it.

Hence any connected subgraph involving nodes of only one colour may be collapsed to a single vertex, with a single value $\alpha$, giving a “spider”. Conversely, a spider may be arbitrarily divided into sub-spiders, provided the total in- and out-degree is preserved, along with the sum of the $\alpha$s. Informally, this can be depicted graphically as the equation:

![Spider theorem diagram]

From this one can derive $n$-fold versions of many of the other equations.

Spiders offer a very intuitive way to manipulate graphs, and are far more compact and convenient in calculations than the graphs built up naively from the generators. However, no finite set of equations suffices to formalise spiders: we must move from finite graphs, where each vertex has bounded degree, and which are subject to a finite number of equations, to a system where nodes may have arbitrarily many edges, and there are infinitely many concrete equations. The desire to retain intuitive reasoning methods for these infinite families of equations motivates the extension from concrete graphs to graph patterns, the main subject developed in this paper.
Comonoid Laws

\[
\begin{align*}
\text{Isometry, Frobenius, and Compact Structure} & \\
\text{Abelian Unitary Group and Bilinearity} & \\
\text{Bialgebra Laws} & \\
\text{Group Actions} & \\
H \quad \text{Property and Colour Duality}
\end{align*}
\]

Figure 1: Graphical Equations for Quantum Systems. In addition, we have a “colour duality”: each equation shown here gives rise to a second, which is obtained by exchanging the two colours. The colour duality is derivable from the equations involving \(H\).
3 Graphs

Definition 2 (Graph). A directed graph consists of a 4-tuple \((V, E, s, t)\) where \(V\) and \(E\) are sets, respectively of vertices and edges, and \(s\) and \(t\) are maps which give the source and target vertices of an edge respectively:

\[
\begin{array}{ccc}
E & \xrightarrow{s} & V \\
\xleftarrow{t} & & \\
\end{array}
\]

We will assume throughout this paper that both \(V\) and \(E\) are finite.

Remark. Note that any number of edges are allowed between vertices, including from a vertex to itself.

Let \(\text{in}(v) := t^{-1}(v)\) and \(\text{out}(v) := s^{-1}(v)\) denote the incoming and outgoing edges at a vertex \(v\). The degree of a vertex \(v\) is \(\text{deg}(v) := |\text{in}(v)| + |\text{out}(v)|\).

To distinguish between elements of different graphs, we will use the subscript notation \(G = (V_G, E_G, s_G, t_G)\).

We say that a vertex \(v\) is a successor of \(u\) if there exists an edge \(e\) such that \(s(e) = u\) and \(t(e) = v\). A pair of vertices are connected, written \(u \sim v\), if they lie in the reflexive, symmetric, transitive closure of the successor relation. The equivalence classes \(V/\sim\) are the connected components of \(G\). We write \(|v|\) to denote the equivalence class containing the vertex \(v\); we write \([v]\) to denote the subgraph determined by \(|v|\).

Definition 3 (Graph Morphism). Given graphs \(G\) and \(H\), a graph morphism \(f : G \to H\) consists of functions \(f_E : E_G \to E_H\) and \(f_V : V_G \to V_H\) such that:

\[
\begin{align*}
\text{s}_H \circ f_E &= f_V \circ \text{s}_G, \\
\text{t}_H \circ f_E &= f_V \circ \text{t}_G.
\end{align*}
\]

These conditions ensure that the structure of the graph is preserved.

Definition 4 (Open Graph, Open Graph Morphism). An open graph \(\Gamma = (G, \partial G)\) consists of a directed graph \(G\), and a set of vertices \(\partial G \subseteq V_G\), such that for each \(v \in \partial G\) we have \(\text{deg}(v) = 1\). The set \(\partial G\) is called the boundary of \(\Gamma\); those vertices in \(V_G \setminus \partial G\) are called the interior of \(\Gamma\), written \(\text{Int} G\).

Given open graphs \((G, \partial G)\) and \((H, \partial H)\) a graph morphism \(f : G \to H\) defines a morphism of open graphs \(f : (G, \partial G) \to (H, \partial H)\) if \(f_V(v) \in \partial H \Rightarrow v \in \partial G\) for all \(v\) in \(V_G\).

We will refer to an open graph \((G, \partial G)\) simply as \(G\) when it is unambiguous to do so.

Definition 5 (Strict Map). Let \(f : (G, \partial G) \to (H, \partial H)\) be an open graph morphism say that \(f\) when strict if \(\forall e \in E_H\), if \(s_H(e) \in f_V(\text{Int} G)\) or \(t_H(e) \in f_V(\text{Int} G)\) then \(\exists e' \in E_G\) such that \(f_E(e') = e\).

\[\text{Equivalently: a directed graph is a functor } G \text{ from } \bullet \xrightarrow{G} \bullet \text{ to Set}; \text{ a graph morphism is then a natural transformation } f : G \Rightarrow H.\]

\[\text{We will use the words “vertex” and “node” interchangeably.}\]
Strictness ensures that there are no additional edges connected to vertices in the image of Int $G$.

We emphasise two points about the distinction between interior and boundary nodes for open graphs. We view graphs as computational objects, built up by connecting smaller objects together; we view the interior vertices as computational primitives. Strict maps ensure that the interior structure—the types and connections of the vertices—is preserved. The boundary of an open graph defines the interface of the system; the boundary nodes indicate this interface, and do not carry computational meaning. Hence boundary nodes have degree one: they simply mark an edge where something may be connected. Morphisms of open graphs preserve this view by not allowing interior nodes to be mapped to the boundary.

We can also view graphs as topological spaces. In this case the boundary nodes can be seen as points which lie outside the space but are needed to define it, similar to the end points of an open interval. From this point of view, morphisms of open graphs are continuous. What then are the open sets of this space? Open subgraphs arise via two graph operations: removing connected components from the graph, and removing single points. We note that it suffices to consider removing points which lie on edges, since vertex removal can be simulated by disconnecting the vertex and then removing the resultant component. Since we are indifferent to which point on the edge is removed, we introduce the notion of splitting an edge. The intuition is that by removing a point from the middle of the edge $e$, we introduce two new boundary points.

**Definition 6** (Splitting an Edge). Let $G$ be an open graph, and suppose $e \in E_G$; we define $G_{\kappa e}$, the splitting of $G$ on $e$, via the graph $G' = (V_G + \{e_1, e_2\}, (E_G \setminus \{e\}) + \{e_1, e_2\}, s', t')$, where $e_1, e_2$ do not occur in $V_G$ or $E_G$, and $s'$ and $t'$ are defined such that

- $s'(e_1) = s_G(e)$, $t'(e_1) = e_1$;
- $s'(e_2) = e_2$, $t'(e_2) = t_G(e)$;

and they otherwise agree with $s_G$ and $t_G$ respectively. Then $G_{\kappa e} := (G', \partial G + \{e_1, e_2\})$.

We define a canonical morphism $i$ embedding $G_{\kappa e}$ back into $G$ as follows:

- $i_V(e_1) = t_G(e_1)$; $i_V(e_2) = s_G(e_2)$; and $i_V(v) = v$ otherwise.
- $i_E(e_1) = i_E(e_2) = e$; and $i_E(e') = e'$ otherwise.

Clearly, $i$ is injective on the portion of $G_{\kappa e}$ excluding $e_1$ and $e_2$, and it is strict.

**Definition 7** (Removing a component). Let $\Gamma = (G, \partial G)$ be an open graph, and suppose that $v \in V_G$. The graph obtained by removing the component $[v]$ is denoted $\Gamma - [v] := (G - [v], \partial G \setminus ([v] \cap \partial G))$ where the underlying graph is given by:

$$G - [v] = (V_G \setminus [v], E_G \setminus s_G^{-1}([v]), s_G|_{(E_G \setminus s_G^{-1}([v]))}, t_G|_{(E_G \setminus s_G^{-1}([v]))}).$$
Writing $G + H$ for the disjoint union of open graphs, it is immediate that we have the isomorphism $G \cong [v] + (G - [v])$, and hence that the coproduct injection $\text{in}_2 : (G - [v]) \hookrightarrow [v] + (G - [v])$ provides a canonical map back into the original graph. A further consequence is that every graph is equivalent to the disjoint union of its connected components.

It is easy to show that the operations of splitting edges and removing components generalise to sets of edges and vertices, and further that any sequence of such operations can be standardised so that all the splittings come first.

**Definition 8 (Open Subgraph).** Let $G$ be an open graph; then each pair $(F, U)$ with $F \subseteq E_G$ and $U \subseteq V_G$ defines an open subgraph $G \downarrow F - [U]$.

Every open subgraph of $G$ has a canonical map embedding it back into $G$, constructed from the canonical embeddings at each step; it is strict, and injective everywhere except the new edges and boundary nodes introduced by splittings.

**Definition 9 (Exact Embedding).** We call an open graph morphism

$$f : (G, \partial G) \hookrightarrow (H, \partial H)$$

an exact embedding if:

1. $f$ is strict;
2. $f_E$ is injective;
3. $f_V$ is injective; and,
4. $f_V(v) \in \partial H \iff v \in \partial G$, for all $v \in V_G$.

**Definition 10 (Matching).** We say that $G$ matches $H$ if there exists an open subgraph $H'$ of $H$, and an exact embedding $e : G \hookrightarrow H'$. In this case we write $G \leq H$; we write $\llbracket G \rrbracket$ for the set of all graphs which $G$ matches.

**Proposition 11.** Let $G$, $H$, and $K$ be open graphs. Then

1. $G \leq G$;
2. $G \leq H$ and $H \leq K$; then $G \leq K$;
3. If $G \leq H$ and $H \leq G$ then $G \cong H$.
4. $G \leq H$ iff $\llbracket H \rrbracket \subseteq \llbracket G \rrbracket$.

**Proof.** The first property follows from the fact that the identity map is an exact embedding; the second and fourth hold because exact embeddings are closed under composition. For the third property: since we can exactly embed $G$ into a subgraph of $H$, and vice versa, we must have that these subgraphs are isomorphic to the original graphs; from here the isomorphism between $G$ and $H$ is easily constructed. \qed
We now present a generalisation of the open graphs described in the previous section. The purpose of this generalisation is to offer more precise control over matching: a graph $G$ will match $H$ when it can be exactly embedded in a given configuration.

**Definition 12.** An *extended open graph*, henceforth abbreviated *e-graph*, is a pair $(G, X)$ where $G$ is a graph and $X \subseteq V_G$ is a distinguished set of vertices. The elements of $X$ are called the *exterior nodes* of $G$; those vertices in $V_G \setminus X$ are called the *interior*.

An e-graph morphism $f : (G, X) \to (H, Y)$ is a graph morphism such that $f_V(v) \in Y$ implies $v \in X$ for all $v \in V_G$.

The exterior nodes of an e-graph generalise the boundary nodes of an open graph and are viewed in the same way: as points outside the graph. As well as marking the edge of the graph, exterior points also constrain how the edges incident at them may be embedded into a larger graph: the must meet at the same point. This will be made explicit below.

**Definition 13 (Splitting a Vertex).** Let $(G, X)$ be an e-graph with $x \in V_G$; we define a new e-graph $G_x$ by *splitting the vertex* $x$ as $G_x := (G', (X \setminus \{x\}) + \text{in}(x) + \text{out}(x)), E_G, s', t')$ and

$$s'(e) = e \quad \text{if } e \in \text{out}(x),$$
$$t'(e) = e \quad \text{if } e \in \text{in}(x),$$
$$s'(e) = s_G(e), \quad t'(e) = t_G(e) \text{ otherwise.}$$

We can define a canonical map $i : G_x \to G$ by $i_E = \text{id}$, and $i_V(v) = x$ if $v \in \text{in}(x) + \text{out}(x)$ and $i_V(v) = v$ otherwise. Evidently, the splitting operation can be lifted to sets of vertices, so we may write $G_{xU}$ when $U \subseteq V_G$. We define a relation $\sqcup$ over the vertices of $G_{xU}$ by $v_1 \sqcup v_2$ iff $i_V(v_1) = i_V(v_2)$.

**Definition 14 (Relaxation of an Extended Graph).** Let $(G, X)$ be an e-graph; define its *relaxation*, $\text{relax}(G) := G_{X,x}$.

Essentially $\text{relax}(G)$ is the open graph that matches $G$ the closest. Note that if $G$ is an open graph itself—i.e. all its exterior points are of degree one—then $\text{relax}(G) \cong G$.

**Definition 15 (Matching an Extended Graph).** We say that $(G, X)$ matches $(H, Y)$ when there exists $H'$, an open subgraph of $\text{relax}(H)$ and an exact embedding $f : \text{relax}(G) \to H'$ such that if $v \sqcup u$ in $\text{relax}(G)$ then $f(v) \sqcup f(u)$ in $\text{relax}(H')$. In this case we write $G \leq_H H$. As before we define $\llbracket G \rrbracket_e := \{H | G \leq_e H\}$

**Proposition 16.** $G \leq_e H \iff \llbracket G \rrbracket_e \supseteq \llbracket H \rrbracket_e$. 


Figure 2: An illustrative example showing the steps involved in the e-graph matching $G \leq_e H$.

Figure 3: The plugging of $G$ and $H$ via the two-sided e-graph $\pi$ with embeddings $p_1$ and $p_2$.

4.1 Composing Graphs

We now introduce a general method for composing graphs which we call plugging; it works equally well for graphs, open graphs, and e-graphs. We will give here the definition for the case of e-graphs, but the reader will have no difficulty in modifying the definitions accordingly.

Let $G$ be a graph (not open or extended), and suppose that we have a partition of its vertices $V_G = F + B$ into a front set and a back set; in this case call the triple $(G, F, B)$ a two-sided graph.

**Definition 17.** A two sided e-graph, $(\pi, V_\pi, F, B)$, with a pair of embeddings $p_1$ and $p_2$ is said the be the plugging of two e-graphs $(G, X)$ and $(H, Y)$, when $\pi \leq_e G$ and $\pi \leq_e H$ by $p_1$ and $p_2$ respectively, such that $p_1(F) \subseteq X$ and $p_2(B) \subseteq Y$. Then we define the plugging, $\pi_p(G, H)$, as via the pushout:

$$
\begin{array}{c}
\pi \\
p_2 \\
p_1 \\
H & G \\
\pi_p(G, H) & \pi_p(G, H)
\end{array}
$$

We let $\pi(G, H)$ abbreviate $\exists p_1, p_2. \pi_p(G, H)$. An example illustrating plugging is given in Figure 3.

**Proposition 18.** Let $\pi$, $G$, and $H$ be as above, and let $K$ be some e-graph; then
\[ \pi(G, H) \cong \pi(H, G); \]
\[ G \leq_e \pi(G, H) \text{ and } H \leq_e \pi(G, H); \]
\[ K \leq_e G \text{ implies } K \leq_e \pi(G, H); \]

5 Compact Closed Categories

**Definition 19.** A strict symmetric monoidal category \( [2] \) is called compact closed \( [11] \) when each object \( A \) has a chosen dual object \( A^* \), and morphisms

\[
\begin{align*}
d_A : I &\rightarrow A^* \otimes A \\
e_A : A \otimes A^* &\rightarrow I
\end{align*}
\]

where \( I \) is the tensor identity of the compact closed category, such that

\[
\begin{align*}
A \cong A \otimes I \xrightarrow{id_A \otimes d_A} A \otimes A^* \otimes A \xrightarrow{\epsilon_A \otimes id_A} I \otimes A \cong A = id_A \tag{3}
\end{align*}
\]

\[
\begin{align*}
A^* \cong I \otimes A^* \xrightarrow{d_A \otimes id_{A^*}} A^* \otimes A \otimes A^* \xrightarrow{id_{A^*} \otimes e_A} A^* \otimes I \cong A^* = id_{A^*}. \tag{4}
\end{align*}
\]

Every arrow \( f : A \rightarrow B \) in a compact closed category \( C \) has a name and coname:

\[
\begin{align*}
\check{f} &\rightarrow I \rightarrow A^* \otimes B, \quad \ph f : A \otimes B^* \rightarrow I,
\end{align*}
\]

which are constructed as \( \check{f} = (id_{A^*} \otimes f) \circ d_A \) and \( \ph f = e_B \circ (f \otimes id_{B^*}) \). Hence there are natural isomorphisms \( C(A, B) \cong C(I, A^* \otimes B) \cong C(A \otimes B^*, I) \) making \( C \) monoidally closed\(^5\). Furthermore, \( f \) has a dual, \( f^* : B^* \rightarrow A^* \), defined by

\[
\begin{align*}
f^* &\rightarrow (id_{A^*} \otimes e_B) \circ (id_{A^*} \otimes f \otimes id_{B^*}) \circ (d_A \otimes id_{B^*})
\end{align*}
\]

By virtue of equations (3) and (4), \( f^{**} = f \). Thus \( (\cdot)^* \) lifts to an involutive functor \( C^{op} \rightarrow C \), making \( C \) equivalent to its opposite.

5.1 Graph Representations for Compact Closed Categories

Open graphs with certain additional structure give a representation for compact closed categories; we now give an overview of this construction. The details omitted here can be found in [9]. Pictorial representations are in Fig. 4. We make the convention that the domain of an arrow is at the top of the picture, and its codomain is at the bottom.

A **concrete graph** \( \Gamma \) is 5-tuple \((G, \text{dom} \Gamma, \text{cod} \Gamma, <_{\text{in}(\cdot)}, <_{\text{out}(\cdot)})\) where:

- \( G = (V, E, s, t) \) is a graph;
- \( \text{dom} \Gamma \) and \( \text{cod} \Gamma \) are totally ordered disjoint sets of degree one vertices of \( G \). Therefore the union of these sets is the **boundary** of the open graph \((G, \text{dom} \Gamma, \text{cod} \Gamma)\);

\(^5\)In general compact closed categories are models of multiplicative linear logic where \( A \multimap B \) is defined as \( A^\perp \otimes B \).
Figure 4: Compact Closed Structure as Graphs.

- $\langle \text{in} \rangle$ is a family of maps, indexed by $V$ such that $\langle \text{in}(v) \rangle \overset{\infty}{\rightarrow} \mathbb{N}_k$ where $k = |\text{in}(v)|$.

- $\langle \text{out} \rangle$ is a family of maps, indexed by $V$ such that $\langle \text{out}(v) \rangle \overset{\infty}{\rightarrow} \mathbb{N}_{k'}$ where $k' = |\text{out}(v)|$.

Since the sets $\text{dom} \Gamma$ and $\text{cod} \Gamma$ consist of vertices of degree one, we can assign a polarity to each one: $v \mapsto +$ if the edge incident at $v$ is an incoming edge; $v \mapsto -$ otherwise. Hence $\text{cod} \Gamma$ and $\text{dom} \Gamma$ are ordered signed sets. Given any ordered signed set $S$ we write $S^*$ for the same ordered set with the opposite signing. Given two such sets we can define their disjoint union $R + S$ as the disjoint union of the underlying sets, inheriting the signing and the order from $R$ and $S$, with the convention that $r < s$ for all $r \in R, s \in S$.

**Proposition 20.** Concrete graphs form a compact closed category whose objects are ordered signed sets and whose arrows $f : A \rightarrow B$ are concrete graphs with $\text{cod } f = B$ and $\text{dom } f = A^*$.

For each ordered signed set $A$, the identity map $\text{id}_A$ has $\text{dom } \text{id}_A = A^*$ and $\text{cod } \text{id}_A = A$; its underlying graph has $E = A$ and $V = A^* + A$ with $t(a) = a$ and $s(a) = a^*$. Given a pair of concrete graphs $f : A \rightarrow B$ and $g : B \rightarrow C$ their composition $g \circ f : A \rightarrow C$ is constructed by merging the two graphs, erasing the vertices of $\text{cod } f$ and $\text{dom } g$ (called the boundary vertices), and identifying the edges previously incident at the deleted vertices. (Due to the opposite polarity of the domain and codomain the edges have compatible direction.) The tensor product on objects $A, B$ is simply $A + B$; given $f : A \rightarrow B$, $g : C \rightarrow D$, the graph of $f \otimes g$ is the disjoint union of the graphs of $f$ and $g$. The unit for the tensor is the empty set. The morphisms $d_A : I \rightarrow A^* \otimes A$, $e_A : A \otimes A^* \rightarrow I$ have the same underlying graph as $\text{id}_A$, but $\text{dom } d = \emptyset$, $\text{cod } d = A^* + A$, $\text{dom } e = A + A^*$ and $\text{cod } e = \emptyset$.

**Remark.** Although we have not written it explicitly, both composition and tensor can both be expressed as plugging. The tensor is the plugging along the empty graph, while composition is plugging along an identity graph. In fact, one can define another compact closed category whose objects are two-sided graphs and whose arrows are e-graphs; sadly, space does not allow it to be described here.
This category captures exactly the axioms for compact closed structure, in the sense that any freely generated compact closed category can be represented by concrete graphs. We will consider a collection of basic terms $F$ whose types are vectors of some set of basic types $T$. Then:

**Definition 21.** A $T,F$-labelling $\theta$ for a concrete graph $\Gamma$ is a pair of maps $\theta_T : E \rightarrow T$ and $\theta_F : (V - \text{cod } \Gamma - \text{dom } \Gamma) \rightarrow F$ such that for each vertex $v$, if $\text{in}(v) = \langle a_1, \ldots, a_n \rangle$ and $\text{out}(v) = \langle b_1, \ldots, b_m \rangle$ then

$$\theta_v : \langle \theta a_1, \ldots, \theta a_n \rangle \rightarrow \langle \theta b_1, \ldots, \theta b_m \rangle$$

We say a concrete graph $\Gamma$ is $T,F$-labellable if there exists an $T,F$-labelling for it; and if $\theta$ is a labelling for $\Gamma$, then the pair $(\Gamma, \theta)$ is called a $T,F$-labelled graph.

The $T,F$-labelled graphs form a compact closed category in the same way as the concrete graphs, subject to the further restriction that arrows are composable only when their labellings agree.

**Theorem 22.** Let $C$ be a compact closed category, freely generated by some set of arrows $F$ and ground types $T$; then $C$ is equivalent to the category of $T,F$-labelled graphs.

Given a compact closed category $C$ generated by some basic set of operations, the arrows of $C$ have a canonical representation as labelled graphs. A consequence of the theorem is then that two arrows are equal by the equations of the compact closed structure if and only if their graph representations are equal.

As a final remark before moving on, note that the external structure of a vertex in a concrete graph is essentially the same as that of a complete graph; hence one can consistently view subgraphs as vertices, and abstract over their internal structure.

### 6 !-Boxes

To support reasoning with spiders we introduce the operation !-boxing (pronounced bang-boxing), on graph representations. Given a graph representation, this introduces a new notation, that of outlining a set of nodes (!-boxing them). We then introduce matching which formalises the idea that a !-box graph can have an arbitrary number of copies of the !-boxed nodes where every copy connects in the same way to the nodes outside the !-box.

**Definition 23 (!-box graph).** A !-box graph is a pair $(G, \mathcal{B}_G)$ where $G$ is a graph and $\mathcal{B}_G$ is the graphs !-boxes which are is a set of disjoint subsets of $V_G$.

---

6See [9] for a more thorough description of the nature of the terms.

7One could consider more expressive notions of nested, or overlapping, node sets in the !-boxes. While such expressivity is interesting, it is not required for the system we formalise here.
Definition 24 (l-box matching). we write \((G, B_G) \leq_! (H, C_H)\), for \((G, B_G)\) matches \((H, B_H)\). This is a binary relation such that \((H, B_H)\) can be obtained from \((G, B_G)\) by the following operations on graphs, performed in order:

\[\text{copy}(c, (G, B_G))\] : the function \(c\) is mapping from \(B_G\) to natural numbers. Each bang box, \(b\), is copied \(c(b)\) times. Any edges between a node, \(n\), inside a l-box \(b\), and a node, \(m\), outside it, get copied so that there is a new edge from \(m\) to the new copy of \(n\). When \(c(b) = 0\), we call it killing as all nodes in the l-box get removed with any incident edges. When \(c(b) = 1\), no additional copies are made and we allow ourselves to omit this case when writing the function.

\[\text{drop}(K, (G, B_G))\] : removes the subset, \(K\) of the l-boxes, but leaves their contents in the graph.

\[\text{merging}(M, (G, B_G))\] : given the set of disjoint subsets of unconnected l-boxes, \(M\), merging simply unions the members.

An illustration of matching with these operations is given in Figure 5.

Proposition 25 (l-box matching is partial order). Reflexivity comes from the trivial matching (no killing, no copying, no dropping and no merging). Transitivity can be proved by constructing combined matching from two existing matches: killing a l-box that was constructed from a copy simply avoids copying the l-box in the first place, copying after merging simply involves additional copying beforehand and merging at the end. Antisymmetry can be proved by constructing from arbitrary matches \(G \leq_! H\) and \(H \leq_! G\) the trivial matching. The construction simply involves removing any killings.

We give a formal semantics to l-box graphs in terms of a set of graphs in the underlying representation. In particular, we denote the interpretation of a l-box graph \((G, B)\) by \([[G, B]]_!\) and say that its members are instances.

Definition 26 (l-box Interpretation). \([[G, B]]_!\) is the set of graphs matched by the l-box graph that have no l-boxes: \([[G, B]]_! = \{H \mid (G, B) \leq_! (H, \emptyset)\}\)

Observe that every instance of a l-box graph can be defined by pairing each l-box with the natural number that defines how many copies are made of it. Thus \([[G]]_!\) is isomorphic to the set of \(k\)-tuples of natural numbers, where \(k\) is
Figure 6: The Spider Theorem, from [2] expressed formally using graph patterns. The !-boxes are named $i$ and $j$. The variable nodes are white and named $a$ and $b$. The non-variable node data (the angle) is written inside the node when non-zero.

the number of !-boxes. The need for the !-box matching operation, rather than using a direct $k$-tuple interpretation, is to allow matching between !-box graphs, and thus to provide a mechanism for derived rules.

**Proposition 27.** !-Matching respects !-box semantics: $G \leq_! H \Leftrightarrow \llbracket G \rrbracket_! \supseteq \llbracket H \rrbracket_!$.

The proof is a simple consequence from the $\leq_!$ being a partial order and the definition of $\llbracket G \rrbracket_!$ being a subset of the graphs that match $G$.

Because !-box graphs correspond to a countably infinite number of concrete graphs, matching cannot be implemented by simply unfolding all interpretations. We now prove that matching is still decidable.

**Theorem 28.** !-box graph Matching is decidable. The key observation is that a graph, $G$, will never match a graph with fewer nodes except by killing. Thus the copying(and killing) operations on $G$ can be bounded by the number of nodes in the graph it is being matched against. While this gives a generate and test style algorithm, it is not efficient. The intuition for an efficient algorithm is to search through $G$ incrementally increasing the matched part.

### 7 Reasoning with Graph Patterns

The representation formed by adding !-boxes to e-graphs, which we call graph patterns, allows us to express, in a finite way, certain infinite families of equations between e-graphs. In particular, the Spider Theorem can now be represented as shown in Figure 6. We now define graph patterns and then describe how they can be used to develop a formal system for reasoning about compact closed categories.

**Definition 29** (Graph Pattern). A graph pattern $G$ is a !-boxed e-graph, i.e. a pair $(eg(G), B_G)$, where $eg(G)$ is an e-graph and $B_G$ is the graph patterns !-boxes.

**Definition 30** (Graph Pattern Interpretation). A graph pattern $G$ represents the set of open concrete graphs: $[G]_p = \bigcup \{[G']_e : G' \in [G]_! \}$.
This definition allows us to lift matching and plugging from e-graphs through !-boxes to develop analogous definitions for graph patterns.

**Definition 31 (Graph Pattern Matching).** We write \( G \leq_p H \) for graph pattern \( G \) matches graph pattern \( H \) and define it to be:

\[
G \leq_p H = \exists G'. G \leq! G' \land G' \leq_e H
\]

**Definition 32 (Graph Pattern Plugging).** Plugging together of two graph patterns is an extension of e-graph plugging where !-boxes membership is respected. It restricts identification of nodes in a plugging to cases when their !-boxes can also be identified:

\[
\pi^{p_2}_{p_1}(G_1, G_2) = H \quad \text{only when, if } b_i \in B_{G_1} \quad \text{and } \exists v. p_i(v) \in b_i \quad \text{then } \forall w \in b_i. \exists v'. p_i(v') = w \land \exists b_j \in B_{G_2}. p_j(v') \in b_j.
\]

This identifies the !-boxes \( b_i \) and \( b_j \) which must each come from a distinct one of \( G_1 \) or \( G_2 \).

These definitions allow the properties of plugging for e-graphs to lift naturally to graph patterns.

The language of graph patterns forms a *meta-level* framework for reasoning about compact closed categories. The meta-level provides generic machinery to manipulate graphs and derive new rules. Following the terminology of logical frameworks, such as Isabelle [14], we call specification of additional structure, beyond the meta-level, the *object-level*. In our setting, this involves providing a set of equations between graphs. These equations are the axioms for the object system. For example, in §8 we define an object level theory for reasoning about quantum computation based on the graphical calculus introduced in §2.

In addition to the axioms, the object level can also provides an appropriate matching or unification operation for data in the nodes and edges.

We now describe the meta-level framework, noting the conditions for a rule to be valid, and prove the systems adequacy. The resulting system forms the basis for an interactive proof assistant that supports reasoning compact closed categories.

### 7.1 Equational Rules

In our framework, the axioms defined by an object-level model, as well as derived rules, are pairs of graph patterns. The elements of the pair represent the left and right hand sides of an equation. Rules are declarative in that they denote a set of equations between the underlying formalism of concrete graphs.

The intuitive idea of substitution with a rule is to replace a subgraph that matches the left hand side with the rule’s right hand side. However, not all pairs of graphs make a valid rule with respect to the underlying semantics. For an equation to be well defined with respect to the compact closed structure it must not be possible to change the type (the boundary nodes in the domain and co-domain) of an concrete graph graph by rewriting. Mapping this restriction back to rules on graph pattern results in the following conditions:

- There has to be a isomorphism between exterior nodes in the left and right hand sides.
• Rules must also define a partial mapping between |-boxes on the left and right hand sides. The intuition for this mapping is that the unfolding used when matching a |-box on the left, is applied to the mapped |-box on the right before replacement.

• When an exterior node appears within a |-box on one side of a rule, it must also appear under a mapped |-box on the other side.

For notational convenience, we annotate |-boxes and exterior nodes in a graph with unique names. For example, see Figure 6 which shows the Spider Theorem, where the mapping between |-boxes is represented by |-boxes having the same. Similarly, the isomorphism between exterior nodes is captured by the set of exterior node names being equal.

### 7.2 Meta-Level Logic and Derived Rules

Having defined what makes a valid rule, we now present the meta-logic of the framework. This is quite simple as it only involves dealing with equations:

\[
\begin{align*}
\Gamma \vdash A = B & \quad \text{trivial} \\
\Gamma \vdash A = B & \quad \text{refl} \\
\Gamma \vdash A = B & \quad \text{sym} \\
\Gamma \vdash (C = D[A/B])\theta & \quad \text{subst} \\
\Gamma \vdash \pi(A, C) = \pi(B, D) & \quad \text{plug}
\end{align*}
\]

where \(\Gamma\) is the set of object-level axioms, \(D[A/B]\) is the graph \(D\) with a matching of \(A\) replaced by \(B\), and \(\theta\) is a matching or unification result defined by object level matching for the node and edge data.

For the reflexivity rule (refl), we assume that \(A\) is a well-formed pattern graph. This rule allows a new graph to be introduced. The plug rule allows graphs to be put together to form larger graphs by plugging in an analogous way to composition in functional programming. By then applying the subst rule, intermediate results are derived which can themselves be used to rewrite other rules and conjectures. Given that the axioms in \(\Gamma\) meet the validity conditions described earlier, the rules all preserve the validity of equations and thus the system as a whole ensures only valid rules are derived.

Given an object-level formalism, a set of equations can be applied automatically to simplify a graph or simulate computation. For such rewriting to terminate, a suitable left-to-right ordering on rules needs to be observed, such as a decrease in the size of the graph. An initial study into this issue has been investigated by Kissinger [12]. An example of simulating a quantum computation is given in [12].

### 7.3 Lifting Axioms and Adequacy

The axioms of an object formalism come from the semantics of the underlying system. For instance, the equations given in Figure 1 can be proved by matrix
calculations in the underlying model. When such rules are expressed as graph patterns, we replace the concrete representation’s boundary nodes with exterior nodes. This operation is called lifting. When a rule contains exterior nodes, the equation on graph patterns corresponds to an infinite family of equations between concrete graphs. Thus we might worry that the lifted equations express too much: they may allow rewrites which are not true. We call the property that the lifted representation is a conservative extension of the initial theory adequacy. For models of compact closed categories, the proof of adequacy is quite simple: given an equation between concrete graphs, \( G = H \), we observe that every instance of the lifted equation has a subgraph matching the original equation such that the instance can be derived by plugging.

8 A Case Study in Quantum Computation

The model of quantum computation introduced in §2 provides an object formalism for our meta-level framework. In particular, the object level axioms come from lifting the equations in Figure 1 and from the formalisation of the Spider Theorem in Figure 6. Our model of quantum computation requires no data for the edges. The nodes on the other hand are either \( H \) (a Hadamard gate) with no additional data, or a Pauli operator which has an angle and a colour. The colour is red operations on the \( X \) basis and a lighter green for those the \( Z \) basis. For their part, angles are expressed as rational numbers which correspond to the coefficient of \( \pi \) in the underlying matrix.

To allow composition of rules to compute the resulting angles we give the \( X \) and \( Z \) nodes an angle expression. When a node is within a \( ! \)-box, the expression is a single angle-variable which gets instantiated to a new angle-variable in each of the unfoldings of the \( ! \)-box. When a node is not within a \( ! \)-box, the angle-expression is a mapping from a set of angle-variables to the corresponding rational coefficient. When an angle-expression contains an angle-variable within a \( ! \)-box, this is interpreted as a sum of the variables that result from its unfolding.

This rather simple expression language has a normal form by ordering the angle-variable by name. Matching then results in angle-variables being instantiated and the expressions in all affected nodes are then (re)normalised. An additional implementation detail must also be observed for the substitution rule: it must ensure that angle-variables in the rule being applied are distinct from those in the expression being rewritten.

The quantum Fourier transform is among the most important quantum algorithms, forming an essential part of Shor’s algorithm [21], famous for providing polynomial factoring. In our graph pattern calculus this circuit becomes the top-left graph in Figure 7. This figure shows how computation can be symbolically performed by rewriting with the lifted equations from Figure 1 and the graph pattern version of the Spider Theorem.
9 Related Work

There are several foundational approaches to graph transformation, including algebraic approaches [8], node-label controlled [10], matrix based [22], and programmed graph replacement [18]. These provide general ways of understanding graph transformations which can then be implemented to provide machinery for a specific application. However, systems based on these theories do not provide machinery for the semantics of compact closed categories. The distinctive feature of our form of graph rewriting is that the graphs capture the structural properties of compact closed categories and our formalism provides a compositional form of rewriting is: it preserves the type of the rewritten subgraph. This allows us to define a plugging operation over which rewriting distributes.

Bundy and Richardson have described an account of ellipses notation for lists [3]. Various authors have also considered ellipses representations for matrices [20, 15], and more recently, Prince, Ghani and McBride have developed a general formalism for ellipses notation using Containers [16]. Providing machinery for rewriting of graphs with ellipses notation, which is needed to represent the Spider Theorem, is a novel contribution of our approach to graph rewriting.

We note that our graphical notation has little connection to graph states as used in various approaches to measurement-based quantum computation [17]. In that approach the graph structure is used to provide a description of the entanglement in a state: it does not provide a complete description of a computation.

10 Conclusions and Further Work

We extended the representation of compact closed categories as graphs to provide a more expressive account of the interface offered by an open graph. This representation enjoys a plugging operation that has sequential and parallel composition as special cases. We also described a formalism for ellipses notations on graphs and showed that matching is decidable. These representations, together,
provide a rich language of graph patterns. This provides the foundation for a simple meta-logic for reasoning about models of compact closed categories.

We use the graphical language to extend existing graphical calculi for quantum computation. In particular, informal reasoning with graphical equations that contain ellipses notation, such as the Spider Theorem, now have a formal graphical representation. We illustrate this by showing how computation can be performed by symbolic graphical rewriting.

We are left with several exciting avenues for further research. The most immediate direction we are pursuing is to provide a full implementation - only a partial one is currently available. Other areas of further work include considering confluence results for sets of rewrite rules, increasing the expressiveness of the representation for graph-patterns, and finding a complete set of rewrite rules for the considered model of quantum computation.

References

[1] S. Abramsky and B. Coecke. A categorical semantics of quantum protocols. In LICS 2004, pages 415–425. IEEE Computer Society, 2004.

[2] A. Asperti and G. Longo. Categories, Types and Structures. MIT Press, 1991.

[3] A. Bundy and J. Richardson. Proofs about lists using ellipsis. In In Proc. of the 6th LPAR, volume 1705 of LNAI, pages 1–12. Springer, 1999.

[4] B. Coecke. Kindergarten quantum mechanics. Lecture Notes, 2005.

[5] B. Coecke and R. Duncan. Interacting quantum observables. In ICALP 2008. LNCS, 2008.

[6] B. Coecke and E. O. Paquette. POVMs and Naimark’s theorem without sums. In Proc. of the 4th International Workshop on Quantum Programming Languages, 2006.

[7] B. Coecke and D. Pavlovic. Quantum measurements without sums. In The Mathematics of Quantum Computation and Technology, CRC Applied Mathematics & Nonlinear Science. Taylor and Francis, 2007.

[8] A. Corradini, H. Ehrig, R. Heckel, M. Korff, M. Löwe, L. Ribeiro, and A. Wagner. Algebraic approaches to graph transformation - part I: Single pushout approach and comparison with double pushout approach. In Handbook of Graph Grammars and Computing by Graph Transformation. Vol. I: Foundations, pages 247–312. World Scientific, 1997.

[9] R Duncan. Types for Quantum Computation. PhD thesis, Oxford University, 2006.

http://dream.inf.ed.ac.uk/projects/quantomatic
[10] D. Janssens and G. Rozenberg. Graph grammars with node-label controlled rewriting and embedding. In Proc. of the 2nd International Workshop on Graph-Grammars and Their Application to Computer Science, pages 186–205. Springer-Verlag, 1983.

[11] G.M. Kelly and M.L. Laplaza. Coherence for compact closed categories. Journal of Pure and Applied Algebra, 19:193–213, 1980.

[12] A. Kissinger. Graph rewrite systems for complementary classical structures in y-symmetric monoidal categories. Master’s thesis, University of Oxford, 2008.

[13] A.K. Pati and S. L. Braunstein. Impossibility of deleting an unknown quantum state. Nature, 404:164–165, 2000.

[14] L. C. Paulson. Isabelle: A generic theorem prover. Springer-Verlag, 1994.

[15] M. Pollet and M. Kerber. Intuitive and formal representations: The case of matrices. In In MKM’04, LNCS 3119, pages 317–331. Springer, 2004.

[16] R. Prince, N. Ghani, and C. McBride. Proving properties about lists using containers. In FLOPS, volume 4989 of LNCS, pages 97–112. Springer, 2008.

[17] R. Raussendorf and H. J. Briegel. A one-way quantum computer. Phys. Rev. Lett., 86:5188–5191, 2001.

[18] A. Schürr. Programmed graph replacement systems, pages 479–546. World Scientific Publishing Co., Inc., River Edge, NJ, USA, 1997.

[19] P. Selinger. Dagger compact closed categories and completely positive maps. In Proc. of the 3rd International Workshop on Quantum Programming Languages, 2005.

[20] A. P. Sexton and V. Sorge. Semantic analysis of matrix structures. In ICDAR ’05: Proceedings of the Eighth International Conference on Document Analysis and Recognition, pages 1141–1145, Washington, DC, USA, 2005. IEEE Computer Society.

[21] P. W. Shor. Polynomial-time algorithms for prime factorization and discrete logarithms on a quantum computer. SIAM J.Sci.Statist.Comput., 26(5), 1997.

[22] P. P. P. Vela and J. de Lara. Matrix approach to graph transformation: Matching and sequences. In ICGT, volume 4178 of LNCS, pages 122–137. Springer, 2006.

[23] W. Wootters and W. Zurek. A single quantum cannot be cloned. Nature, 299:802–803, 1982.